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Enumeration of cospectral and coinvariant graphs

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ABSTRACT

We present enumeration results on the number of connected graphs up to 10 vertices for which there is at least one other graph with the same spectrum (cospectral mate), or at least one other graph with the same Smith normal form (coinvariant mate) with respect to several matrices associated to a graph. The presented numerical data give some indication that possibly the Smith normal form of the distance Laplacian and the signless distance Laplacian matrices could be a finer invariant than the spectrum to distinguish graphs. Finally, we prove a graph characterization using the Smith normal form of the distance signless Laplacian matrix.

1. Introduction

Spectral graph theory aims to understand to what extent graphs are characterized by their spectra. Starting from the eigenvalues of a matrix associated to a graph, it seeks to deduce combinatorial properties of the graph. For this, we associate a graph G to a matrix M and analyze the eigenvalues of M. These eigenvalues are called the *spectrum* of G with respect to the matrix M, and its multiset is denoted by M-spectrum(G). *M-cospectral graphs* are graphs that share M-spectrum. A graph G is *determined by its M-spectrum*, M-DS, if only isomorphic graphs are cospectral with G.

Motivated by the graph isomorphism problem, it is of interest what fraction of all graphs is uniquely determined by its spectrum. Haemers conjectured that the fraction of graphs on n vertices with a M-cospectral mate tends to zero as n tends to infinity. A numerical study for $n \leq 9$ was given by Godsil and McKay [16], for $n = 10, 11$ by Haemers and Spence [18] and for $n = 12$ by Brouwer and Spence [12]. Aouchiche and Hansen [6] presented computational results in which they studied cospectrality for the distance, distance Laplacian and distance signless Laplacian matrices of all the connected graphs on up to 10 vertices. Recently, Pinheiro, Souza and Trevisan [26] provided some numerical evidence that the complementary spectrum of a graph distinguishes more graphs than other standard graph spectra, but they also showed that it is hard to compute the complementary spectrum.

The main question is whether it is possible to define a matrix M of G such that every graph becomes M-DS. In [14] it was shown that the answer to this question is positive. However, in this case it is more work to check cospectrality of the matrices than testing isomorphism. If there would be an easily computable matrix M for which every graph becomes M-

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Table 1
Number of connected graphs with at least one cospectral mate for A, L, Q and D.

n	5	6	7	8	9	10
$\lvert\mathcal{G}_n\rvert$	21	112	853	11,117	261,080	11,716,571
$\lvert\mathcal{G}_n^{sp}(A)\rvert$	0	2	63	1353	46,930	2,462,141
$\lvert\mathcal{G}_n^{sp}(L)\rvert$	0	4	115	1611	40,560	1,367,215
$\lvert\mathcal{G}_n^{sp}(Q)\rvert$	2	10	80	1047	17,627	615,919
$\lvert\mathcal{G}_n^{sp}(D)\rvert$	0	0	22	658	25,058	1,389,986

DS, the graph isomorphism problem would be solved. Hence, when M is one of the commonly used matrices associated to graphs (adjacency, Laplacian, distance matrices, signless Laplacian, normalized Laplacian), one can say that there is not such a matrix M for which all graphs are M-DS, since there exist many examples of non-isomorphic graphs that share the same M-spectrum. This leaves open the possibility of amplifying or replacing spectra with the use of more refined representations for obtaining more faithful graph information.

The main goal of this article is to propose a new way of representing a graph using the Smith normal form (SNF) of certain distance matrices. We provide some numerical evidence that this new algebraic graph representation may do a better job in distinguishing graphs. For this we first need to recall some definitions. Two matrices M, N are *equivalent* if there exist unimodular matrices P and Q with entries in $\mathbb{Z}$ satisfying $M = PNQ$. The Smith normal form of a integer matrix M, denoted by SNF(M), is the unique diagonal matrix $\text{diag}(f_1, \dots, f_r, 0, \dots, 0)$ equivalent to M such that $r = rank(M)$ and $f_i | f_j$ for $i < j$. The *invariant factors* (or *elementary divisors*) of M are the integers in the diagonal of the SNF(M). If M is an integer symmetric matrix associated to a graph, then we say that the graphs G and H are M-*coinvariant* if the SNFs of $M(G)$ and $M(H)$, computed over $\mathbb{Z}$, are the same. Coinvariant graphs were introduced in [28]. Note that related to the SNF there is the p-*rank*, i.e., the rank of the matrix considered over the finite field $\mathbb{F}_p$. We should note that the p-rank has also been used in the literature to distinguish graphs; for instance, the 2-rank and the spectrum characterize symplectic graphs over $\mathbb{F}_2$ [24], the 2-rank can be used to distinguish strongly regular graphs with the same parameters as the symplectic graph [1], and some p-ranks and the spectrum were used to characterize distance-regular graphs [25].

In particular, in this work we study if there is a matrix M (say adjacency, Laplacian, signless Laplacian, etc.) whose SNF distinguishes more graphs. Broadly speaking, the idea is to verify whether the portion of graphs that have a M-coinvariant mate is smaller than the portion of graphs having a M-cospectral mate for a particular matrix M. Cospectrality and coinvariancy both play an important role in the famous graph isomorphism problem. While it is unknown whether testing graph isomorphism is a hard problem or not, determining whether two graphs are cospectral or coinvariant can be done in polynomial time [20,27]. It is also known that testing coinvariancy is experimentally faster than testing cospectrality [2]. Thus, one can focus on testing isomorphism among coinvariant graphs.

Our results show that the invariant factors of the distance signless Laplacian matrix provide a way of representing graphs which does a better job than the spectrum in distinguishing them. The distance Laplacian and the distance signless Laplacian matrices have received quite a lot of attention over the last years [7,8,10,15,22,23]. This article is a sequel to the work by Aouchiche and Hansen [6]. Numerical data on the number of cospectral and coinvariant graphs is given for several matrices, and we also take the opportunity to correct an earlier value. This paper also complements the work by Haemers and Spence [18], LepovicitePLXBIB0022 and Godsil and McKay [17] on enumerating cospectral graphs.

In particular, we extend the computer enumeration for cospectral graphs of [17,18,21] and [6] to all connected graphs on at most 10 vertices that have at least a cospectral mate with respect to the distance Laplacian matrix and the distance signless Laplacian matrix. We also enumerate graphs with at most 10 vertices which have at least a coinvariant mate for several associated matrices. Finally, we present a novel method to show a graph characterization using the SNF of the distance Laplacian and distance signless Laplacian matrix, illustrating the power of the proposed graph invariant.

2. Enumeration

Since we will use several graph distance matrices, we focus on connected graphs such that our enumeration results are comparable. Denote by $\mathcal{G}_n$ the set of connected graphs with n vertices. Given a connected graph G, we will study the following associated matrices: the adjacency matrix $A(G)$, the Laplacian matrix $L(G)$, the distance matrix $D(G)$, the signless Laplacian matrix $Q(G)$, the distance Laplacian matrix $D^L(G)$ and the distance signless Laplacian matrix $D^Q(G)$.

Let $\mathcal{G}_n^{sp}(M)$ be the set of graphs in $\mathcal{G}_n$ which have at least one cospectral mate in $\mathcal{G}_n$ with respect to the matrix M. Table 1 provides the number of cospectral mates of connected graphs with respect to several associated matrices.

Analogously, let $\mathcal{G}_n^{in}(M)$ be the set of graphs in $\mathcal{G}_n$ which have at least one coinvariant mate in $\mathcal{G}_n$ with respect to the matrix M. Table 2 shows the enumeration of $\mathcal{G}_n^{in}(M)$ for several associated matrices.

Extensive research has been devoted to understand cospectral graphs, but much less has been dedicated to understand coinvariant mates and its potential to characterize graphs. The reason for this could be that for matrices A, L, Q and D, there is a large proportion of connected graphs having a M-coinvariant mate, as Fig. 1 shows. We follow [13] in defining the

Table 2
Number of connected graphs with at least one coinvariant mate for A, L, Q and D.

n	4	5	6	7	8	9	10
$\lvert\mathcal{G}_n\rvert$	6	21	112	853	11,117	261,080	11,716,571
$\lvert\mathcal{G}_n^{in}(A)\rvert$	4	20	112	853	11,117	261,080	11,716,571
$\lvert\mathcal{G}_n^{in}(L)\rvert$	2	8	57	526	8027	221,834	11,036,261
$\lvert\mathcal{G}_n^{in}(Q)\rvert$	2	11	78	620	7962	201,282	10,086,812
$\lvert\mathcal{G}_n^{in}(D)\rvert$	2	15	102	835	11,080	260,991	11,716,249

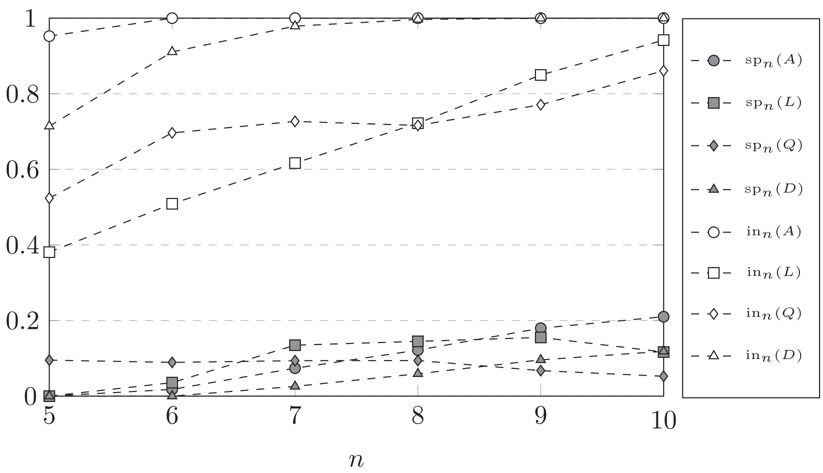


Fig. 1. The fraction of graphs on n vertices that have at least one cospectral mate with respect to a certain associated matrix is denoted as *sp*. The fraction of graphs on n vertices with respect to a certain associated matrix that have at least one coinvariant mate is denoted as *in*.

Table 3
Number of connected graphs with a cospectral or a coinvariant mate for D^L and D^Q.

n	5	6	7	8	9	10
$\lvert\mathcal{G}_n^{sp}(D^L)\rvert$	0	0	43	745	20,455	787,851
$\lvert\mathcal{G}_n^{in}(D^L)\rvert$	0	0	18	455	16,505	642,002
$\lvert\mathcal{G}_n^{sp-in}(D^L)\rvert$	0	0	14	435	16,006	611,987
$\lvert\mathcal{G}_n^{sp}(D^Q)\rvert$	2	6	38	453	8168	319,324
$\lvert\mathcal{G}_n^{in}(D^Q)\rvert$	2	4	20	259	7444	264,955
$\lvert\mathcal{G}_n^{sp-in}(D^Q)\rvert$	2	4	20	243	6676	255,964

spectral uncertainty $\mathrm{sp}_n(M)$ with respect to M as the ratio $|\mathcal{G}_n^{sp}(M)|/|\mathcal{G}_n|$, and the *invariant uncertainty* $\mathrm{in}_n(M)$ with respect to M as the ratio $|\mathcal{G}_n^{in}(M)|/|\mathcal{G}_n|$.

Table 3 presents the number of connected graphs having at least one cospectral or at least one coinvariant mate for D^L and D^Q. Here, $|\mathcal{G}_n^{sp-in}(M)|$ denotes the amount of graphs with a cospectral mate which is also a coinvariant mate with respect to the corresponding matrix M. Aouchiche and Hansen [6] enumerated cospectral graphs for D, D^L and D^Q of all connected graphs with at most 10 vertices. While most of their results are consistent with ours, in Table 3 we obtain 20,455 cospectral graphs with 9 vertices with respect to D^L, while they reported that there are 19,778 of such graphs.

Fig. 2 displays the spectral and the invariant uncertainty for D^L and D^Q. We also include the spectral uncertainty for Q, since according to Table 1, this would be the best invariant for distinguishing graphs using the spectrum. According to our results, the SNF of D^Q performs better than the spectrum for distinguishing graphs for all considered matrices. We should also note that there is no significant improvement when both the spectrum and the SNF are used together, as the parameter $\mathcal{G}_n^{sp-in}(M)$ indicates in Table 3, thus this has not been added in Fig. 2.

In this work we also tested the discrimination power of the p-rank on distinguishing graphs. However, since the p-rank can take values from 0 to n, in general, it seems not such a good graph invariant. Thus we performed an enumeration of graphs with the same SNF for the matrices introduced above over F_p with $p \in 2, 3, 5, 7$. We used this since the p-rank follows from the SNF of a matrix M over F_p, but not viceversa. The enumeration results showed a clear tendency to claim that, for any matrix $M \in \{A, L, Q, D, D^L, D^Q\}$, almost all graphs on n vertices have another graph with the same SNF of M over F_p. Thus, we decided not to include these numerical results on the tables.

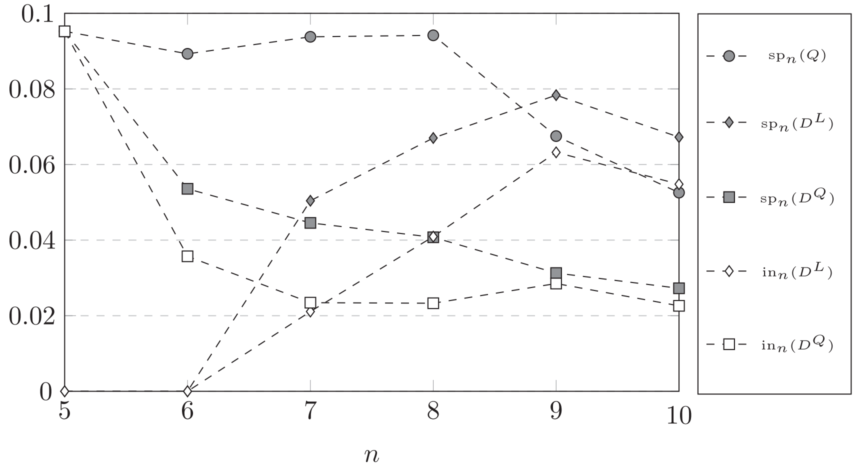


Fig. 2. The fraction of graphs on n vertices that have at least one cospectral mate with respect to a certain associated matrix is denoted as *sp*. The fraction of graphs on n vertices with respect to a certain associated matrix that have at least one coinvariant mate is denoted as *in*.

Table 4
Number of connected graphs with a cospectral and a coinvariant mate for D^L and D^Q.

n	7	8	9	10
$\lvert\mathcal{G}_n^{sp}(D^L, D^Q)\rvert$	0	90	1965	61,909
$\lvert\mathcal{G}_n^{in}(D^L, D^Q)\rvert$	0	44	1447	46,239
$\lvert\mathcal{G}_n^{sp}(D, D^L)\rvert$	0	0	32	9449
$\lvert\mathcal{G}_n^{in}(D, D^L)\rvert$	0	32	1770	92,915
$\lvert\mathcal{G}_n^{sp}(D, D^Q)\rvert$	0	0	0	7712
$\lvert\mathcal{G}_n^{in}(D, D^Q)\rvert$	0	20	432	24,517
$\lvert\mathcal{G}_n^{sp}(D, D^L, D^Q)\rvert$	0	0	0	7622
$\lvert\mathcal{G}_n^{in}(D, D^L, D^Q)\rvert$	0	0	138	12,246

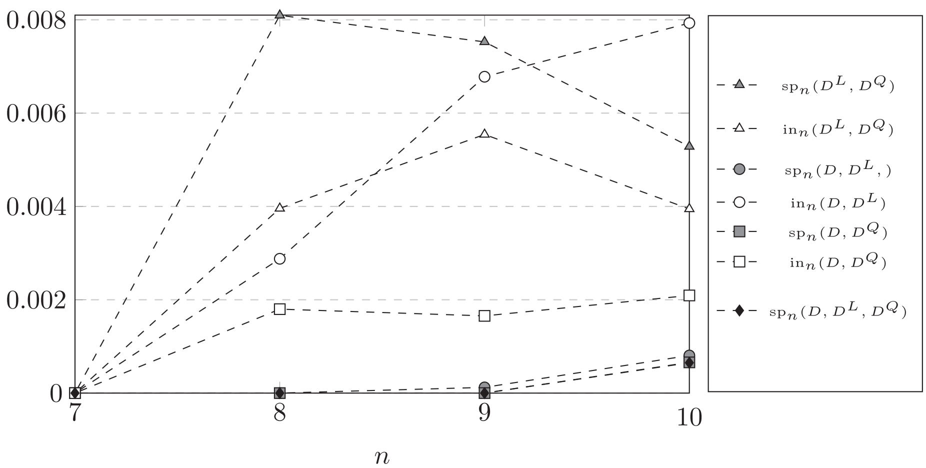


Fig. 3. The fraction of graphs on n vertices that have at least one cospectral mate with respect to a certain associated matrix is denoted as sp. The fraction of graphs on n vertices with respect to a certain associated matrix that have at least one coinvariant mate is denoted as in.

Aouchiche and Hansen [6] also explored how to improve the spectral uncertainty by considering two and three matrices together. Analogously as it was done in [6], in Table 4 we show the number of cospectral and coinvariant graphs when two matrices are considered. Let $\mathcal{G}_n^{sp}(M,N)$ be the set of graphs in $\mathcal{G}_n$ which have a cospectral mate in $\mathcal{G}_n$ with respect to the matrices M and N, and let $\mathcal{G}_n^{in}(M,N)$ be the set of graphs in $\mathcal{G}_n$ which have a coinvariant mate in $\mathcal{G}_n$ with respect to the matrices M and N. Thus, $\mathrm{sp}_n(M,N) = |\mathcal{G}_n^{sp}(M,N)|/|\mathcal{G}_n|$ and $\mathrm{in}_n(M,N) = |\mathcal{G}_n^{in}(M,N)|/|\mathcal{G}_n|$.

Fig. 3 shows the spectral and invariant uncertainty of the pairs of matrices obtained in Table 4. For the pair (D^L, D^Q), we see and advantage in considering the SNF. But for the other pairs, we observe that the spectrum is much better. There is

Table 5
$|\mathcal{G}_{10}^{sp-in}(M,N)|$.

$M\backslash N$	A	L	Q	D	D^L	D^Q
A	2,151,957	24,021	22,764	1,113,103	9253	7688
L	521,200	1,059,992	121,708	192,455	562,943	44,398
Q	136,347	84,058	486,524	48,413	44,848	250,068
D	1,073,185	15,176	13,496	1,145,275	8935	7646
D^L	300,596	563,219	52,757	110,574	611,989	47,004
D^Q	65,627	44,475	245,529	28,061	46,941	255,964

Table 6
Number of connected graphs with a cospectral and a coinvariant mate for several matrices combination.

n	8	9	10
$\lvert\mathcal{G}_n^{sp-in}(A,D^L)\rvert$	0	32	9,253
$\lvert\mathcal{G}_n^{sp-in}(D,D^L)\rvert$	0	32	8,935
$\lvert\mathcal{G}_n^{sp-in}(A,D^Q)\rvert$	0	2	7,688
$\lvert\mathcal{G}_n^{sp-in}(D,D^Q)\rvert$	0	0	7,646
$\lvert\mathcal{G}_n^{sp-sp-in}(A,D,D^L)\rvert$	0	32	8,743
$\lvert\mathcal{G}_n^{sp-sp-in}(A,D,D^Q)\rvert$	0	0	7,550
$\lvert\mathcal{G}_n^{sp-in-in}(A,D^L,D^Q)\rvert$	0	0	7,490
$\lvert\mathcal{G}_n^{sp-in-in}(D,D^L,D^Q)\rvert$	0	0	7,510

a clear improvement by taking the spectrum of the distance matrix together with the spectrum of either D^L or D^Q to the same obtained by the SNF. This will also stand in the following analysis.

Let $|\mathcal{G}_n^{sp-in}(M,N)|$ denote the number of graphs with a cospectral mate with respect to the matrix M that is also a coinvariant mate with respect to the matrix N. In Table 5, we compute $|\mathcal{G}_{10}^{sp-in}(M,N)|$ for all possible pairs of associated matrices. The lowest values are $|\mathcal{G}_{10}^{sp-in}(A,D^L)|$, $|\mathcal{G}_{10}^{sp-in}(D,D^L)|$, $|\mathcal{G}_{10}^{sp-in}(A,D^Q)|$ and $|\mathcal{G}_{10}^{sp-in}(A,D^Q)|$. It is interesting to observe that the combination of the spectrum of D with the SNF of D^Q gives better results than using only the spectrum of the two matrices. Therefore, this suggests that when distinguishing graphs, we should compute first the SNF of their distance signless Laplacian matrices and then the spectrum of their distance matrices.

In order to improve the value obtained for $|\mathcal{G}_{10}^{sp}(D,D^L,D^Q)|$, we explore the use of the following parameters. Let $|\mathcal{G}_n^{sp-sp-in}(M_1,M_2,M_3)|$ be the number of graphs with a cospectral mate for the matrix M_1 which is also a cospectral mate with respect to M_2, and that is also a coinvariant mate with respect to the matrix M_3. Let $|\mathcal{G}_n^{sp-in-in}(M_1,M_2,M_3)|$ be the number of graphs with a cospectral mate for the matrix M_1 which is also a coinvariant mate with respect to M_2, and is also a coinvariant mate with respect to the matrix M_3. The results from this analysis are shown in Table 6.

From Table 6, we can see that $|\mathcal{G}_{10}^{sp-sp-in}(A,D,D^Q)|$, $|\mathcal{G}_{10}^{sp-in-in}(A,D^L,D^Q)|$ and $|\mathcal{G}_{10}^{sp-in-in}(D,D^L,D^Q)|$ are better than $|\mathcal{G}_{10}^{sp}(D,D^L,D^Q)| = 7,622$. Actually, the best performance is obtained with $|\mathcal{G}_{10}^{sp-in-in}(A,D^L,D^Q)| = 7,490$. Note that the order in computing each parameter matters only in the ability of the parameter to distinguish graphs.

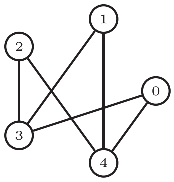
To sum up, from the above computational results one can conclude that the best procedure to distinguish graphs using the spectrum and the SNF is first to compute the SNF of their D^Q matrices, since $\mathrm{in}_n(D^Q)$ has the best performance over the spectral and invariant uncertainty of all matrices. Then, if necessary, compute the spectrum of their A matrices, since $|\mathcal{G}_n^{sp-in}(A,D^L)|$ is lower than $|\mathcal{G}_n^{in}(D^L,D^Q)|$ for $n \leq 10$. Finally compute the SNF of the D^L matrices.

2.1. Coinvariant trees

We end up Section 2 with an observation on coinvariant trees. Aouchiche and Hansen [8] reported enumeration results on cospectral trees with at most 20 vertices with respect to D, D^L and D^Q. For D, they found that among the 123,867 trees on 18 vertices, there are two pairs of D-cospectral mates. Among the 317,955 trees on 19 vertices, there are six pairs of D-cospectral mates. There are 14 pairs of D-cospectral mates over all the 823,065 trees on 20 vertices. And surprisingly, after the enumeration of all 1,346,023 trees on at most 20 vertices, they found no D^L-cospectral mates and no D^Q-cospectral mates. This fact lead Aouchiche and Hansen to conjecture that every tree is determined by its distance Laplacian spectrum, and by its distance signless Laplacian spectrum.

Analogously, for the SNF of D, D^L and D^Q of trees one can obtain some similar insights. But for that, first we need to state a result by Hou and Woo [19], who extended the Graham and Pollak celebrated formula $\det(D(T_{n+1})) = (-1)^n n 2^{n-1}$ for any tree T_{n+1} with $n+1$ vertices to the SNF of the distance matrix.

Theorem 1 ([19]). *Let T_{n+1} be a tree with $n+1$ vertices, then* $\mathrm{SNF}(D(T_{n+1})) = \mathsf{I}_2 \oplus 2\mathsf{I}_{n-2} \oplus (2n)$.



$$\begin{bmatrix} x_0 & 2 & 2 & 1 & 1 \\ 2 & x_1 & 2 & 1 & 1 \\ 2 & 2 & x_2 & 1 & 1 \\ 1 & 1 & 1 & x_3 & 2 \\ 1 & 1 & 1 & 2 & x_4 \end{bmatrix}$$

Fig. 4. A graph and its generalized distance matrix.

The following is a straight forward consequence from Theorem 1, since this implies that all trees on n vertices have the same SNF of its distance matrix D.

Corollary 2. *All trees with n vertices are D-coinvariant mates.*

After enumerating coinvariant trees with at most 20 vertices with respect to D^L and D^Q, we found no D^L-coinvariant mates and no D^Q-coinvariant mates among all trees with up to 20 vertices. This fact lead us to conjecture that almost all trees are determined by the SNF of its D^L, and analogously, by the SNF of its D^Q.

3. Graphs determined by the SNF

Not much is known regarding graph characterizations using the SNF. A few examples of graphs characterized by the SNF of the adjacency and the Laplacian matrices appear in [5] or [11]. However, our computational results from Section 2 provide an indication that possibly almost no graph has a coinvariant mate when $n \to \infty$ for the matrices D^L and D^Q. While the SNF of D^L has been recently used to characterize complete graphs and star graphs [2], to our knowledge there is not yet any graph characterization result using the SNF of D^Q. In this section we will show that complete graphs can be determined by considering the SNF of D^Q.

As mentioned before, it is known that complete graphs and star graphs are determined by the SNF of the D^L matrix [2].

Theorem 3 ([2])**.** *Complete graphs are determined by the SNF of the D^L matrix.*

Theorem 4 ([2])**.** *Star graphs are determined by the SNF of the D^L matrix.*

In this section we show an analogous result to Theorem 3, but using the SNF of the distance signless Laplacian matrix. In order to do so we need to define the distance ideals of a graph, which were first introduced in [4].

Let $G = (V, E)$ be a connected graph and let $X_G = \{x_u : u \in V(G)\}$ be a set of indeterminates associated with the vertices of G. We denote by $\operatorname{diag}(X_G)$, the diagonal matrix whose entries are the indeterminates in X_G. The matrix $\operatorname{diag}(X_G) + D(G)$ is known as *generalized distance matrix* of G. From this matrix we can recover the matrices D, D^L and D^Q just by evaluating the indeterminates X_G at the zero or transmission vectors. Recall that the *transmission* $tr(u)$ of a vertex u is $\sum_{v\in V} d_G(u, v)$, and the transmission vector $tr(G)$ is the vector whose entries are associated with the transmission of the vertices of G. Then, $D(G) = D(G, \mathbf{0})$, $D^L(G) = -D(G, -tr(G))$ and $D^Q(G) = D(G, tr(G))$.

Let n be the number of vertices of G. For $k \in \{1, \dots, n\}$, the *k-th distance ideal* $I_k(G, X_G)$ of the graph G is defined as the ideal generated by the k-minors of $D(G, X_G)$ in $\mathbb{Z}[X_G]$, that is, $\langle \text{minors}_k(D(G, X_G))\rangle$, where $\text{minors}_k(D(G, X_G))$ is the set of the determinants of the $k \times k$ submatrices of $D(G, X_G)$. A distance ideal is said to be *unit* or *trivial* if the ideal is equal to $\mathbb{Z}[X_G]$, equivalently, the ideal is generated by the unit.

Example 5. Let G be the graph in Fig. 4. The second distance ideal $I_2(G, X_G)$ has as generating set the following Gröbner basis

$$\langle x_0 + 1, x_1 + 1, x_2 + 1, x_3 + 1, x_4 + 1, 3\rangle$$

The third distance ideal is generated by the following Gröbner basis

$$\begin{aligned} \langle x_0x_1 - 2x_0 - 2x_1 + 4, x_0x_2 - 2x_0 - 2x_2 + 4, x_0x_3 - 2x_0 - 2x_3 + 4,\\ x_0x_4 - 2x_0 - 2x_4 + 4, 3x_0 - 6, x_1x_2 - 2x_1 - 2x_2 + 4, x_1x_3 - 2x_1 - 2x_3 + 4,\\ x_1x_4 - 2x_1 - 2x_4 + 4, 3x_1 - 6, x_2x_3 - 2x_2 - 2x_3 + 4,\\ x_2x_4 - 2x_2 - 2x_4 + 4, 3x_2 - 6, 2x_3x_4 - x_3 - x_4 - 4\rangle. \end{aligned}$$

The fourth distance ideal is generated by the following Gröbner basis

$$\begin{aligned} &\langle 2x_0x_1x_2 - x_0x_1 - x_0x_2 - 4x_0 - x_1x_2 - 4x_1 - 4x_2 + 20,\\ &x_0x_1x_3 - 2x_0x_1 - 2x_0x_3 + 4x_0 - 2x_1x_3 + 4x_1 + 4x_3 - 8,\\ &x_0x_1x_4 - 2x_0x_1 - 2x_0x_4 + 4x_0 - 2x_1x_4 + 4x_1 + 4x_4 - 8,\\ &x_0x_2x_3 - 2x_0x_2 - 2x_0x_3 + 4x_0 - 2x_2x_3 + 4x_2 + 4x_3 - 8, \end{aligned}$$

$$\begin{aligned}
&x_0x_2x_4 - 2x_0x_2 - 2x_0x_4 + 4x_0 - 2x_2x_4 + 4x_2 + 4x_4 - 8,\\
&2x_0x_3x_4 - x_0x_3 - x_0x_4 - 4x_0 - 4x_3x_4 + 2x_3 + 2x_4 + 8,\\
&x_1x_2x_3 - 2x_1x_2 - 2x_1x_3 + 4x_1 - 2x_2x_3 + 4x_2 + 4x_3 - 8,\\
&x_1x_2x_4 - 2x_1x_2 - 2x_1x_4 + 4x_1 - 2x_2x_4 + 4x_2 + 4x_4 - 8,\\
&2x_1x_3x_4 - x_1x_3 - x_1x_4 - 4x_1 - 4x_3x_4 + 2x_3 + 2x_4 + 8,\\
&2x_2x_3x_4 - x_2x_3 - x_2x_4 - 4x_2 - 4x_3x_4 + 2x_3 + 2x_4 + 8\rangle.
\end{aligned}$$

The last distance ideal is generated by the following Gröbner basis

$$\begin{aligned}
&\langle x_0x_1x_2x_3x_4 - 4x_0x_1x_2 - x_0x_1x_3 - x_0x_1x_4 + 4x_0x_1 - x_0x_2x_3 - x_0x_2x_4\\
&+4x_0x_2 - 4x_0x_3x_4 + 4x_0x_3 + 4x_0x_4 - x_1x_2x_3 - x_1x_2x_4 + 4x_1x_2 - 4x_1x_3x_4\\
&+4x_1x_3 + 4x_1x_4 - 4x_2x_3x_4 + 4x_2x_3 + 4x_2x_4 + 16x_3x_4 - 12x_3 - 12x_4 - 16\rangle.
\end{aligned}$$

An alternative way of computing the SNF of a matrix M is the following. Let us denote by $\Delta_k(M)$, the *greatest common divisor* of all minors of size k of the matrix M. It is known [2] that the *k-th* invariant factor of the matrix M is equal to $\Delta_k(M)/\Delta_{k-1}(M)$, where $\Delta_0(M) = 1$.

The following result shows a relation between the SNF of the distance matrix and the distance ideals.

Proposition 6 ([4]). *Let* $\mathbf{d} \in \mathbb{Z}^{V(G)}$. *If* $f_1 \mid \cdots \mid f_r$ *are the non-zero invariant factors of the SNF of the matrix* $D(G, \mathbf{d})$, *then*

$$I_k(G, \mathbf{d}) = \left\langle \prod_{j=1}^{k} f_j \right\rangle = \langle \Delta_k(D(G, \mathbf{d}))\rangle \text{ for all } 1 \le k \le r.$$

In this way, distance ideals can be regarded as a generalization of the SNF of the distance, distance Laplacian and distance signless Laplacian matrices. Thus, we can recover the SNF of the matrices $D(G)$, $D^L(G)$ and $D^Q(G)$ by evaluating the distance ideals at X_G equal to $\mathbf{0}$, $-tr(G)$ and $tr(G)$, respectively.

In order to show our main result of this section we need the following theorem.

Theorem 7 ([4]). *Let* K_n *be the complete graph with n vertices. The k-th distance ideal of* K_n *is generated by*

$$\begin{cases} \prod_{j=1}^{n}(x_j - 1) + \sum_{i=1}^{n}\prod_{j\neq i}(x_j - 1) & \text{if } k = n,\\ \left\{\prod_{j\in\mathcal{I}}(x_j - 1) : \mathcal{I} \subset [n] \text{ and } |\mathcal{I}| = i - 1\right\} & \text{if } k < n. \end{cases}$$

From Theorem 7 we can recover the SNFs of the distance (D), distance Laplacian (D^L) and distance signless Laplacian (D^Q) matrices of the complete graph by evaluating their distance ideals. An evaluation at $x_v = 0$ for each $v \in V$, we obtain that $\Delta_k(D(K_n)) = 1$, for $k \in [n-1]$, and $\Delta_n(D(K_n)) = \left|(-1)^n + n(-1)^{n-1}\right| = n - 1$. From which follows that the SNF of $D(K_n)$ is $\mathsf{I}_{n-1} \oplus (n-1)$. By evaluating the distance ideals at $x_v = -n + 1$ for each $v \in V$, we obtain the SNF of $D^L(K_n)$ is $1 \oplus n\mathsf{I}_{n-2} \oplus 0$. And by evaluating the distance ideals at $x_v = n - 1$ for each $v \in V$, we obtain the SNF of $D^Q(K_n)$ is $1 \oplus (n-2)\mathsf{I}_{n-2} \oplus 2(n-1)(n-2)$.

Other consequence of Proposition 6 is that if *k-th* invariant factor of a matrix obtained of an evaluation of the generalized distance matrix of G, then the *k-th* distance ideal of G is not trivial. Thus, for any graph G and any $\mathbf{d} \in \mathbb{Z}^{V(G)}$, the number of invariant factors equal to 1 of the matrix $D(G, \mathbf{d})$ is at least the number of trivial distance ideals of G. Therefore, the family of graphs with at most k trivial distance ideals contains the families of graphs whose matrices D, D^L and D^Q have at most k invariant factors equal to 1. We are going to use this property to obtain a characterization of the graphs whose D^Q matrices have at least one invariant factor equal to 1. For this, we need the following result.

Theorem 8 ([4]). *Let G be a connected graph. G has only one trivial distance ideal if and only if G is either a complete graph or a complete bipartite graph.*

Therefore, to find family of graphs such that their D^Q matrices have at most one invariant factor equal to 1, then we only need to consider the families of complete graphs and complete bipartite graphs. We have already seen that the SNF of $D^Q(K_n)$ is $1 \oplus (n-2)\mathsf{I}_{n-2} \oplus 2(n-1)(n-2)$. From which follows that complete graphs with at least 4 vertices have one invariant factor of SNF of D^Q equal to one. Now we are going to prove that this family is contains all the graphs whose distance signless Laplacian matrix have only one invariant factor equal to one.

Theorem 9. *Let G be a connected graph. The SNF of* $D^Q(G)$ *has only one invariant factor equal to 1 if and only if G is a complete graph with* $n \neq 3$ *vertices.*

Proof. It only remains to verify that the second invariant factor of complete bipartite graphs is equal to one. In [4], the second distance ideal of complete bipartite graphs were computed. Let $D(K_{m,n}, \{x_1, \ldots, x_m, y_1, \ldots, y_n\})$ be the generalized distance matrix of $K_{m,n}$, which is equal to the following matrix

$$\begin{bmatrix} \operatorname{diag}(x_1, \ldots, x_m) - 2\mathsf{I}_m + 2\mathsf{J}_m & \mathsf{J}_{m,n}\\ \mathsf{J}_{n,m} & \operatorname{diag}(y_1, \ldots, y_n) - 2\mathsf{I}_n + 2\mathsf{J}_n \end{bmatrix}.$$

If $m \geq 2$ and $n = 1$, then

$$I_2(K_{m,1}, \{x_1, \ldots, x_m, y_1\}) = \langle x_1 - 2, \ldots, x_m - 2, 2y_1 - 1 \rangle.$$

After evaluating the ideal at $x_i = 2m - 1$, and $y_1 = m$, we obtain the ideal $\langle 2m-3, 2m-1 \rangle \subseteq \mathbb{Z}$. Since the $\gcd(2m-3, 2m-1) = 1$, it follows that the second invariant factor of $\text{SNF}(D^Q(K_{m,1}))$ is 1. If $m \geq 2$ and $n \geq 2$, then

$$I_2(K_{m,n}, \{x_1, \ldots, x_m, y_1, \ldots, y_n\}) = \langle x_1 - 2, \ldots, x_m - 2, y_1 - 2, \ldots, y_n - 2, 3 \rangle.$$

After evaluating the ideal at $x_i = 2m + n - 2$ and $y_i = 2n + m - 2$, we obtain the ideal $\langle 2m + n - 4, m + 2n - 4, 3 \rangle \subseteq \mathbb{Z}$. Since the $\gcd(2m + n - 4, m + 2n - 4, 3) = 1$, it follows that the second invariant factor of $\text{SNF}(D^Q(K_{m,n}))$ is 1. □

Now we are ready to state the main result of this section.

Corollary 10. *Complete graphs are determined by the SNF of the distance signless Laplacian matrix.*

It would be interesting to obtain a characterization of graphs whose SNF of D^L and D^Q has two invariant factors equal to 1. This could be obtained after showing a characterization of graphs having two trivial distance ideals. However, the latter problem seems to be difficult, since there exist infinitely many minimal induced forbidden graphs [3] (most of them are the same needed in the characterization of the well-known Strong Perfect Graph Theorem).

4. Concluding remarks

While the adjacency, Laplacian and signless Laplacian matrices have attracted a lot of attention in the field of spectral characterizations of graphs, for such matrices, the SNF does not seem useful to distinguish graphs, since almost all graphs on 10 vertices have a coinvariant mate. However, our enumeration results suggest that the invariant factors of the distance Laplacian and the distance signless Laplacian matrices could be a finer invariant to distinguish graphs in cases where other algebraic invariants, such as those derived from the spectrum, fail. This confirms what was suggested by Biggs [9]. Another argument to consider the SNF as a parameter to distinguish graphs is that this is a finer invariant than the p-rank: the p-rank is just the number of invariant factors not divisible by p.

In this work we show that the results by Aouchiche and Hansen [6] can be extended even further. In particular, we provide numerical evidence that using the invariant factors of the SNF of certain distance matrices one can improve some of the results by Aouchiche and Hansen. In this regard, our computational results suggest that possibly almost no graph has a coinvariant mate when $n \to \infty$ for the matrices D^L and D^Q.

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