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SOME GRAPHS DETERMINED BY THEIR DISTANCE SPECTRUM*

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Abstract. Let G be a connected graph with order n. Let $\lambda_1(D(G)) \geq \cdots \geq \lambda_n(D(G))$ be the distance spectrum of G. In this paper, it is shown that the complements of P_n and C_n are determined by their D-spectrum. Moreover, it is shown that the cycle C_n (n odd) is also determined by its D-spectrum.

Key words. Distance spectrum, Complement, Cospectral.

AMS subject classifications. 05C50.

1. Introduction. For M be a Hermitian matrix of order n we denote by p_M the characteristic polynomial of M defined by $p_M(\lambda) = \det(\lambda I_n - M)$, where I_n is the $n \times n$ identity matrix. Its characteristic roots are all real and will be denoted in nonincreasing order by

$$\lambda_1(M) \geq \lambda_2(M) \geq \cdots \geq \lambda_n(M),$$

where possible duplicates have not been suppressed. They are eigenvalues of M. We define Spec_M the M-spectrum by the multiset $\{\lambda_1(M), \lambda_2(M), \ldots, \lambda_n(M)\}$. The matrices that we are interested in relate to graphs.

All graphs considered here are simple, connected (so loops or multiple edges are not allowed), undirected and finite. Let $G = (V(G), E(G))$ be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. For a graph G, let $M = M(G)$ be a graph matrix defined in a prescribed way (typically $M(G) = A(G)$ for the adjacency matrix of G and $M(G) = D(G)$ for the distance matrix of G). Two graphs G and H are said to be M-cospectral if they have the same M-spectrum.

As usual, we use P_n and C_n to denote the path and cycle with order n, respectively. We denote by $\delta(G)$ the minimum degree of G. We also denote $\overline{G}$ the complement of the graph G and we will write $G \cong H$ to mean that G and H are isomorphic graphs. Other matrix notations that we use in this article are J for the matrix in which every entry is 1, $\mathbb{1}$ the vector of ones, $\mathrm{Adj}(M)$ for the classical adjoint of the matrix M and $\|M\|_{\mathrm{HS}}$ for the Hilbert–Schmidt (Frobenius) norm of a matrix M.

Since we know that if G is A-cospectral with H, then G and H have the same size, it is natural to ask the following problem.

Question 1.1. *Let G and H be two connected graphs of order n with size $m(G)$ and $m(H)$, respectively. When G is D-cospectral with H, does $m(G) = m(H)$ hold?*

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Unfortunately, the answer to Question 1.1 is negative. The following two graphs G_1 and G_2 have the same distance characteristic polynomial

$$\lambda^8 - 138\lambda^6 - 868\lambda^5 - 2196\lambda^4 - 2672\lambda^3 - 1520\lambda^2 - 320\lambda,$$

but G_1 has 10 edges and G_2 has 11 edges.

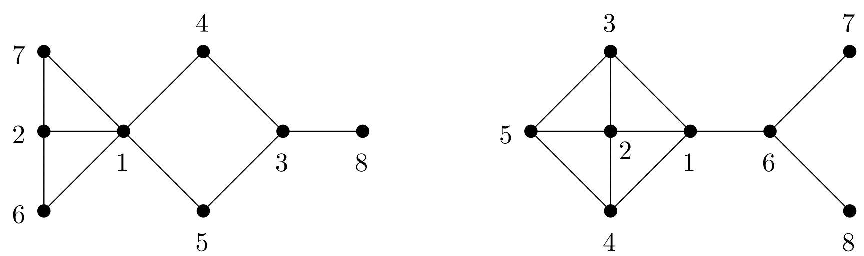

Fig. 1. The graphs G_1 and G_2.

We believe that this is the smallest order example of this phenomenon. The reader may consult Heysse[11] for other examples.

Graphs G and H with the same spectrum of a graph matrix M are called M-cospectral graphs. A graph G is said to be determined by its M-spectrum if there is no other non-isomorphic graph with the same spectrum, that is, $\mathrm{Spec}M(H) = \mathrm{Spec}M(G)$ implies $H \cong G$. The following problem is very interesting but difficult.

Problem 1.2. *Which connected graphs are determined by their M-spectrum?*

The background of this problem originates from chemistry. In 1956, Günthard and Primas [9] raised this question in the context of Hückel's theory. It is an old problem yet far from solved. For additional remarks on this topic we refer the reader to the excellent surveys by van Dam and W.H. Haemers [5, 6]. The following results are about the graphs which are determined by their A-spectra or D-spectra.

Jin and Zhang [13] proved that the complete multipartite graph is determined by its D-spectra which was conjectured by Lin, Hong, Wang and Shu [15]. However, the complete multipartite graph is not determined by its A-spectra, ($C_4 \cup K_1$ and $K_{1,4}$ have the same A-spectrum).

Let F_k denote the friendship graph. Cioabă, Haemers, Vermette, Wong [3] showed that F_k ($k \neq 16$) is determined by its A-spectrum. Very recently, Lu, Huang and Huang [18] proved that F_k is determined by its D-spectrum.

Hoffman [12] showed that hypercubes are determined by their A-spectrum in dimension less than or equal to 3 but not for higher dimensions. Koolen, Hayat and Iqbal [14] showed that the hypercubes are determined by their D-spectrum.

Let $K_{s,t}$ denote the complete bipartite graph. Cámara and Haemers [2] and Lin, Zhai and Gong [17] showed the complement of $K_{s,t} \vee (n-s-t)K_1$ ($s+t < n$) is determined by its A-spectrum and its D-spectrum respectively.

Doob and Haemers [7] proved that the complement of P_n is determined by its A-spectrum. In this paper,

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we prove that the complement of P_n is determined by its D-spectrum.

The rest of the paper is organized as follows. In Section 2, we show that the graphs $\overline{C_n}$ and $\overline{P_n}$ are determined by their D-spectrum. In Section 3, we show that the cycle C_n (n odd) is also determined by its D-spectrum.

2. The graphs $\overline{C_n}$ and $\overline{P_n}$ are determined by their distance spectra.

2.1. Basic facts about the D-spectra of $\overline{C_n}$ and $\overline{P_n}$.

LEMMA 2.1. (Cauchy Interlace Theorem) *Let A be a Hermitian matrix with order n and let B be a principal submatrix of A with order m. If $\lambda_1(A) \geq \lambda_2(A) \geq \cdots \geq \lambda_n(A)$ list the eigenvalues of A and $\mu_1(B) \geq \mu_2(B) \geq \cdots \geq \mu_m(B)$ list the eigenvalues of B, then*

$$\lambda_{n-m+i}(A) \leq \mu_i(B) \leq \lambda_i(A)$$

for $i = 1, \ldots, m$.

The D-spectrum of $\overline{C_n}$ is easily calculated by a discrete Fourier transform. We obtain

$$\begin{aligned}
&\lambda_1(D(\overline{C_n})) = n + 1\\
&\lambda_{2j}(D(\overline{C_n})) = -1 + 2\cos\left(\frac{2\pi j}{n}\right), \quad j = 1, \ldots, \left\lfloor \frac{n}{2} \right\rfloor\\
&\lambda_{2j+1}(D(\overline{C_n})) = -1 + 2\cos\left(\frac{2\pi j}{n}\right), \quad j = 1, \ldots, \left\lfloor \frac{n-1}{2} \right\rfloor
\end{aligned}$$

with most of the eigenvalues being repeated. In case n is even, we have $\lambda_n(D(\overline{C_n}) = -3$.

The following observations are motivated by Doob and Haemers [7]. It is easily observed that $D(\overline{P_n})$ occurs as a principal $n \times n$ submatrix of $D(\overline{C_{n+1}})$. The Cauchy Interlacing Theorem gives

$$\lambda_{2j}(D(\overline{P_n})) = \lambda_{2j}(D(\overline{C_{n+1}}) = -1 + 2\cos\left(\frac{2\pi j}{n+1}\right), \quad j = 1, \ldots, \left\lfloor \frac{n}{2} \right\rfloor.$$

For the remaining eigenvalues of $D(\overline{P_n})$, the strict form of the Cauchy Interlacing Theorem [10] gives

$$\lambda_{2j-1}(D(\overline{C_{n+1}})) > \lambda_{2j-1}(D(\overline{P_n})) > \lambda_{2j}(D(\overline{C_{n+1}}))), \quad j = 1, \ldots, \left\lfloor \frac{n+1}{2} \right\rfloor.$$

which implies in particular that the eigenvalues of $D(\overline{P_n})$ are all simple.

We denote by $\operatorname{diam}(H)$ the diameter of the graph H.

LEMMA 2.2. *Let $G = \overline{C_n}$ or $G = \overline{P_n}$, and let H be D-cospectral to G. Then* $\operatorname{diam}(H) = 2$ *and* $m(H) = m(G)$.

Proof. We have $\lambda_n(D(H)) = \lambda_n(D(G)) > -2 - \sqrt{2}$. It follows from [16, Theorem 2.3] that $\operatorname{diam}(H) = 2$. Since

$$\sum_{i=1}^{n} \lambda_i^2(D(H)) = \sum_{i=1}^{n} \lambda_i^2(D(G))$$

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and

$$\sum_{i=1}^{n} \lambda_i^2(D(H)) = \sum_{1\le i,j\le n} d_{ij}^2(H) = 2m(H) + 4[n(n-1) - 2m(H)],$$

it follows that $m(G) = m(H)$. ∎

LEMMA 2.3. *Let $A = A(H)$ be the adjacency matrix of a graph H with n vertices and m edges. Then we have*

$$\begin{aligned}
\operatorname{tr}\left((A+J-I)^3\right) &= \operatorname{tr}(A^3) + 3\operatorname{tr}(A^2J) + (3n-6)\operatorname{tr}(AJ) - 3\operatorname{tr}(A^2) + n^3 - 3n^2 + 2n \\
&= 6m(n-3) + n^3 - 3n^2 + 2n + \operatorname{tr}(A^3) + 3\sum_{j=1}^{n}\sum_{k=1}^{n}\sum_{\ell=1}^{n} a_{jk}a_{k\ell} \\
&= 6mn + n^3 - 3n^2 + 8n + \operatorname{tr}(A^3) + 3\sum_{k=1}^{n}(d_k-1)(d_k-2), \qquad (2.1)
\end{aligned}$$

where d_k denotes the degree of the k^{th} vertex.

Proof. The result follows by routine calculation. ∎

In particular, if $\operatorname{diam}(H) = 2$ and $m(H) = m$, then $D(H) = A(\overline{H}) + J - I$ and it follows that

$$\operatorname{tr}\left(D(H)^3\right) = 4n^3 - 6n^2 + 8n - 6mn + \operatorname{tr}(A(\overline{H})^3) + 3\sum_{k=1}^{n}(d_k(\overline{H})-1)(d_k(\overline{H})-2).$$

PROPOSITION 2.4. *Let $G = \overline{C_n}$ with $n \ge 4$ or $G = \overline{P_n}$, and let H be D-cospectral to G. Then $\overline{H}$ is a disjoint union of paths and cycles.*

Proof. By Lemma 2.2, we have $\operatorname{diam}(H) = 2$ and $m(G) = m(H)$. Since G and H are D-cospectral, we have $\operatorname{tr}\left(D(G)^3\right) = \operatorname{tr}\left(D(H)^3\right)$. Since $\operatorname{tr}(A(\overline{G})^3) = 0$ and $d_k(\overline{G}) \in \{1,2\}$, it follows that

$$\operatorname{tr}(A(\overline{H})^3) + 3\sum_{k=1}^{n}(d_k(\overline{H})-1)(d_k(\overline{H})-2) = 0.$$

But every term on the left is nonnegative. We deduce that $\operatorname{tr}(A(\overline{H})^3) = 0$ and that $d_k(\overline{H}) \in \{1,2\}$ for all $k = 1,\ldots,n$. Hence, the result holds. ∎

2.2. The complement of P_n is determined by its distance spectrum.

LEMMA 2.5. *Let $G = \overline{P_n}$ and let H be distance cospectral to G. Then $\overline{H}$ is a disjoint union of a path and a number (possibly zero) of cycles.*

Proof. This follows from Proposition 2.4 and the fact that $m(\overline{G}) = m(\overline{H})$. ∎

LEMMA 2.6. *We have*

$$p\det(\lambda I - D(\overline{C_p})) = (\lambda - (p+1))\mathbb{1}'\operatorname{Adj}(\lambda I - D(\overline{C_p}))\mathbb{1}.$$

Proof. This is an immediate consequence of the fact that $\mathbb{1}$ is the Perron eigenvector of $D(\overline{C_p})$ for the Perron eigenvalue $p+1$. ∎

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THEOREM 2.7. *The complement of P_n is determined by its distance spectra.*

Proof. Let H be a graph cospectral with $\overline{P_n}$. By virtue of Lemma 2.5, it will suffice to assume that $\overline{H}$ is the disjoint union of C_p and an unknown graph Q and obtain a contradiction. Towards this, we have by a standard Schur Complement formula

$$\det(\lambda I - D(H)) = \det(\lambda I - D(\overline{C_p}))\det(\lambda I - D(\overline{Q})) - \left(\mathbb{1}'\mathrm{Adj}(\lambda I - D(\overline{C_p}))\mathbb{1}\right)\left(\mathbb{1}'\mathrm{Adj}(\lambda I - D(\overline{Q}))\mathbb{1}\right).$$

By Lemma 2.6, the polynomial $\mathbb{1}'\mathrm{Adj}(\lambda I - D(\overline{C_p}))\mathbb{1}$ is a factor of $\det(\lambda I - D(H)) = \det(\lambda I - D(\overline{P_n}))$, and hence, $\det(\lambda I - D(\overline{P_n}))$ has all the roots of $\det(\lambda I - D(\overline{C_p}))$ (counted according to multiplicity) with the exception of the Perron root $p+1$. But this forces $D(\overline{P_n})$ to have at least one multiple characteristic root, a contradiction. ∎

2.3. The complement of C_n is determined by its distance spectrum.

LEMMA 2.8. *Let $G = \overline{C_n}$ and let H be D-cospectral to G. Then $\overline{H}$ is a disjoint union of a number of cycles.*

Proof. This follows from Proposition 2.4 and the fact that $m(\overline{G}) = m(\overline{H})$. ∎

The following result is a case of Weyl's Inequality [1, Theorem III.2.1].

LEMMA 2.9. [19] *Let A and B be $n\times n$ Hermitian matrices and $C = A + B$. Then*

$$\lambda_k(C) \geq \lambda_j(A) + \lambda_{k-j+n}(B)\ (n \geq j \geq k \geq 1).$$

LEMMA 2.10. *Let $G = \overline{C_n}$ and let H be D-cospectral to G. Then $\overline{H}$ does not contain the union of two disjoint cycles.*

Proof. If not, we may suppose that $\overline{H}$ contains the union of two disjoint cycles, then $\lambda_2(A(\overline{H})) \geq 2$. Note that $D(H) = J_n - I_n + A(\overline{H})$. Then by Lemma 2.9, we have

$$\lambda_2(D(G)) = \lambda_2(D(H)) \geq \lambda_2(A(\overline{H})) + \lambda_n(J_n - I_n) \geq 1,$$

a contradiction. ∎

THEOREM 2.11. *The complement of C_n is determined by its distance spectra.*

Proof. For $n = 3$, the proof is by direct calculation. We assume $n \geq 4$. Let H be a graph cospectral with $\overline{C_n}$. By virtue of Lemma 2.8, $\overline{H}$ is a disjoint union of cycles. By Lemma 2.10, $\overline{H}$ is a single cycle. ∎

REMARK 2.12. An interesting situation arises when G is the complement of the union of C_6 and an isolated vertex and H is the complement of the graph obtained by taking three disjoint copies of P_3 and identifying a pendent vertex from each copy. These graphs are D-cospectral. Their complements have seven vertices and six edges. All the vertices of the complements except one have degree one or two. The exceptional vertex of $\overline{G}$ has degree 0 and that of $\overline{H}$ has degree 3. Thus, the identity

$$\mathrm{tr}(A(\overline{G})^3) + 3\sum_{k=1}^{n}(d_k(\overline{G}) - 1)(d_k(\overline{G}) - 2) = \mathrm{tr}(A(\overline{H})^3) + 3\sum_{k=1}^{n}(d_k(\overline{H}) - 1)(d_k(\overline{H}) - 2)$$

holds.

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3. The graph P_n is determined by its distance spectrum.

THEOREM 3.1. *Let G be a connected graph with n vertices. Then $\|D(G)\|_{\mathrm{HS}}^2 \leq \dfrac{n^4-n^2}{6}$ with equality if and only if G is a path. In particular P_n is determined by its distance spectrum.*

Proof. The proof is by induction on the number n of vertices. Since the theorem is easy to check for small n, induction starts.

Replacing G by a spanning tree of G increases the distance matrix elementwise. Hence, without loss of generality, we may assume that G is a tree. Select a pendent vertex v of G and let H be the tree obtained by removing v from G. Then, by the induction hypothesis,

$$\|D(H)\|_{\mathrm{HS}}^2 \leq \frac{(n-1)^2(n-2)n}{6},$$

with equality only if H is a path. Now clearly,

$$\sum_{u\neq v} d_G(u,v)^2 \leq \sum_{k=1}^{n-1} k^2 = \frac{n(2n-1)(n-1)}{6},$$

with equality if and only if there is a vertex u of G such that $d_G(u,v)=n-1$. It now follows that

$$\|D(G)\|_{\mathrm{HS}}^2 \leq \|D(H)\|_{\mathrm{HS}}^2 + 2\sum_{u\neq v} d_G(u,v)^2 \leq \frac{(n-1)^2(n-2)n}{6} + \frac{n(2n-1)(n-1)}{3} = \frac{n^4-n^2}{6},$$

with equality implying $\mathrm{diam}(G)=n-1$ and forcing G to be a path. This completes the induction step. ☐

4. The graph C_n (n odd) is determined by its distance spectrum. In [16], it is shown that $D(G)\mathbb{1} \leq \lambda_1(D(C_n))\mathbb{1}$ for every 2-connected graph G of order n. Using much the same methods, we will establish the following theorem.

THEOREM 4.1. *For every 2-edge connected graph G of order n, $\|D(G)\|_{\mathrm{HS}} \leq \|D(C_n)\|_{\mathrm{HS}}$ with equality only if $G \cong C_n$.*

LEMMA 4.2. *Let G be a 2-connected graph of order n and v any vertex. Then the following hold:*

1. $\sum_{k=1}^n d_{v,k} \leq \alpha_1(n) = \begin{cases} \frac{n^2-1}{4} & \text{if } n \text{ is odd,} \\ \frac{n^2}{4} & \text{if } n \text{ is even.}\end{cases}$
2. $\sum_{k=1}^n d_{v,k}^2 \leq \alpha_2(n) = \begin{cases} \frac{n^3-n}{12} & \text{if } n \text{ is odd,} \\ \frac{n^3+2n}{12} & \text{if } n \text{ is even.}\end{cases}$

Proof. We note that part 1 is already established in [16]. We let $d = \max\limits_{1\leq k\leq n} d_{v,k}$ and let S_i be the set of vertices at exactly distance i from v for $i=0,\ldots,d$. Lin et al. note that S_i is a cut set for $i=1,\ldots,d-1$ and deduce that $|S_i|\geq 2$ in the same range. Starting from

$$\sum_{k=1}^n d_{v,k}^2 = \sum_{i=1}^d |S_i| i^2, \qquad n-1 = \sum_{i=1}^d |S_i|,$$

we find

$$(n-1)d^2 - \sum_{i=1}^d |S_i| i^2 = \sum_{i=1}^d |S_i|(d^2-i^2) \geq \sum_{i=1}^d 2(d^2-i^2) = \frac{4}{3}d^3 - d^2 - \frac{1}{3}d.$$

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Therefore,

$$\sum_{k=1}^{n} d_{v,k}^2 \leq (n-1)d^2 - \frac{4}{3}d^3 + d^2 + \frac{1}{3}d.$$

This quantity attains its maximum value of $\frac{n^3-n}{12}$ when $d = \frac{n-1}{2}$ or $d = \frac{n+1}{2}$ if n is odd and $\frac{n^3+2n}{12}$ at $d = \frac{n}{2}$ if n is even. It is easy to see that these values are attained for $G = C_n$ and if equality obtains, then $|S_i| = 2$ for $i = 1, \ldots, \frac{n-1}{2}$ (case n odd) and for $i = 1, \ldots, \frac{n-2}{2}$ (case n even). Thus, $G \cong C_n$. ∎

Corollary 4.3. *Let G be a 2-connected graph of order n. Then $\|D(G)\|_{\mathrm{HS}} \leq \|D(C_n)\|_{\mathrm{HS}}$ with equality only if $G \cong C_n$.*

The proof is immediate.

Lemma 4.4. *Let G be a 2-edge connected graph of order n and v any vertex. Then*

1. $\sum_{k=1}^{n} d_{v,k} \leq \beta_1(n) = \begin{cases} \frac{n^2-n}{3} & \text{if } n \cong 0 \text{ or } 1 \pmod 3, \\ \frac{n^2-n-2}{3} & \text{if } n \cong 2 \pmod 3. \end{cases}$
2. $\sum_{k=1}^{n} d_{v,k}^2 \leq \beta_2(n) = \begin{cases} \frac{4n^3-6n^2}{27} & \text{if } n \cong 0 \pmod 3, \\ \frac{4n^3-6n^2+2}{27} & \text{if } n \cong 1 \pmod 3, \\ \frac{4n^3-6n^2-24n+40}{27} & \text{if } n \cong 2 \pmod 3. \end{cases}$

Proof. Using the same notations as before, we note that $|S_1| \geq 2$ and that for $i = 1, \ldots, d-1$, either $|S_i| \geq 2$ or $|S_{i+1}| \geq 2$ since if both $|S_i| = 1$ and $|S_{i+1}| = 1$, then removal of the unique edge joining S_i to S_{i+1} will disconnect the graph. In obtaining a lower bound for $\sum_{i=1}^{d} |S_i|(d-i)$, we see that the worst case scenario is when $|S_i| = 2$ for i odd and $|S_i| = 1$ for i even. Thus, we obtain

$$(n-1)d - \sum_{i=1}^{d} |S_i| i = \sum_{i=1}^{d} |S_i|(d-i) \geq \frac{3}{4}d^2 - \frac{1}{2}d - \frac{1}{8} + \frac{1}{8}(-1)^d,$$

and hence,

$$\sum_{k=1}^{n} d_{v,k} \leq (n-1)d - \frac{3}{4}d^2 + \frac{1}{2}d + \frac{1}{8} - \frac{1}{8}(-1)^d.$$

The maximum value of this quantity is obtained with $d = \frac{2n}{3}$ even when $n \cong 0 \pmod 3$, $d = \frac{2n-2}{3}$ even when $n \cong 1 \pmod 3$ and $d = \frac{2n-1}{3}$ odd when $n \cong 2 \pmod 3$. A moment's thought shows that in case $n \cong 2 \pmod 3$, $d = \frac{2n-1}{3}$ is unattainable. It is not difficult to see that the largest value is obtained from $|S_i| = 1$ for $i = 0, 2, 4, \ldots, d-2$ and $|S_i| = 2$ for $i = 1, 3, \ldots, d-3, d-1, d$, where $d = \frac{2n-4}{3}$ is even. The second assertion follows in the same way after finding

$$\sum_{k=1}^{n} d_{v,k}^2 \leq \frac{1}{4}d(4dn - 2d - 4d^2 + 1 - (-1)^d)$$

and arguing as above. ∎

Lemma 4.5. *If G is a 2-edge connected graph that is not 2-connected, then there exists a vertex v whose removal disconnects G and such that there is a 2-connected subgraph K of G and a 2-edge connected subgraph H of G with vertex sets meeting only in v.*

Proof. Consider the set M of maximal 2-connected induced subgraphs of G. Since G is not 2-connected, M has at least two elements. Clearly two such subgraphs are either vertex disjoint or meet in a single

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Volume 34, pp. 320-330, July 2018.

vertex. Thus, we may define a graph on the vertex set M. Two vertices of M are adjacent if and only if the intersection of the vertex sets of the corresponding subgraphs is a singleton. Clearly this graph is connected and cannot have a cycle since this would contradict the maximality of at least one of the graphs in M. So, the graph is a tree. We choose one of the subgraphs corresponding to a leaf of this tree. This is the graph K and it links to exactly one element of M at a vertex v. The union of the remaining subgraphs is H. Then K and H meet only in v and H is 2-edge connected since G is. ◻

PROPOSITION 4.6. *If G is a 2-edge connected graph that is not 2-connected, then*

$$\|D(G)\|_{\mathrm{HS}} < \|D(C_n)\|_{\mathrm{HS}}.$$

Proof. We prove this by induction on n. For small values of n it is easily verified. We apply Lemma 4.5 and use the induction hypothesis to deduce

$$\|D(H)\|_{\mathrm{HS}}^2 \le q\alpha_2(q) = \|D(C_q)\|_{\mathrm{HS}}^2,$$

where q is the order of H. We find an upper bound for the square of the Hilbert–Schmidt norm of G by

$$\|D(G)\|_{\mathrm{HS}}^2 = \|D(K)\|_{\mathrm{HS}}^2 + \|D(H)\|_{\mathrm{HS}}^2 + 2\sum_{k\in V(K)\setminus\{v\}}\ \sum_{\ell\in V(H)\setminus\{v\}} (d_{v,k}+d_{v,\ell})^2$$

since for $k \in V(K)$ and $\ell \in V(H)$, $d_{k,\ell} = d_{v,k} + d_{v,\ell}$. We may assume that K has $p \ge 3$ vertices and H has $q \ge 3$ vertices. Then

$$\begin{aligned}\|D(G)\|_{\mathrm{HS}}^2 = \|D(K)\|_{\mathrm{HS}}^2 + \|D(H)\|_{\mathrm{HS}}^2 + 2(q-1)\sum_{k\in V(K)} d_{v,k}^2 \\ + 2(p-1)\sum_{\ell\in V(H)} d_{v,\ell}^2 + 4\left(\sum_{k\in V(K)} d_{v,k}\right)\left(\sum_{\ell\in V(H)} d_{v,\ell}\right).\end{aligned}$$

Therefore, we wish to show

$$p\alpha_2(p) + q\alpha_2(q) + 2(q-1)\alpha_2(p) + 2(p-1)\beta_2(q) + 4\alpha_1(p)\beta_1(q) < n\alpha_2(n)$$

where $n = p+q-1$. For moderate values of n (say $n \le 10$) this can be done by checking all possible values of p and q. For large n, we use the worst case estimates for the quantities. Explicitly we need to check that

$$\frac{1}{12}p^2(p^2+2) + \frac{1}{12}q^2(q^2+2) + \frac{1}{6}(q-1)p(p^2+2) + \frac{2}{27}(p-1)(4q^3-6q^2+2) + \frac{p^2}{3}\left(q^2-q\right) < \frac{n^2(n^2-1)}{12}.$$

for $n = p+q-1$, $p, q \ge 3$ and $p+q > 11$. This amounts to showing that

$$\frac{1}{6}p^3q + \frac{1}{6}p^2q^2 + \frac{1}{27}pq^3 - \frac{1}{6}p^3 - \frac{2}{3}p^2q - \frac{5}{9}pq^2 - \frac{1}{27}q^3 + \frac{1}{4}p^2 - \frac{7}{36}q^2 + \frac{1}{2}pq - \frac{1}{6}q + \frac{1}{54}p + \frac{4}{27} > 0$$

in the same range. This is a lengthy exercise in differential calculus which we omit. ◻

Proof of Theorem 4.1. If G is 2-connected, the result follows from Corollary 4.3, if not, then from Proposition 4.6. ◻

Furthermore, we have:

PROPOSITION 4.7. *For n odd, the coefficient of λ in the characteristic polynomial* $\det(\lambda I - D(C_n))$ *is odd.*

Electronic Journal of Linear Algebra, ISSN 1081-3810
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Volume 34, pp. 320-330, July 2018.

Proof. The coefficient of λ in the characteristic polynomial $\det(\lambda I - D(C_n))$ is the sum of n principal minors of oder $n-1$. All these minors are equivalent, so it suffices to show that a typical such minor written with coefficients in $GF(2)$ has determinant 1. One reduces such a minor by applying row operations in the central four rows in such a way that the central two rows and the first and last columns can be removed. This results in a minor of a similar type, so that the result follows by an induction hypothesis.

As an example, consider the case $n = 9$. Then

$$\begin{vmatrix} 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 \end{vmatrix} = \begin{vmatrix} 1 & 0 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 \end{vmatrix}$$

in $GF(2)$ by applying the row operations $R_4 \to R_4 - R_3$ and $R_5 \to R_5 - R_6$. ∎

PROPOSITION 4.8. *For G a graph which is not 2-edge connected, the coefficient of λ in the characteristic polynomial $\det(\lambda I - D(G))$ is even.*

LEMMA 4.9. *Let A be a symmetric $n \times n$ matrix with coefficients in $GF(2)$ with zero diagonal. Then if n is odd, $\det(A) = 0$. If n is even, then $\det(A) = \sum \prod_{j=1}^{\frac{n}{2}} a_{p_j,q_j}$ where the sum is over all sets of $\frac{n}{2}$ disjoint pairs (p_j, q_j).*

Proof. Consider the expansion $\det(A) = \sum_{\sigma \in S_n} \prod_{j=1}^{n} a_{j,\sigma(j)}$. The term corresponding to σ in this expansion is the same as the term corresponding to σ^{-1}. So, if $\sigma \neq \sigma^{-1}$ the terms cancel. Since only permutations σ with no fixed points can make a contribution, the result follows. ∎

COROLLARY 4.10. *Let A be a symmetric $n \times n$ matrix with coefficients in $GF(2)$. Suppose that $a_{1,k} = 1$ for $k = 2, \ldots, n$, $a_{1,1} = 0$ and $a_{j,j} = \lambda$ for $j = 2, \ldots, n$. Then the coefficient of λ in $\det(A)$ is zero.*

Proof. The coefficient of λ in $\det(A)$ is $\sum_{k=2}^{n} \det(A_k)$, where A_k is the matrix obtained by striking out the kth row and column from A and setting the diagonal elements to zero. If n is even, then $\det(A_k) = 0$ for all k. If n is odd, then $\det(A_j) = \sum \prod_{j=1}^{\frac{n}{2}} a_{p_j,q_j}$ where the sum is over all sets of $\frac{n-2}{2}$ disjoint pairs (p_j, q_j) from $\{2, \ldots, n\} \setminus \{k\}$. It is easy to see that each such set of pairs occurs exactly twice. ∎

Proof of Proposition 4.8. The characteristic polynomial of $D(G)$ where G can be disconnected by the removal of an edge e has the form modulo $GF(2)$

$$\begin{vmatrix} \lambda I + A & x & \mathbb{1} + x & Z \\ x' & \lambda & 1 & \mathbb{1}' + y' \\ \mathbb{1}' + x' & 1 & \lambda & y' \\ Z' & \mathbb{1} + y & y & \lambda I + B \end{vmatrix},$$

where x and y are column vectors and A and B are symmetric matrices with zero diagonal. The second and third row and columns correspond to the vertices adjoining the edge e. After applying a simultaneous row

Electronic Journal of Linear Algebra, ISSN 1081-3810
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and column operation, this becomes

$$\begin{vmatrix} \lambda I+A & x & \mathbb{1} & Z \\ x' & \lambda & 1-\lambda & \mathbb{1}'+y' \\ \mathbb{1}' & 1-\lambda & 2(\lambda-1) & -\mathbb{1}' \\ Z' & \mathbb{1}+y & -\mathbb{1} & \lambda I+B \end{vmatrix}.$$

Clearly, we may replace $2(\lambda-1)$ with zero and the contribution to the coefficient of λ of the λ term in the (2,3) entry is the same as that in the (3,2) entry. Therefore, the determinant

$$\begin{vmatrix} \lambda I+A & x & \mathbb{1} & Z \\ x' & \lambda & 1 & \mathbb{1}'+y' \\ \mathbb{1}' & 1 & 0 & \mathbb{1}' \\ Z' & \mathbb{1}+y & \mathbb{1} & \lambda I+B \end{vmatrix}$$

will have the same coefficient of λ modulo 2. The result now follows from Corollary 4.10. ∎

THEOREM 4.11. *For n odd, the graph C_n is uniquely determined by its distance spectrum.*

Proof. Let G be a graph with the same order and distance spectrum as C_n. Then if G is 2-edge connected, the result follows from Theorem 4.1, if not, then from Propositions 4.7 and 4.8. ∎

5. Concluding remarks. Suppose that G is D-cospectral with H, we know that $m(G)$ is not always equal to $m(H)$. So we have the following problem.

PROBLEM 5.1. *Suppose that G is D-cospectral with H. Under which condition, we have $m(G) = m(H)$?*

From the paper, we know that if both G and H have diameter 2, then $m(G) = m(H)$. But when the diameter is greater than 3, then the size is not always equal. So it is interesting to consider the connected graphs with larger diameter, such as C_n. In the paper, when n is odd, we show that C_n is determined by its D-spectra, but when it comes to n even, we leave the following problem.

PROBLEM 5.2. *For n even, is the graph C_n uniquely determined by its distance spectrum?*

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