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Research Article

The Distance Matrices of Some Graphs Related to Wheel Graphs

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Let D denote the distance matrix of a connected graph G. The inertia of D is the triple of integers $(n_+(D), n_0(D), n_-(D))$, where $n_+(D)$, $n_0(D)$, and $n_-(D)$ denote the number of positive, 0, and negative eigenvalues of D, respectively. In this paper, we mainly study the inertia of distance matrices of some graphs related to wheel graphs and give a construction for graphs whose distance matrices have exactly one positive eigenvalue.

1. Introduction

A simple graph $G = (V, E)$ consists of V, a nonempty set of vertices, and E, a set of unordered pairs of distinct elements of V called edges. All graphs considered here are simple and connected. Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The distance between two vertices u, $v \in V(G)$ is denoted by d_{uv} and is defined as the length of the shortest path between u and v in G. The *distance matrix* of G is denoted by $D(G)$ and is defined by $D(G) = (d_{uv})_{u,v\in V(G)}$. Since $D(G)$ is a symmetric matrix, its *inertia* is the triple of integers $(n_+(D(G)), n_0(D(G)), n_-(D(G)))$, where $n_+(D(G))$, $n_0(D(G))$, and $n_-(D(G))$ denote the number of positive, 0, and negative eigenvalues of $D(G)$, respectively.

The distance matrix of a graph has numerous applications to chemistry [1]. It contains information on various walks and self-avoiding walks of chemical graphs. Moreover, the distance matrix is not only immensely useful in the computation of topological indices such as the Wiener index [1] but also useful in the computation of thermodynamic properties such as pressure and temperature virial coefficients [2]. The distance matrix of a graph contains more structural information compared to a simple adjacency matrix. Consequently, it seems to be a more powerful structure discriminator than the adjacency matrix. In some cases, it can differentiate isospectral graphs although there are nonisomorphic trees with the same distance polynomials [3]. In addition to such applications in chemical sciences, distance matrices find applications in music theory, ornithology [4], molecular biology [5], psychology [4], archeology [6], sociology [7], and so forth. For more information, we can see [1] which is an excellent recent review on the topic and various uses of distance matrices.

Since the distance matrix of a general graph is a complicated matrix, it is very difficult to compute its eigenvalues. People focus on studying the inertia of the distance matrices of some graphs. Unfortunately, up to now, only few graphs are known to have exactly one positive D-eigenvalue, such as trees [8], connected unicyclic graphs [9], the polyacenes, honeycomb and square lattices [10], complete bipartite graphs [11], K_n, and iterated line graphs of some regular graphs [12], and cacti [13]. This inspires us to find more graphs whose distance matrices have exactly one positive eigenvalue.

The *wheel graph* of n vertices W_n is a graph that contains a cycle of length $n-1$ plus a vertex v (sometimes called the hub) not in the cycle such that v is connected to every other vertex. In this paper, we first study the inertia of the distance matrices in wheel graphs if one or more edges are removed from the graph, and then, with the help of the structural characteristics of wheel graphs, we give a construction for graphs whose distance matrices have exactly one positive eigenvalue.

2. Preliminaries

We first give some lemmas that will be used in the main results.

Lemma 1 (see [14]). *Let A be a Hermitian matrix with eigenvalues $\lambda_1 \geqslant \cdots \geqslant \lambda_n$ and B one of its principal submatrices. Let B have eigenvalues $\mu_1 \geqslant \cdots \geqslant \mu_m$. Then the inequalities $\lambda_{n-m+i} \leqslant \mu_i \leqslant \lambda_i$ $(i = 1, \ldots, m)$ hold.*

For a square matrix, let $\operatorname{cof}(A)$ denote the sum of cofactors of A. Form the matrix $\widetilde{A}$ by subtracting the first row from all other rows then the first column from all other columns and let $\widetilde{A}_{11}$ denote the principle submatrix obtained from $\widetilde{A}$ by deleting the first row and first column.

Lemma 2 (see [15]). $cof(A) = \det \widetilde{A}_{11}$.

A cut vertex is a vertex the removal of which would disconnect the remaining graph; a block of a graph is defined to be a maximal subgraph having no cut vertices.

Lemma 3 (see [15]). *If G is a strongly connected directed graph with blocks $G_1, G_2, \ldots, G_r$, then*

$$\begin{aligned} cof\, D(G) &= \prod_{i=1}^{r} cof\, D(G_i), \\ \det D(G) &= \sum_{i=1}^{r} \det D(G_i) \prod_{j \neq i} cof\, D(G_i). \end{aligned} \tag{1}$$

Lemma 4. *Let*

$$C = \begin{bmatrix} 1 & 1 & 1 & 1 & \cdots & 1 & 1 \\ -1 & -2 & -1 & 0 & \cdots & 0 & 0 \\ 0 & -1 & -2 & -1 & \cdots & 0 & 0 \\ 0 & 0 & -1 & -2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -2 & -1 \\ 0 & 0 & 0 & 0 & \cdots & -1 & -2 \end{bmatrix}_{n\times n}. \tag{2}$$

Then

$$\det C = \begin{cases} -\dfrac{n}{2}, & \text{if } n \text{ is even}, \\ \dfrac{n+1}{2}, & \text{if } n \text{ is odd}. \end{cases} \tag{3}$$

Proof. Let

$$\begin{aligned} C_n &= \begin{vmatrix} 1 & 1 & 1 & 1 & \cdots & 1 & 1 \\ -1 & -2 & -1 & 0 & \cdots & 0 & 0 \\ 0 & -1 & -2 & -1 & \cdots & 0 & 0 \\ 0 & 0 & -1 & -2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -2 & -1 \\ 0 & 0 & 0 & 0 & \cdots & -1 & -2 \end{vmatrix}_{n\times n}, \\ D_n &= \begin{vmatrix} \frac{1}{2} & -1 & 0 & 0 & \cdots & 0 & 0 \\ 1 & -2 & -1 & 0 & \cdots & 0 & 0 \\ 1 & -1 & -2 & -1 & \cdots & 0 & 0 \\ 1 & 0 & -1 & -2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 0 & 0 & 0 & \cdots & -2 & -1 \\ 1 & 0 & 0 & 0 & \cdots & -1 & -2 \end{vmatrix}_{n\times n}. \end{aligned} \tag{4}$$

Comparing C_n to D_n, we get the following:

$$C_n = D_n + \frac{n}{2} \times (-1)^{n-1}. \tag{5}$$

Expanding the determinant D_n according to the last column and then the last line, we get the following incursion:

$$D_n = -2D_{n-1} - D_{n-2} + 1; \tag{6}$$

that is,

$$D_n + D_{n-1} = -\left(D_{n-1} + D_{n-2}\right) + 1. \tag{7}$$

Since $D_1 = 1/2$, $D_2 = 0$, and $D_3 = 1/2$, from the above incursion, we get the following:

$$D_n = \begin{cases} 0, & \text{if } n \text{ is even}, \\ \dfrac{1}{2}, & \text{if } n \text{ is odd}. \end{cases} \tag{8}$$

So, we have the following:

$$C_n = \begin{cases} -\dfrac{n}{2}, & \text{if } n \text{ is even}, \\ \dfrac{n+1}{2}, & \text{if } n \text{ is odd}. \end{cases} \tag{9}$$

This completes the proof. □

3. Main Results

In the following, we always assume that $V(W_n) = \{v_0, v_1, \ldots, v_{n-1}\}$, where v_0 is the hub of W_n.

Theorem 5. *Let $e = v_i v_{i+1 \bmod (n-1)}$ $(1 \leqslant i \leqslant n-1)$. Then*

$$\det D(W_n - e) = \begin{cases} -\dfrac{n^2}{4}, & \text{if } n \text{ is even}, \\ \dfrac{n^2-1}{4}, & \text{if } n \text{ is odd}, \end{cases} \tag{10}$$

where $n \geqslant 3$.

Proof. Without loss of generality, we may assume that $e = v_1 v_{n-1}$. Let

$$A_n = \det D(W_n - e) = \begin{vmatrix} 0 & 1 & 1 & 1 & \cdots & 1 & 1 \\ 1 & 0 & 1 & 2 & \cdots & 2 & 2 \\ 1 & 1 & 0 & 1 & \cdots & 2 & 2 \\ 1 & 2 & 1 & 0 & \cdots & 2 & 2 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 2 & 2 & 2 & \cdots & 0 & 1 \\ 1 & 2 & 2 & 2 & \cdots & 1 & 0 \end{vmatrix}_{n\times n}. \tag{11}$$

Then

$$A_n = \begin{vmatrix} 0 & 1 & 1-\frac{1}{2} & 1 & \cdots & 1 & 1 \\ 1 & -2 & 0 & 0 & \cdots & 0 & 0 \\ 1-\frac{1}{2} & 0 & -2+\frac{1}{2} & -1 & \cdots & 0 & 0 \\ 1 & 0 & -1 & -2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 0 & 0 & 0 & \cdots & -2 & -1 \\ 1 & 0 & 0 & 0 & \cdots & -1 & -2 \end{vmatrix}_{n\times n}. \tag{12}$$

Expanding the determinant A_n according to the second line, we get the following incursion:

$$A_n = (-1)^{n-1}\frac{n}{2} - 2A_{n-1} - C_{n-2} - D_{n-2} - A_{n-2}, \tag{13}$$

where C_n and D_n are defined as in Lemma 4.

By Lemma 4, we get the following:

$$A_n = \begin{cases} -1 - 2A_{n-1} - A_{n-2}, & \text{if } n \text{ is even}, \\ -2A_{n-1} - A_{n-2}, & \text{if } n \text{ is odd}. \end{cases} \tag{14}$$

Since $A_3 = 2$, $A_4 = -4$, $A_5 = 6$, and $A_6 = -9$, according to the above incursion, we get the following:

$$A_n = \begin{cases} -\dfrac{n^2}{4}, & \text{if } n \text{ is even}, \\ \dfrac{n^2-1}{4}, & \text{if } n \text{ is odd}, \end{cases} \tag{15}$$

where $n \geqslant 3$. This completes the proof. □

Corollary 6. *Let $e = v_i v_{i+1 \bmod (n-1)}$ $(1 \leqslant i \leqslant n-1)$. Then*

$$n_+(D(W_n - e)) = 1, \qquad n_0(D(W_n - e)) = 0, \qquad n_-(D(W_n - e)) = n - 1. \tag{16}$$

Proof. We will prove the result by induction on n.

If $n = 3$, $W_3 - e \cong P_3$ is obviously true.

Suppose that the result is true for $n-1$; that is, $n_+(D(W_{n-1} - e)) = 1$, $n_0(D(W_{n-1} - e)) = 0$, $n_-(D(W_{n-1} - e)) = n - 2$.

Since $D(W_{n-1} - e)$ is a principle submatrix of $D(W_n - e)$, by Lemma 1, the eigenvalues of $D(W_{n-1} - e)$ interlace the eigenvalues of $D(W_n - e)$. By Theorem 5, $\det D(W_{n-1} - e) \det D(W_n - e) < 0$. So, $D(W_n - e)$ has one negative eigenvalue more than $D(W_{n-1} - e)$. According to the induction hypothesis, we get $n_+(D(W_n - e)) = 1$, $n_0(D(W_n - e)) = 0$, and $n_-(D(W_n - e)) = n - 1$. This completes the proof. □

Theorem 7. *One has*

$$\det D(W_n) = \begin{cases} 1 - n, & \text{if } n \text{ is even}, \\ 0, & \text{if } n \text{ is odd}, \end{cases} \tag{17}$$

where $n \geqslant 3$.

Proof. Consider the following

$$\begin{aligned} \det D(W_n) &= \begin{vmatrix} 0 & 1 & 1 & 1 & \cdots & 1 & 1 \\ 1 & 0 & 1 & 2 & \cdots & 2 & 1 \\ 1 & 1 & 0 & 1 & \cdots & 2 & 2 \\ 1 & 2 & 1 & 0 & \cdots & 2 & 2 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 2 & 2 & 2 & \cdots & 0 & 1 \\ 1 & 1 & 2 & 2 & \cdots & 1 & 0 \end{vmatrix}_{n\times n} \\ &= \begin{vmatrix} 0 & 1 & 1 & 1 & \cdots & 1 & 1 \\ 1 & -2 & -1 & 0 & \cdots & 0 & -1 \\ 1 & -1 & -2 & -1 & \cdots & 0 & 0 \\ 1 & 0 & -1 & -2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 0 & 0 & 0 & \cdots & -2 & -1 \\ 1 & -1 & 0 & 0 & \cdots & -1 & -2 \end{vmatrix}_{n\times n} \\ &= \begin{vmatrix} 0 & n-1 & 1 & 1 & \cdots & 1 & 1 \\ n-1 & -4(n-1) & -4 & -4 & \cdots & -4 & -4 \\ 1 & -4 & -2 & -1 & \cdots & 0 & 0 \\ 1 & -4 & -1 & -2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & -4 & 0 & 0 & \cdots & -2 & -1 \\ 1 & -4 & 0 & 0 & \cdots & -1 & -2 \end{vmatrix}_{n\times n} \\ &= \begin{vmatrix} 0 & n-1 & 1 & 1 & \cdots & 1 & 1 \\ n-1 & 4(n-1) & 0 & 0 & \cdots & 0 & 0 \\ 1 & 0 & -2 & -1 & \cdots & 0 & 0 \\ 1 & 0 & -1 & -2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 0 & 0 & 0 & \cdots & -2 & -1 \\ 1 & 0 & 0 & 0 & \cdots & -1 & -2 \end{vmatrix}_{n\times n}. \end{aligned} \tag{18}$$

Expanding the above determinant according to the second line, we get the following:

$$\det D(W_n) = (-1)^{n-1}(n-1)^3 + 4(n-1)A_{n-1}, \tag{19}$$

where A_n is defined as in Theorem 5.

By Theorem 5, when $n \geqslant 3$, we get the following:

$$\det D(W_n) = \begin{cases} 1 - n, & \text{if } n \text{ is even}, \\ 0, & \text{if } n \text{ is odd}. \end{cases} \tag{20}$$

This completes the proof. □

Similar to Corollary 6, we can get the following corollary.

Corollary 8. *(i) If n is even, $n_+(D(W_n)) = 1$, $n_0(D(W_n)) = 0$, $n_-(D(W_n)) = n - 1$.*

(ii) If n is odd, $n_+(D(W_n)) = 1$, $n_0(D(W_n)) = 1$, $n_-(D(W_n)) = n - 2$.

Denote by $W_n - v_0$ the graph obtained from W_n by deleting the vertex v_0 and all the edges adjacent to v_0; that is, $W_n - v_0 \cong C_{n-1}$. Let E_k $(1 \leqslant k \leqslant n)$ be any subset of $E(W_n - v_0)$ with $|E_k| = k$. In the following, we always denote by $W_n - E_k$ the graph obtained from W_n by deleting all the edges in E_k.

Theorem 9. *One has $n_+(D(W_n - E_k)) = 1$, $n_0(D(W_n - E_k)) = 0$, $n_-(D(W_n - E_k)) = n - 1$.*

Proof. Denote the components of $W_n - E_k - v_0$ by $C_1, \ldots, C_s$. Let G_i denote the graph that contains C_i plus the vertex v_0 such that v_0 is connected to every other vertex, $1 \leqslant i \leqslant s$. Then each G_i $(1 \leqslant i \leqslant s)$ is isomorphism to $W_{|V(G_i)|} - e_i$ or K_2, where e_i is an edge of $W_{|V(G_i)|} - v_0$. By Lemma 2 and some direct calculations, we get the following:

$$\operatorname{cof}(G_i) = \det D\left(\widetilde{W_{|V(G_i)|} - e_i}\right)_{11} = (-1)^{|V(G_i)|-1}\left|V(G_i)\right|. \tag{21}$$

It is easy to check that $\operatorname{cof}(G_i) = (-1)^{|V(G_i)|-1}|V(G_i)|$ is also true when G_i is isomorphism to K_2.

In the following, we will prove the theorem by introduction on s.

For $s = 1$, $G \cong W_n - e$, where e is an edge of $W_n - v_0$, by Corollary 6, we get the result.

Suppose the result is true for $s - 1$.

For s, let $G' = G_1 \cup G_2 \cup \cdots \cup G_{s-1}$. Then by the induction hypothesis, $n_+(D(G')) = 1$, $n_0(D(G')) = 0$, and $n_-(D(G')) = |V(G')| - 1$, which implies that

$$\det D\left(G'\right) = (-1)^{|V(G')|-1}a, \tag{22}$$

where a is a positive integer.

Since

$$\operatorname{cof}(G_i) = (-1)^{|V(G_i)|-1}\left|V(G_i)\right|, \quad 1 \leqslant i \leqslant s, \tag{23}$$

by Lemma 3,

$$\operatorname{cof} D\left(G'\right) = \prod_{j=1}^{s-1}\operatorname{cof} D\left(G_j\right) = (-1)^{|V(G')|-1}\prod_{j=1}^{s-1}\left|V\left(G_j\right)\right|. \tag{24}$$

Then

$$\begin{aligned}
&\det D\left(W_n - E_k\right)\\
&\quad = \det D\left(G'\right)\operatorname{cof} D\left(G_i\right) + \det D\left(G_i\right)\operatorname{cof} D\left(G'\right)\\
&\quad = (-1)^{|V(G')|-1}a \times (-1)^{|V(G_i)|-1}\left|V\left(G_i\right)\right|\\
&\qquad + (-1)^{|V(G_i)|-1}b \times (-1)^{|V(G')|-1}\prod_{j=1}^{s-1}\left|V\left(G_j\right)\right|\\
&\quad = (-1)^{n-1}\left(a\left|V\left(G_i\right)\right| + b\prod_{j=1}^{s-1}\left|V\left(G_j\right)\right|\right),
\end{aligned} \tag{25}$$

where $b = n^2/4$, if n is even and $b = (n^2 - 1)/4$, if n is odd.

In this case, similar to Corollary 6, we can easily get $n_+(D(W_n - E_k)) = 1$, $n_0(D(W_n - E_k)) = 0$, and $n_-(D(W_n - E_k)) = n - 1$.

Up to now, we have proved the result. □

Let $Gu_i \cdot v_jH$ denote the graph formed by only identifying the vertex u_i of G with the vertex v_j of H, where u_i and v_j are arbitrary vertices of G and H, respectively.

Lemma 10 (see [13]). *Let $G \times H$ denote the Cartesian product of connected graphs G and H, where $V(G) = \{u_1, \ldots, u_m\}$ and $V(H) = \{v_1, \ldots, v_n\}$. Then we have*

(i) $n_+(G \times H) = n_+(Gu_i \cdot v_jH)$;

(ii) $n_0(G \times H) = (m-1)(n-1) + n_0(Gu_i \cdot v_jH)$;

(iii) $n_-(G \times H) = n_-(Gu_i \cdot v_jH)$.

Theorem 11. *Let u_0 and v_0 be the hubs of W_n and W_m, respectively. Suppose E_p $(0 \leqslant p \leqslant n-1)$ and E_q $(0 \leqslant q \leqslant m-1)$ are any subsets of $E(W_n - u_0)$ and $E(W_m - v_0)$ with $|E_p| = p$, $|E_q| = q$, respectively. Then, the distance matrix of the graph $(W_n - E_p) \times (W_m - E_q)$ has exactly one positive eigenvalue.*

Proof. Since u_0 and v_0 are the hubs of W_n and W_m, respectively, $(W_n - E_p)u_0 \cdot v_0(W_m - E_q)$ must be isomorphism to some $W_{n+m-1} - E_{p+q}$, where w_0 is the hub of W_{n+m-1} and E_{p+q} is any subset of $E(W_{n+m-1} - w_0)$ with $|E_{p+q}| = p + q$. By Theorem 9 and Lemma 10, we get the result. □

Given an arbitrary integer m, for $1 \leqslant i \leqslant m$, let v_{i0} be the hub of W_{n_i} and E_{p_i} any subset of $E(W_{n_i} - v_{i0})$. Suppose $V(W_{n_i}) = \{v_{i0}, v_{i1}, \ldots, v_{i(n_i-1)}\}$.

Theorem 12. *For an arbitrary integer m, the distance matrix of the graph $G = (W_{n_1} - E_{p_1})v_{1k} \cdot v_{2j}(W_{n_2} - E_{p_2})v_{2h} \cdots v_{(m-1)r}(W_{n_{m-1}} - E_{p_{m-1}})v_{(m-1)t} \cdot v_{ms}(W_{n_m} - E_{p_m})$ has exactly one positive eigenvalue.*

Proof. We will prove the conclusion by induction on m.

If $m = 1$, by Theorem 9, the conclusion is true.

Suppose the conclusion is true for $m-1$. For convenience, let $H = (W_{n_1} - E_{p_1})v_{1k} \cdot v_{2j}(W_{n_2} - E_{p_2})v_{2h} \cdots v_{(m-2)i}(W_{n_{m-2}} - E_{p_{m-2}})$. Then $G = Hv_{(m-2)g} \cdot v_{(m-1)r}(W_{n_{m-1}} - E_{p_{m-1}})v_{(m-1)t} \cdot v_{ms}(W_{n_m} - E_{p_m})$. By Lemma 10, we have the following:

$$\begin{aligned}
n_+(G) &= n_+\left(H\left(W_{n_{m-1}} - E_{p_{m-1}}\right)v_{(m-1)t} \cdot v_{ms}\left(W_{n_m} - E_{p_m}\right)\right)\\
&= n_+\left(H\left(W_{n_{m-1}} - E_{p_{m-1}}\right)v_{(m-1)0} \cdot v_{m0}\left(W_{n_m} - E_{p_m}\right)\right).
\end{aligned} \tag{26}$$

Since $(W_{n_{m-1}} - E_{p_{m-1}})v_{(m-1)0} \cdot v_{m0}(W_{n_m} - E_{p_m}) = W_{n_{m-1}+n_m-1} - E_{p_{m-1}} - E_{p_m}$, we get $n_+(G) = n_+(Hv_{(m-2)g} \cdot v_{(m-1)r}(W_{n_{m-1}+n_m-1} - E_{p_{m-1}} - E_{p_m}))$. By the induction hypothesis, we get $n_+(G) = 1$. This completes the proof. □

Remark 13. Let G_1 and G_2 be any two graphs with the same form as G in Theorem 12. Making Cartesian product of graphs G_1 and G_2, by Lemma 10 and Theorem 12, we get a series of graphs whose distance matrices have exactly one positive eigenvalue.

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