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## Structural properties of minimal strong digraphs versus trees <sup>☆</sup>



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### ABSTRACT

In this article, we focus on structural properties of minimal strong digraphs (MSDs). We carry out a comparative study of properties of MSDs versus (undirected) trees. For some of these properties, we give the matrix version, regarding nearly reducible matrices. We give bounds for the coefficients of the characteristic polynomial corresponding to the adjacency matrix of trees, and we conjecture bounds for MSDs. We also propose two different representations of an MSD in terms of trees (the union of a spanning tree and a directed forest; and a double directed tree whose vertices are given by the contraction of connected Hasse diagrams).

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## 1. Introduction

A digraph is *strongly connected* or (simply) *strong* (SD) if every pair of vertices are joined by a directed path. An SD is *minimal* (MSD) if it loses the strong connection property when any of their arcs is suppressed. This class of digraphs has been considered under different points of view. See, for instance, [2,5,6,8,10–15].

It is well known that a digraph is SD if and only if its adjacency matrix is irreducible [6]. The set of SDs of order  $n$  with vertex set  $V$  can be partially ordered by the relation of inclusion among their sets of arcs. Then, the MSDs are the minimal elements of this partially ordered set. Analogously, the set of irreducible  $(0,1)$ -matrices of order  $n$  with zero trace can be partially ordered by means of the coordinatewise ordering. The minimal elements of this partially ordered set are *nearly reducible matrices*. Hence, nearly reducible matrices are irreducible matrices which cease to be so if we make any of their 1-entries zero, and so a digraph is an MSD if and only if its adjacency matrix is a nearly reducible matrix [6,15]. Hartfiel [13] gives a remarkable canonical form for nearly reducible matrices.

We are also interested in the following nonnegative inverse eigenvalue problem [18]: given real numbers  $k_1, k_2, \dots, k_n$ , find necessary and sufficient conditions for the existence of a nonnegative matrix  $A$  of order  $n$  with characteristic polynomial  $x^n + k_1 x^{n-1} + k_2 x^{n-2} + \dots + k_n$ . The coefficients of the characteristic polynomial are closely related to the cycle structure of the weighted digraph with adjacency matrix  $A$  by means of the Theorem of the coefficients [7], and the irreducible matricial realizations of the polynomial are identified with strongly connected digraphs [6]. The class of strong digraphs can easily be reduced to the class of minimal strong digraphs, so we are interested in any theoretical or constructive characterization of these classes of digraphs.

In [10], a sequentially generative procedure for the constructive characterization of the classes of MSDs is given. In addition, algorithms to compute unlabeled MSDs and their isospectral classes are described. These algorithms have been implemented to calculate the said classes of digraphs up to order 15, classified by their order and size [20]. We are also interested in properties regarding the spectral structure of this class of digraphs, mainly about the coefficients of the characteristic polynomial.

MSDs can be seen as a generalization of trees, as we pass from simple graphs to directed graphs. Although the structure of MSDs is much richer than that of trees, many analogies remain between the properties of both families. Other properties, nevertheless, undergo radical changes when passing from trees to MSDs.

In this article, we focus on structural properties of MSDs. We carry out a comparative study of properties of MSDs versus trees. For some of the properties, we also give an interpretation in terms of nearly reducible matrices, via the adjacency matrices. We also conjecture a generalization of the bounds on the coefficients of characteristic polynomials of trees to MSDs. As a particular case, the independent coefficient of the characteristic polynomial of a tree or an MSD must be  $-1$ ,  $0$  or  $1$ . For trees, this means that a tree has at most one perfect matching; for MSDs, it means that an MSD has at most one

covering by disjoint cycles. Finally, we use the properties described to give two possible representations of an MSD: every MSD can be factored into a rooted spanning tree and a forest of reversed rooted trees; and also as a double directed tree whose vertices are connected Hasse diagrams. In our opinion, the analogies described suppose a significant change in the traditional point of view about this class of digraphs.

The outline of the article is as follows: In section 2, we set up some notations and recall basic properties of MSDs. In section 3, we study structural analogies and differences between MSDs and trees. In section 4, we establish sharp bounds for the coefficients of the characteristic polynomials of trees, and we conjecture a generalization of these bounds for MSDs. In section 5, we describe the two distinct representations of MSDs.

**2. Notations and basic properties**

In this paper we use some standard basic concepts and results about graphs. We list them now, so as to fix the notations.

A *digraph*  $D$  is a pair  $D = (V, A)$ , where  $V$  is a finite nonempty set and  $A \subset V \times V - \{(v, v) : v \in V\}$ . Elements in  $V$  and  $A$  are called *vertices* and *arcs*, respectively, and  $|V|$  and  $|A|$  are the *order* and *size* of  $D$ . If  $u, v \in V$  we denote  $(u, v)$  by  $uv$  and we write  $D - uv$  for the digraphs  $(V, A - \{(u, v)\})$ . For a vertex  $v \in V$ , the subdigraph  $D - v$  consists of all vertices of  $D$  except  $v$  and all arcs of  $D$  except those incident with  $v$ . A *path* in  $D$  is a sequence of distinct vertices  $v_1v_2 \dots v_q, q \geq 2$ , such that  $v_iv_{i+1}$  is an arc for  $i = 1, 2, \dots, q - 1$ . We denote a path from the vertex  $u$  to the vertex  $v$  by  $uv$ -path. A *cycle of length*  $q$  or a  *$q$ -cycle* is a path  $v_1v_2 \dots v_q$  closed by the arc  $v_qv_1$ . It is denoted by  $C_q$ . A *double directed tree* is the digraph  $\overleftrightarrow{T}$  obtained from a tree  $T$  by replacing each edge  $\{u, v\}$  with the two arcs  $(u, v)$  and  $(v, u)$  (we follow the notation introduced in [6], but keep the term “directed tree” to have its usual meaning). The *linear graph*  $L_n$  is the undirected path over  $n$  vertices. The corresponding double directed tree is denoted by  $\overleftrightarrow{L}_n$ . A *perfect matching* in a graph  $G$  is a set of mutually non-adjacent edges of  $G$  covering all vertices of  $G$ .

A *cut vertex* in a graph or digraph is a vertex whose deletion increments the number of connected components. An edge of a graph (or an arc of a digraph) is a *cut* if its deletion increments the number of connected components. A *2-cut* is a pair of edges (or arcs) whose concurrent deletion increments the number of connected components.

We now record a number of basic facts about the strong digraphs (see [10] and the references therein). In an SD of order  $n \geq 2$ , the indegree and outdegree of the vertices are bigger than or equal to 1. A vertex is *linear* if it has indegree and outdegree equal to 1. Equivalently, in a  $(0, 1)$ -irreducible matrix, the index  $i$  is *linear* if the row and the column  $i$  have only one 1-entry. In a tree, the leaves are also linear vertices by considering the edges as two arcs.

If  $D$  is an MSD and there is an arc  $uv$  in  $D$ , then there cannot be another  $uv$ -path joining the vertex  $u$  to the vertex  $v$ . In general, an arc  $uv$  in a digraph  $D$  is *transitive* if there is another  $uv$ -path distinct from the arc  $uv$ . The semicycle consisting of a  $uv$ -path

together with the arc  $uv$  is a *pseudocycle*. So an MSD has no transitive arcs or pseudocycles; moreover, this condition characterizes the minimality of the strong connection (see [11,14]). In matrix terms,  $A = (a_{ij})$  is a nearly reducible matrix if and only if  $a_{ij} = 1$  implies  $a_{ij}^{(l)} = 0$ , for all  $l \geq 2$ , being  $A^l = (a_{ij}^{(l)})$ . Consequently, if  $D$  is an MSD then so is every strong subdigraph of  $D$ . Furthermore, every subdigraph that is an MSD is an induced subdigraph.

The *contraction of a cycle* of length  $k$  in a strong digraph consists of the reduction of the cycle to a unique vertex, so that  $k - 1$  of its vertices and its  $k$  arcs are eliminated. The contraction obviously preserves the SD property.

**Lemma 1.** (Berge [2]) *The contraction of a cycle in an MSD preserves the minimality, that is, it produces another MSD.*

**Lemma 2.** (Gupta [12]) *The size of a minimal strong digraph  $D$  of order  $n \geq 2$  satisfies  $n \leq |A| \leq 2(n - 1)$ . The size of  $D$  is  $n$  if and only if  $D$  is an  $n$ -cycle. The size of  $D$  is  $2(n - 1)$  if and only if  $D$  is a double directed tree.*

Brualdi and Hedrick [5] also proved that there exists an MSD of order  $n \geq 2$  and size  $m$  if and only if  $n \leq m \leq 2(n - 1)$  and characterized the MSDs of order  $n$  and size  $2n - 3$ .

The next result was first proved by Dirac [8] and independently by Plummer [17] in the context of minimal two connected graphs and by Berge and by Brualdi and Ryser [6] for MSDs. A simplified proof by induction over the order  $n$  is given in [10].

**Lemma 3.** *Every MSD of order  $n \geq 2$  has at least two linear vertices.*

The following results will be useful tools in the proofs of the results of this paper.

An *ear decomposition* [1, 7.2] of a strong digraph  $D = (V, A)$  is a sequence of digraphs  $P_0, P_1, \dots, P_k$ , where  $P_0 = (V_0, A_0)$  is a cycle and each  $P_i = (V_i, A_i)$ ,  $1 \leq i \leq k$ , is a path or a cycle with the following properties:

- (a)  $P_i$  and  $P_j$  are arc-disjoint if  $i \neq j$ .
- (b) For each  $i = 1, \dots, k$ : if  $P_i$  is a cycle, then it has just one vertex in common with  $\cup_{j=0}^{i-1} V_j$ . Otherwise the end-vertices of  $P_i$  are distinct vertices of  $\cup_{j=0}^{i-1} V_j$  and no other vertex of  $P_i$  belongs to  $\cup_{j=0}^{i-1} V_j$ .
- (c)  $\cup_{i=0}^k A_i = A$ .

Each  $P_i$  is called an *ear*.

Such a decomposition exists for every SD. In fact, for every vertex  $u$  and every cycle  $C$  through  $u$ ,  $C$  is  $P_0$  for certain ear decompositions [1, Theorem 7.2.2]. MSDs satisfy that every ear has at least a new vertex and two arcs. Lemmas 1 and 2 can be proven in a relatively simple fashion by using this kind of decomposition.

*The Theorem of the coefficients* [7]. Let  $D$  be a digraph with characteristic polynomial  $x^n + k_1x^{n-1} + k_2x^{n-2} + \dots + k_{n-1}x + k_n$ . Then

$$k_i = \sum_{CS \in \mathcal{L}_i} (-1)^{P(CS)}, \quad i = 1, \dots, n$$

where  $CS$  denotes a *cyclic structure* i.e., a set of disjoint unlabeled cycles of  $D$ ,  $\mathcal{L}_i = \{CSs \text{ covering } i \text{ vertices of } D\}$ , and  $P(CS)$  is the number of cycles in  $CS$ .

### 3. Minimal strong digraphs versus trees

Trees and MSDs are defined in a similar way. They are minimal connected graphs and minimal strong digraphs respectively, such that, in every case, the deletion of any edge and arc, respectively, implies strong connectivity loss. Despite the analogy in the definition, it is expected that the properties of these two kinds of graphs are very different because, while trees have no cycles, in every MSD, each arc belongs to a cycle.

However, surprisingly, there are many analogies between these two families of graphs. We explore the properties of both kind of graph, so as to deeply understand the structure of MSDs, by using the very well-known structure of trees.

- (i) Trees and MSDs have a linear number  $m$  of edges and arcs respectively, related to the number of vertices  $n$ . The order  $n$  of a tree determines the number of edges,  $m = n - 1$ , whereas this does not hold for MSDs. In this case, the number of arcs satisfies  $n \leq m \leq 2(n - 1)$ .

So, the number of arcs of a (double-directed)  $n$ -tree is the maximum size of an MSD of order  $n$ .

As a consequence of [Lemma 2](#), considering the adjacency matrix of an MSD with maximal number of arcs  $m = 2(n - 1)$  (which must be a double directed tree), we can state the following property:

**Corollary 4.**

1. *If  $m$  is an integer, then there exists an  $n \times n$  nearly reducible matrix of size  $m$  if and only if  $n \leq m \leq 2(n - 1)$ .*
2. *Every  $n \times n$  nearly reducible matrix with just  $n$  1-entries is permutation congruent to an  $n$ -cycle matrix.*
3. *An  $n \times n$  nearly reducible matrix has just  $2(n - 1)$  1-entries if and only if it is symmetric.*

- (ii) There is an equivalent definition of trees: they are connected graphs with  $n - 1$  edges. This fact is related to the following property of MSDs: a strong digraph with  $n$  arcs is an MSD ([Lemma 2](#)).
- (iii) Furthermore, the two families of graphs (with at least two vertices) satisfy that they have at least two linear vertices, i.e. vertices with degree one (the leaves of the tree) and indegree and outdegree one ([Lemma 3](#)), respectively.
- (iv) In both cases, there are configurations with a maximum number of linear vertices related to the order: tree stars have  $n - 1$  linear vertices and directed cycles have  $n$ .

- (v) Also, in both cases, there are configurations with a vertex with maximum degree: both tree and MSD stars.
- (vi) On the other hand, there is a unique tree of order  $n$  with minimum number of linear vertices: the linear graph  $L_n$ . The MSDs with just two linear vertices are also linear configurations, in the following sense.

**Definition 5.** An MSD is *simple linear* if it is the cycle  $C_2$ , the MSD  $C_3C_3$  with a common arc, or it is composed of a sequence of  $p \geq 3$  cycles  $C_3C_4C_4 \cdots C_4C_3$ , where each  $C_4$  cycle shares two disjoint arcs with the preceding and the following cycle, respectively, in the sequence. An MSD is *linear* if it can be obtained from the linear graph  $L_n$  by the substitution of each edge by a simple linear MSD, identifying the endpoints of each edge with the linear vertices of the simple linear MSD.

**Lemma 6.** *In an MSD with just two linear vertices, each of them belongs to a unique cycle. Furthermore, these cycles are  $C_2$  or  $C_3$ .*

**Proof.** Let  $D$  be an MSD with just two linear vertices. Let  $u$  be one of them, and let  $C$  be a cycle containing  $u$ . If the other linear vertex belongs to  $C$ , then  $D = C$  (otherwise, the contraction of  $C$  would result in an MSD with only one linear vertex). Hence,  $D$  is a cycle with exactly two linear vertices, that is,  $D = C_2$ .

Assume now that the other linear vertex of  $D$  does not belong to  $C$ . The contraction of  $C$  into a vertex  $z$  implies that  $z$  is a linear vertex in the contracted MSD  $D'$  (otherwise,  $D'$  has only one linear vertex). Let  $v_1$  and  $v_2$  be the vertices in  $C$  incident with the two arcs through  $z$ . As  $u$  is the only linear vertex in the cycle,  $C$  must be either the 3-cycle  $uv_1v_2u$  (or  $uv_2v_1u$ ), or the 2-cycle  $uv_1u$ , if  $v_1 = v_2$ . The uniqueness of the cycle holds trivially.  $\square$

**Theorem 7.** *An MSD is linear if and only if it has just two linear vertices.*

**Proof.** Let  $D$  be an MSD. If  $D$  is linear, then  $D$  has just two linear vertices. For the reciprocal, we shall prove it by induction on the number  $n$  of vertices.

If  $n = 2$ , then  $D = C_2$  is a simple linear MSD.

If  $n > 2$ , let  $D$  be an MSD with  $n + 1$  vertices, and with just two linear vertices,  $u$  and  $w$ . By the Lemma above,  $u$  belongs to a unique cycle  $C_2$  or  $C_3$ .

If  $u$  belongs to a 2-cycle  $uvu$ , then  $v$  is a linear vertex in  $D' = D - u$ , and the cycle  $uvu$  is a simple linear MSD. By the induction hypothesis,  $D'$  is a linear MSD and, hence, so is  $D$ .

If  $u$  belongs to a 3-cycle  $uv_1v_2u$ , then the MSD  $D'$ , obtained from  $D$  by the contraction of the 3-cycle into the vertex  $z$ , has just two linear vertices,  $z$  and  $w$ . Hence, by the induction hypothesis,  $D'$  is a linear MSD. Then, two cases are possible, as illustrated in Fig. 2. This cycle  $C_3$  belongs to a linear MSD of the form  $C_3C_3 \cdots$  or  $C_3C_4 \cdots$ . In both cases, it is clear that  $D$  is linear.  $\square$

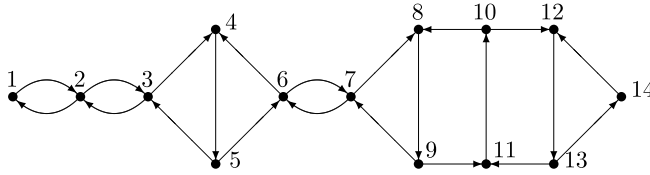


Fig. 1. A linear MSD composed by five simple linear MSDs.

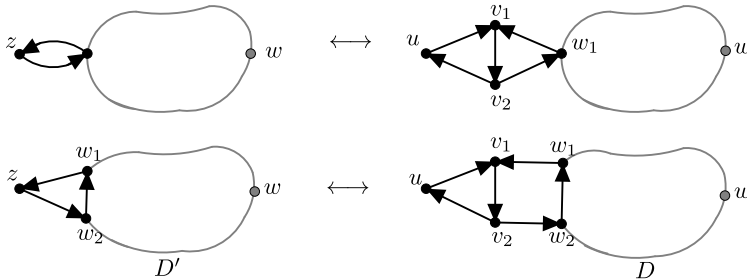


Fig. 2. The two cases in proof of Theorem 7.

As a consequence of the two previous results we have:

**Corollary 8.**

1. If an MSD has a linear vertex in a  $q$ -cycle with  $q \geq 4$ , then it has at least three linear vertices.
2. If an MSD has a  $q$ -cycle with  $q \geq 5$ , then it has at least three linear vertices.

Note that the vertices of a linear MSD can be labeled so that the corresponding adjacency matrix is pentadiagonal (see the labeling of the linear MSD in Fig. 1). Hence, we can state the following property:

**Corollary 9.** A nearly reducible matrix with only two linear indices is permutation congruent to a pentadiagonal matrix.

- (vii) In a tree, each vertex belongs to a 2-cycle (considering the edges as two arcs), and hence it is either linear or a cut vertex. In a linear MSD, each vertex contained in a 2-cycle is either linear or a cut vertex. Even more, for every 3-cycle in a linear MSD, exactly one of its vertices is either linear or a cut vertex. And for every 4-cycle in a linear MSD, exactly two of its vertices have indegree 2 and outdegree 1, while the other two have indegree 1 and outdegree 2. None of them is a cut vertex.
- (viii) In a tree, every edge is a cut. In the associated double directed tree, the arcs of each 2-cycle constitute a 2-cut. For MSDs, the situation is as follows:

**Theorem 10.** Each cycle in an MSD has a 2-cut.

**Proof.** Let  $D$  be an MSD. We shall prove the result by induction on the number  $n$  of vertices of  $D$ .

If  $n = 2$ , then  $D = C_2$ , and its arcs are a 2-cut.

If  $n > 2$ , and  $D$  is a double directed tree, then the result is known.

In any other case, there exists in  $D$  a cycle  $C_q$  with  $q > 2$ . If  $D = C_q$ , then any pair of arcs is a 2-cut.

In addition, there exists another cycle  $C$  sharing some vertices (and maybe arcs) with  $C_q$ . Let  $D'$  be the digraph obtained from  $D$  by the contraction of  $C$  on a vertex  $z$ . Then  $C_q$  is transformed into one or several cycles with a common vertex  $z$ . We choose one of those cycles and, by induction hypothesis, it has a 2-cut, that is, there exist two arcs  $u'_1v'_1$  and  $u'_2v'_2$  such that  $D' - u'_1v'_1 - u'_2v'_2$  has two connected components, say  $D'_1$  and  $D'_2$ . The vertex  $z$  lies in one of the components. If  $u'_j, v'_j \neq z$  for  $j = 1, 2$ , then  $u'_j = u_j$  and  $v'_j = v_j$  are vertices of  $D$ , and the original arcs  $u_1v_1, u_2v_2$  are a 2-cut. If  $u'_j = z$  (resp.  $v'_j = z$ ) for  $j = 1, 2$  or both, then there is only one vertex  $w_j$  in  $C$  such that  $w_jv_j$  (resp.  $u_jw_j$ ) is an arc in  $C_q$ . The couple of arcs given by the appropriate  $u_jv_j, w_jv_j$  or  $u_jw_j$  (for  $j = 1, 2$ ) constitute a 2-cut.  $\square$

In general, every nearly reducible matrix is permutation congruent to a matrix with the form

$$\left( \begin{array}{c|c} * & E_{ij} \\ \hline * & * \end{array} \right),$$

where  $E_{ij}$  is a matrix with its  $(i, j)$ -entry equal to 1, and the rest equal to 0. This is consequence of the fact that the vanishing of any 1-entry makes the matrix reducible.

By considering the adjacency matrix of an MSD, [Theorem 10](#) may be stated as follows:

**Corollary 11.** *A nearly reducible matrix with a cycle submatrix  $C$  is permutation congruent to a matrix of the form*

$$\left( \begin{array}{c|c} * & E_{ij} \\ \hline E_{kl} & * \end{array} \right),$$

where the 1-entries of the blocks  $E_{ij}$  and  $E_{kl}$  correspond to arcs in  $C$ . Hence, making these two entries zero, we obtain a totally reducible matrix (i.e., a matrix which is permutation congruent to a nontrivial block diagonal matrix).

- (ix) Given two vertices  $u$  and  $v$  in any tree, there is a unique path connecting them. We generalize this fact as *path-tree property* for both graphs and digraphs: for every two vertices  $u$  and  $v$  in a graph (resp. a digraph) there is a unique path connecting



them (resp. a unique directed path from  $u$  to  $v$ ). Then trees satisfy the path-tree property, while MSDs do not. If  $uv$  is an arc in an MSD then this path is the unique path connecting the vertex  $u$  to the vertex  $v$ , but we cannot say the same if the arc  $uv$  does not belong to the MSD. Nevertheless, there exists a subfamily of the MSD class where the property holds. It is defined below.

In the following definition, a topological cycle means a cycle in the graph obtained by the substitution of every arc by an edge.

**Definition 12.** A *directed cycle digraph* is an SD in which every topological cycle comes from a directed cycle.

Clearly, every directed cycle digraph is an MSD. However, we also prove below that the class of MSDs satisfying the path-tree property is just the directed cycle digraph class.

**Theorem 13.** A *strong digraph* satisfies the path-tree property if and only if it is a directed cycle digraph.

**Proof.** Let  $D$  be an SD. We first prove that if  $D$  is a directed cycle digraph then  $D$  satisfies the path-tree property. Suppose that  $D$  does not satisfy the path-tree property. Let  $u$  and  $v$  be vertices between which there are two different directed paths. Without loss of generality, we can assume that the paths only match at the end vertices. Therefore, they constitute a topological cycle that is not a directed cycle in  $D$ .

Let  $D$  now be an SD that satisfies the path-tree property. Let us consider an ear decomposition of  $D$ . Then the end vertices of any ear are equal, or else there would be two directed paths between them. We conclude that in  $D$  there are no other topological cycles than the ears. Therefore  $D$  is a directed cycle digraph.  $\square$

- (x) Another meaningful difference between trees and MSDs is the complexity of the following algorithmic problem: Given a weighted connected graph and a weighted strong digraph, find a minimal spanning tree (MST) and a minimal spanning strong subdigraph (MSSS), respectively. While there are many polynomial algorithms to solve the MST problem [4], the MSSS problem belongs to the NP-hard class (see [1] and the references therein), even when all weights are one.
- (xi) Every tree has at most one perfect matching. We prove below that an MSD has at most one covering by disjoint cycles. This property becomes the previous one if we consider each edge in the tree as two arcs.

**Theorem 14.** An MSD has at most one covering by disjoint cycles.

**Proof.** Let  $D$  be an MSD. Suppose that  $D$  has two different coverings by disjoint cycles,  $\mathcal{C}_1$  and  $\mathcal{C}_2$ . Without loss of generality, we can suppose that  $\mathcal{C}_1$  and  $\mathcal{C}_2$  have

no common cycles: if there were any common cycles, we could iteratively delete the vertices of each cycle, and then reset the strong connection, while preserving the minimality, by adding non-transitive arcs.

Let us denote the order of  $D$  by  $n$ , the size by  $m$ , the number of cycles in  $\mathcal{C}_1$  by  $k_1$ , the number of cycles in  $\mathcal{C}_2$  by  $k_2$  and suppose, without loss of generality, that  $k_1 \leq k_2$ . Contracting the cycles of  $D$  belonging to  $\mathcal{C}_1$  we can conclude that  $m \leq n + 2(k_1 - 1)$ , since the number of vertices  $n$  is also the number of contracted arcs, and there are  $k_1$  vertices in the contracted digraph  $D'$  and hence, at most, another  $2(k_1 - 1)$  arcs in  $D$ . On the other hand, the cycles of  $\mathcal{C}_1$  have altogether exactly  $n$  arcs and each cycle in  $\mathcal{C}_2$  adds at least two new arcs. Hence, it holds that  $m \geq n + 2k_2$ . Finally, we obtain the contradiction:  $m \leq n + 2(k_1 - 1) < n + 2k_2 \leq m$ .  $\square$

In terms of the adjacency matrix of  $D$ , we can state it as follows:

**Corollary 15.** *The determinant of a nearly reducible matrix is 1,  $-1$  or 0.*

- (xii) The covering of a strong digraph  $D$  with  $\alpha$  cycles, not necessarily disjoint, where  $\alpha$  is the stability number or the independence number of  $D$ , constitutes the Gallai conjecture [9]. This was proved by Bessy and Thomassé [3] and the proof also applies to MSDs and trees if we consider, in the last case, that edges are equivalent to two arcs. There are examples of MSDs and trees where  $\alpha$  cycles are needed in order to cover the corresponding digraph: MSD and tree stars.
- (xiii) The covering of a strong digraph  $D$  with  $\alpha - 1$  disjoint paths, where  $\alpha$  is, as above, the stability number or the independence number of  $D$ , constitutes the Las Vergnas conjecture [16]. This was proved by Thomassé [19] and the proof also applies to MSDs and trees if we consider, in the last case, that edges are equivalent to two arcs. There are examples of MSDs and trees where  $\alpha - 1$  disjoint paths are needed in order to cover the corresponding digraph: MSD and tree stars.
- (xiv) The next property will be developed in the next section. Given the characteristic polynomial corresponding to the adjacency matrix of a tree or an MSD,  $x^n + k_1x^{n-1} + k_2x^{n-2} + \dots + k_n$ , we prove, for trees, that the coefficients are bounded as follows:

$$k_m = 0 \quad \text{if } m \text{ is odd,} \quad k_m \leq \binom{n - \frac{m}{2}}{\frac{m}{2}} \quad \text{if } m \text{ is even.}$$

For MSDs, we conjecture that  $k_m \leq \binom{n - \lceil \frac{m}{2} \rceil}{\lfloor \frac{m}{2} \rfloor}$ .

#### 4. Bounds on the coefficients of the characteristic polynomials of MSDs

##### 4.1. Double directed trees

Let  $\overleftrightarrow{T} = (V, A)$  be a double directed tree with  $n$  vertices and let  $k_m(\overleftrightarrow{T})$  be the coefficient of  $x^{n-m}$  in the monic characteristic polynomial of the adjacency matrix of  $\overleftrightarrow{T}$ .

As double directed trees have only cycles of length 2, it follows, by the Theorem of the coefficients, that  $k_m(\overleftrightarrow{T}) = 0$  for  $m$  odd; if  $m$  is even, all possible cycle structures covering  $m$  vertices have exactly  $m/2$  disjoint 2-cycles, and hence all their contributions to  $k_m(\overleftrightarrow{T})$  have the same sign. So, for  $m$  even,  $|k_m(\overleftrightarrow{T})|$  is the number of coverings of  $m$  vertices of  $\overleftrightarrow{T}$  by  $m/2$  disjoint 2-cycles. For any  $m$  (even or odd), we denote the number of coverings of  $m$  vertices of  $\overleftrightarrow{T}$  by disjoint 2-cycles by  $K_m(\overleftrightarrow{T})$ .

**Theorem 16.** *Let  $T$  be a tree with  $n$  vertices,  $n \geq 2$ . Then:*

1.  $K_m(\overleftrightarrow{T}) = 0$  for all  $m$  odd such that  $1 \leq m \leq n$ .
2.  $K_m(\overleftrightarrow{T}) \leq \binom{n - \frac{m}{2}}{\frac{m}{2}}$  for all  $m$  even such that  $2 \leq m \leq n$ .
3.  $K_m(\overleftrightarrow{T}) = \binom{n - \frac{m}{2}}{\frac{m}{2}}$  for all  $m$  even such that  $2 \leq m \leq n$  if and only if  $T$  is the linear graph  $L_n$ .
4. If  $T \neq L_n$ , then  $K_m(\overleftrightarrow{T}) < \binom{n - \frac{m}{2}}{\frac{m}{2}}$  for some  $m \geq 4$ .

**Proof.** As stated above, the case  $m$  odd is straightforward. The case  $m$  even remains to be studied. We shall prove the result by induction on  $n$ , the number of vertices.

a)  $n = 2$  and  $n = 3$ .

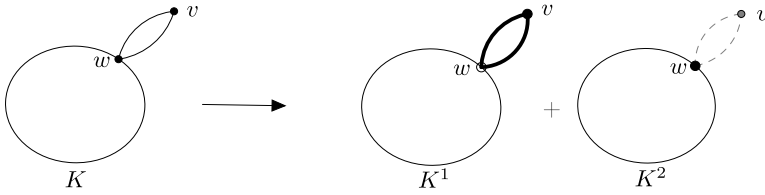
1. If  $n = 2$ , then  $m = 2$  and  $K_2(\overleftrightarrow{T}) = 1 = \binom{1}{1}$  holds.

2. If  $n = 3$ , then  $m = 2$  and  $K_2(\overleftrightarrow{T}) = 2 = \binom{2}{1}$  holds.

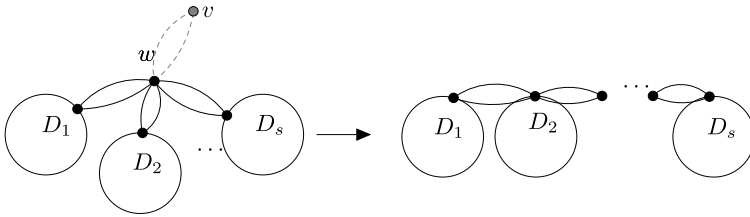
b) Let  $n \geq 3$  and assume (induction hypothesis) that for all  $2 \leq l \leq n$ , all  $m$  even such that  $2 \leq m \leq l$  and all double directed trees with  $l$  vertices, the following inequality holds:

$$K_m(\overleftrightarrow{T}) \leq \binom{l - \frac{m}{2}}{\frac{m}{2}}.$$

Let  $\overleftrightarrow{T} = (V, A)$  be a double directed tree with  $n + 1$  vertices and let  $m$  be even with  $2 \leq m \leq n + 1$ .



**Fig. 3.**  $K^1$  and  $K^2$ .



**Fig. 4.** Joining all the vertices adjacent to  $w$  by means of a path of 2-cycles.

We consider a linear vertex  $v \in V$ , and the vertex  $w$  that forms a 2-cycle  $C$  with  $v$ . We denote by  $K_m^1(\overleftrightarrow{T})$  and  $K_m^2(\overleftrightarrow{T})$  the number of coverings of  $m$  vertices of  $\overleftrightarrow{T}$  by  $m/2$  disjoint 2-cycles including and excluding  $C$ , respectively (see Fig. 3). Clearly,  $K_m(\overleftrightarrow{T}) = K_m^1(\overleftrightarrow{T}) + K_m^2(\overleftrightarrow{T})$ .

If we consider the double directed tree  $\overleftrightarrow{T}'$ , obtained from  $\overleftrightarrow{T}$  by deleting  $v$  and  $w$  and joining all the vertices adjacent to  $w$  by means of a path of 2-cycles (see Fig. 4), then  $K_m^1(\overleftrightarrow{T}) \leq K_{m-2}(\overleftrightarrow{T}')$  and hence

$$K_m^1(\overleftrightarrow{T}) \leq \binom{n-1-\frac{m-2}{2}}{\frac{m-2}{2}} = \binom{n-\frac{m}{2}}{\frac{m}{2}-1}$$

for  $m \geq 4$  and also for  $m = 2$  as, in this case,  $K_m^1(\overleftrightarrow{T}) = 1$ .

For the double directed tree  $\overleftrightarrow{T}'' = \overleftrightarrow{T} - v$ , we have that  $K_m^2(\overleftrightarrow{T}) = K_m(\overleftrightarrow{T}'')$  and hence:

$$K_m^2(\overleftrightarrow{T}) \leq \binom{n-\frac{m}{2}}{\frac{m}{2}}, \text{ if } m \leq n, \text{ and } K_m^2(\overleftrightarrow{T}) = 0, \text{ if } m = n + 1.$$

Finally, we complete the induction step by studying the following two cases:

1. If  $m = n + 1$ :  $K_m(\overleftrightarrow{T}) \leq \binom{n-\frac{n+1}{2}}{\frac{n+1}{2}-1} + 0 = 1 = \binom{n+1-\frac{n+1}{2}}{\frac{n+1}{2}}$ .
2. If  $m \leq n$ :  $K_m(\overleftrightarrow{T}) \leq \binom{n-\frac{m}{2}}{\frac{m}{2}-1} + \binom{n-\frac{m}{2}}{\frac{m}{2}} = \binom{n+1-\frac{m}{2}}{\frac{m}{2}}$ .

To prove (3), if  $T$  is the linear graph  $L_n = v_1 \cdots v_n$ , we denote the consecutive sequence of 2-cycles of the directed tree  $\overleftrightarrow{T}$  by  $C_1, \dots, C_{n-1}$ , where  $C_i = v_i v_{i+1} v_i, i = 1, \dots, n-1$ . Then  $K_m(\overleftrightarrow{T})$  is the number of cycle structures  $\{C_{i_1}, C_{i_2}, \dots, C_{i_{m/2}}\} \in \mathcal{L}_m$  such that  $i_1, i_2, \dots, i_{m/2}$  is an increasing sequence of non consecutive terms of  $\{1, 2, \dots, n-1\}$  with  $1 \leq i_1$  and  $i_{m/2} \leq n-1$  or, equivalently, such that  $i_1, i_2-1, i_3-2, \dots, i_{m/2}-(m/2-1)$  is an increasing sequence of distinct terms with  $1 \leq i_1$  and  $i_{m/2} \leq n-1 - ((m/2-1)) = n - m/2$ , and hence  $K_m(\overleftrightarrow{T}) = \binom{n - \frac{m}{2}}{\frac{m}{2}}$ .

Finally, let us prove (4). Let  $T = (V, E) \neq L_n$ . We consider the case  $m = 4$ , and we shall prove that  $K_4(\overleftrightarrow{T}) < \binom{n-2}{2}$ . It is not difficult to obtain the closed formula  $K_4(\overleftrightarrow{T}) = \frac{1}{2} \sum_{v_1 v_2 \in E} (n - \deg(v_1) - \deg(v_2))$ , from which the following formula can be derived:

$$K_4(\overleftrightarrow{T}) = \frac{1}{2} \left( n(n-1) - \sum_{v \in V} (\deg(v))^2 \right).$$

We claim that the strict maximum of this expression, constrained to the condition  $\frac{1}{2} \sum_{v \in V} \deg(v) = n - 1$ , is attained for the following sequence of degrees of  $T$ :  $2, 2, 2, \dots, 2, 1, 1$ ; that is, for  $T = L_n$ . Indeed, if we consider a different degree sequence, we could increase the value of the corresponding  $K_4$  by decreasing by 1 a degree  $a$  and increasing by 1 another degree  $b$ , such that  $a - b \geq 2$  (note that, for any tree other than  $L_n$ , there is at least one vertex  $v_a$  with  $a = \deg(v_a) \geq 3$ , and also there are leaves  $v_b$ , with  $b = \deg(v_b) = 1$ , so there exist degrees  $a, b$  such that  $a - b \geq 2$ ). The value of  $K_4$  would thus increase by  $2(a - b - 1)$ . Repeated application of this procedure yields that the strict maximum of  $K_4$  is attained for the degree sequence of  $L_n$ .  $\square$

**Corollary 17.** *The independent term  $k_n$  of the characteristic polynomial of a double directed tree  $\overleftrightarrow{T}$  of order  $n$  satisfies  $k_n \in \{-1, 0, 1\}$  and*

- i)  $k_n = 0$  if and only if there is no perfect matching in  $T$ .
- ii)  $k_n = 1$  if and only if there is a perfect matching in  $T$  and  $n = 4p$ , for some integer  $p$ .
- iii)  $k_n = -1$  if and only if there is a perfect matching in  $T$  and  $n = 4p + 2$ , for some integer  $p$ .

**Corollary 18** (from [Theorem 14](#)). *The independent term  $k_n$  of the characteristic polynomial of an MSD  $D$  of order  $n$  satisfies  $k_n \in \{-1, 0, 1\}$  and*

- i)  $k_n = 0$  if and only if there is no covering of  $D$  by disjoint cycles.
- ii)  $k_n = 1$  if and only if there is a covering of  $D$  with an even number of disjoint cycles.
- iii)  $k_n = -1$  if and only if there is a covering of  $D$  with an odd number of disjoint cycles.

4.2. General case

Let  $D = (V, A)$  be an MSD with  $n$  vertices,  $n \geq 2$ , and  $m$  be an integer with  $2 \leq m \leq n$ . We denote by  $K_m(D)$  the number of cycle structures covering  $m$  vertices of  $D$ . Obviously,  $|k_m(D)| \leq K_m(D)$ ,  $k_m(D)$  being the coefficient of  $x^{n-m}$  in the characteristic polynomial of the adjacency matrix of  $D$ .

We conjecture that the upper bound on the value  $K_m(D)$  for double directed trees ( $m$  even) also holds for MSDs, both for even and odd  $m$ .

**Conjecture 19.** *Let  $D$  be an MSD with  $n$  vertices,  $n \geq 2$ , and  $m$  an integer such that  $2 \leq m \leq n$ . Then the following inequality holds:*

$$K_m(D) \leq \binom{n - \lceil \frac{m}{2} \rceil}{\lfloor \frac{m}{2} \rfloor}$$

Using the generative procedure for MSDs described in [10], whose results are listed in [20], we have obtained the maxima of the absolute value of  $k_m(D)$  for all MSDs  $D$  of order  $n$ , for  $n \leq 15$ . In the following table, we give these maxima and, when it is different, the upper bound given by Conjecture 19 (in brackets).

$n$	$ k_n $	$ k_{n-1} $	$ k_{n-2} $	$ k_{n-3} $	$ k_{n-4} $	$ k_{n-5} $	$ k_{n-6} $
2	1						
3	1	2					
4	1	2	3				
5	1	3	3	4			
6	1	3	6	4	5		
7	1	4	5 (6)	10	5	6	
8	1	4	10	8 (10)	15	6	7
9	1	5	9 (10)	20	11 (15)	21	7
10	1	5	15	16 (20)	35	15 (21)	28
11	1	6	14 (15)	35	26 (35)	56	19 (28)
12	1	6	21	30 (35)	70	40 (56)	84
13	1	7	20 (21)	56	55 (70)	126	57 (84)
14	1	7	28	50 (56)	126	91 (126)	210
15	1	8	27 (28)	84	105 (126)	252	147 (210)

$n$	$ k_{n-7} $	$ k_{n-8} $	$ k_{n-9} $	$ k_{n-10} $	$ k_{n-11} $	$ k_{n-12} $	$ k_{n-13} $
9	8						
10	8	9					
11	36	9	10				
12	24 (36)	45	10	11			
13	120	29 (45)	55	11	12		
14	78 (120)	165	35 (55)	66	12	13	
15	330	105 (165)	220	41 (66)	78	13	14

5. Representations of MSDs

The fact that a double directed tree has  $2(n - 1)$  arcs suggests that we can decompose it into two directed trees, each of them having  $n - 1$  arcs. Furthermore, this decomposition

is a factorization, and it can be done in such a way that, given any vertex  $u$ , the first directed tree is a rooted tree with root  $u$  and the second is a reversed rooted tree with root  $u$ . By a *reversed rooted tree* we mean the resulting directed tree after reversing the orientation of all arcs in a rooted tree.

This property can be generalized to MSDs but, in general, the factorization cannot yield two directed trees, because an MSD can have less than  $2(n - 1)$  arcs. The Theorem below establishes said generalization.

**Theorem 20.** *An MSD factors into a rooted spanning tree and a forest of reversed rooted trees.*

**Proof.** Let  $D$  be an MSD. Let us consider an ear decomposition of  $D$ ,  $\mathcal{E} = \{P_0, \dots, P_k\}$ . Since  $D$  is an MSD, each ear  $P_j$  ( $1 \leq j \leq k$ ) contains at least one new vertex and two new arcs, with respect to  $\bigcup_{i=0}^{j-1} V_i$  and  $\bigcup_{i=0}^{j-1} A_i$ , respectively.

The first ear is a cycle,  $P_0 = v_0^0 v_1^0 \cdots v_{s_0-1}^0 v_0^0$ . Let  $T$  be the path  $v_0^0 v_1^0 \cdots v_{s_0-1}^0$  and let  $F$  be the arc  $v_{s_0-1}^0 v_0^0$ . Then,  $T$  is a rooted tree, with root  $v_0^0$ , and  $F$  is a reversed rooted tree, with reversed root  $v_0^0$ . For each ear  $P_j = v_0^j v_1^j \cdots v_{s_j}^j$ ,  $1 \leq j \leq k$ , we add the path  $v_0^j v_1^j \cdots v_{s_j-1}^j$  to  $T$  and the arc  $v_{s_j-1}^j v_{s_j}^j$  to  $F$ . Note that all the new vertices of  $P_j$  are added to  $T$ , they are connected to  $T$  only by the first vertex of the path  $v_0^j$  and they have indegree one. Note also that the arc  $v_{s_j-1}^j v_{s_j}^j$  is joined to one of the connected components of  $F$ , if the vertex  $v_{s_j}^j$  belongs to  $F$ , and it constitutes a new connected component, if  $v_{s_j}^j$  does not belong to  $F$ . Then it is clear, by construction, that  $T$  is a rooted spanning tree, with root  $v_0^0$ , and that  $F$  is a forest of reversed rooted trees.  $\square$

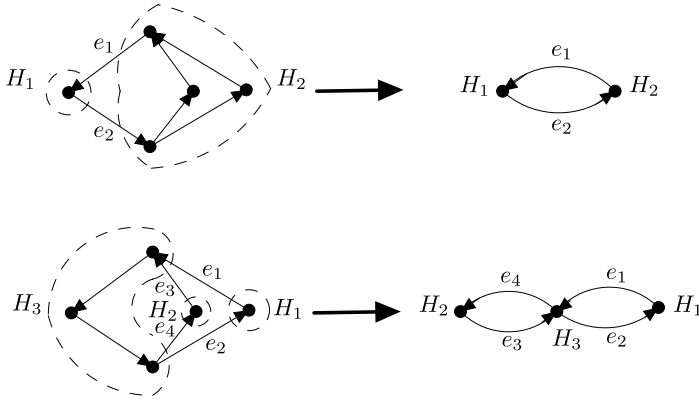
Note that this factorization depends on the labeling of the first ear  $P_0$ . In fact, there exist  $s_0$  possible different factorizations,  $s_0$  being the length of the cycle  $P_0$ .

For the next theorem, we need to introduce Hasse diagrams. A *Hasse diagram* is an acyclic digraph with no transitive arcs. The *contraction of a Hasse diagram* as a subdigraph consists on its reduction to a unique vertex (in a similar way to the contraction of a cycle).

In every MSD of order  $n$ , an underlying double directed tree exists, with  $k \leq n$  vertices; and  $k$  disjoint Hasse diagrams, contained in the MSD, whose contraction generates a vertex of the double directed tree. The arcs of the 2-cycles of the underlying double directed tree come from the arcs of the 2-cuts of cycles in the MSD. In the case of the MSD being a double directed tree, the underlying double directed tree is the MSD itself, and each Hasse diagram is just a vertex. We show in the Fig. 5 two different underlying double directed trees for the same MSD.

**Theorem 21.** *An MSD has an underlying double directed tree whose vertices are given by the contraction of connected Hasse diagrams.*

**Proof.** Let  $D$  be an MSD. We describe a process to depict  $D$  as a double directed tree of Hasse diagrams. We shall recursively construct a double directed tree  $\overset{\leftrightarrow}{T} = (V, A)$ , whose



**Fig. 5.** Two different underlying double directed trees for the same MSD.

vertices are connected subdigraphs of  $D$ . We initialize  $\overleftrightarrow{T}$  with vertex set  $V = \{D\}$  and arc set  $A = \emptyset$ , and then we perform the following decomposition with every vertex  $N$  of  $\overleftrightarrow{T}$  which is cyclic:

1. Take a cycle  $C$  from  $N$ .
2. Choose two arcs  $u_1u_2, v_2v_1$  in  $C$  that build up a 2-cut of  $D$  (using [Theorem 10](#)). Let  $N_1, N_2$  be the intersection of  $N$  with the two connected components of  $D - u_1u_2 - v_2v_1$  ( $u_i, v_i \in N_i$ , for  $i \in \{1, 2\}$ ). We claim that  $N_1, N_2$  are connected. Let  $C_1$  and  $C_2$  be the paths resulting from the cycle  $C$  after deleting  $u_1u_2$  and  $v_2v_1$ . Then, every vertex of  $N$  belongs either to the connected component of  $C_1$  or to the connected component of  $C_2$ , as the connection of  $N$  implies that  $N$  is connected to  $C$ . Hence, the deletion of  $u_1u_2, v_2v_1$  generates exactly two connected components in  $N$ : one containing  $C_1$  and the other containing  $C_2$ .
3. Update  $\overleftrightarrow{T}$  as follows: delete  $N$  from  $V$ , and add  $N_1$  and  $N_2$ ; add the arcs  $N_1N_2$  and  $N_2N_1$  to  $A$  (they correspond to the arcs  $u_1u_2$  and  $v_2v_1$ , respectively).
4. Also, all the arcs in  $A$  having  $N$  as an endpoint have to be updated. Let  $M \in V, NM, MN \in A$ , corresponding to the arcs  $w_1w'_1$  and  $w'_2w_2$  in  $D$  ( $w_1, w_2 \in N, w'_1, w'_2 \in M$ ). Without loss of generality, assume that  $w_1 \in N_1$ . We claim that then  $w_2 \in N_1$ . Otherwise, as  $M$  is connected, we could construct an undirected path in  $M$  joining  $w'_1$  to  $w'_2$ , and hence we would have an undirected path—disjoint to the cycle  $C$ —joining  $w_1$  and  $w_2$ . This contradicts the fact that  $u_1u_2, v_2v_1$  in  $C$  are a 2-cut of  $D$ . As a consequence, we can substitute the arcs  $NM, MN \in A$  by  $N_1M, MN_1$ , corresponding to the same original arcs  $w_1w'_1$  and  $w'_2w_2$  of  $D$ .

We continue this process until no cyclic digraphs are left in  $V$ . The final result of this procedure is a double directed tree whose vertices are connected acyclic digraphs. These vertices are also Hasse diagrams, as none of their arcs can be transitive.  $\square$



**Remark 22.** In the representation of an MSD as a double directed tree of connected Hasse diagrams given by [Theorem 21](#), the Hasse diagrams fulfill the following properties:

1. The maximals of the Hasse diagrams are initial vertices of the arcs of the underlying double directed tree.
2. The minimals of the Hasse diagrams are final vertices of the arcs of the underlying double directed tree.
3. The Hasse diagrams corresponding to linear vertices of the underlying double directed tree have exactly one minimal and one maximal.
4. For every linear MSD, the underlying double directed tree is unique, because for every cycle, the arcs of the 2-cuts are uniquely determined. The underlying double directed tree is  $\overset{\leftrightarrow}{L}_{j+1}$ , where  $j$  is the number of cycles of the linear MSD.

## 6. Final remarks

Every digraph can be seen as an acyclic digraph whose vertices are the strongly connected components of the digraph: the condensation digraph. Every SD vertex of the condensation digraph can be generated from an MSD by adding the corresponding transitive arcs. Consequently, it seems very important to undertake a deeper study of the structural properties of MSDs.

In this paper, we have looked at MSDs as a generalization of trees. We have studied the analogies and differences between both of them, and we have started a promising research on the coefficients of the characteristic polynomials of these digraphs.

We have also considered other representations of MSDs, whose study can be helpful to understand the acyclic order structure (condensation digraph) and the cyclic structure of a digraph.

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