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RECONSTRUCTING A GRAPH FROM THE BOUNDARY DISTANCE MATRIX

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Abstract

A vertex v of a connected graph G is said to be a boundary vertex of G if for some other vertex u of G, no neighbor of v is further away from u than v. The boundary $\partial(G)$ of G is the set of all of its boundary vertices.

The boundary distance matrix $\hat{D}_G$ of a graph $G = ([n], E)$ is the square matrix of order κ, with κ being the order of $\partial(G)$, such that for every $i, j \in \partial(G)$, $[\hat{D}_G]_{ij} = d_G(i, j)$.

Given a square matrix $\hat{B}$ of order κ, we prove under which conditions $\hat{B}$ is the distance matrix $\hat{D}_T$ of the set of leaves of a tree T, which is precisely its boundary.

We show that if G is either a block graph or a unicyclic graph, then G is uniquely determined by the boundary distance matrix $\hat{D}_G$ of G and we also conjecture that this statement holds for every connected graph G, whenever both the order n and the boundary (and thus also the boundary distance matrix) of G are prefixed.

Moreover, an algorithm for reconstructing a 1-block graph (respectively, a unicyclic graph) from its boundary distance matrix is given, whose time complexity in the worst case is $O(n)$ (respectively, $O(n^2)$).

Keywords: boundary, distance matrix, block graph, unicyclic graph, realizability.

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1. Introduction

While typically a graph is defined by its lists of vertices and edges, significant research has been dedicated to minimizing the necessary information required to uniquely determine a graph. For example, various approaches include reconstructing metric graphs from density functions [9], road networks from a set of trajectories [1], graphs utilizing shortest paths or distance oracles [16], labeled graphs from all r-neighborhoods [21], or reconstructing phylogenetic trees [2]. Of particular note is the graph reconstruction conjecture [17, 32] which states the possibility of reconstructing any graph on at least three vertices (up to isomorphism) from the multiset of all unlabeled subgraphs obtained through the removal of a single vertex. Indeed, a search with the word "graph reconstruction" returns more than 3 million entries.

In this paper, our focus lies in the reconstruction of graphs from the distance matrix of their boundary vertices and the graph's order. We are persuaded that this process could hold true for all graphs, and we state it as a conjecture (see Conjecture 12). It is accordingly of particular interest to explore whether this conjecture holds for specific families of graphs. Our objective herein is to establish its validity for block graphs and also for unicyclic graphs.

There is a similar line of research in the continuous setting, known as the *boundary rigidity problem* (introduced in [11, 20]), which can be stated as follows. Given a compact Riemannian manifold (M, g) with boundary ∂M, establish under which assumptions on ∂M, the geodesic distance $d_g|_{\partial M \times \partial M}$, uniquely determines g. For further details on this topic, see [23, 29, 31].

The concept of a graph's boundary was introduced by Chartrand, Erwin, Johns and Zhang in 2003 [7]. Initially conceived to identify local maxima of vertex distances, the boundary has since revealed a host of intriguing properties. It has been recognized as geodetic [4], serving as a resolving set [14], as a strong resolving set [24] and also as doubly resolving set (see Proposition 4). Put simply, each vertex lies in the shortest path between two boundary vertices and, given any pair of vertices x and y, there exists a boundary vertex v such that either x lies on the shortest path between v and y, or vice versa. With such properties, it is unsurprising that the boundary emerges as a promising candidate for reconstructing the entire graph.

Graph distance matrices represent a fundamental tool for graph users, enabling the solution of problems such as finding the shortest path between two nodes. However, our focus here shifts mainly towards their realizability. That is, given a matrix (integer, positive and symmetric), we inquire whether there exists a corresponding graph where the matrix entries represent the distances between vertices. In 1965, Hakimi and Yau [12] presented a straightforward additional condition that the matrix must satisfy to be realizable (see Theorem 1).

Building upon this, in 1974, Buneman [3] provided the matrix characterization for being the distance matrix of a tree once we know that the graph is K_3-free, and Graham and Pollack [10] computed the determinant of the distance matrix of a tree (see Theorem 17). Additionally, Howorka [15] in 1979, formulated conditions for the distance matrix of a block graph (see Theorem 15), and Lin, Liu and Lu [19] provided the determinant of such matrices (see Theorem 16). Incidentally, we use their result to derive the converse of the Graham and Pollack's theorem. Furthermore, we also give an algorithmic approach to the characterization of the distance matrix of a unicyclic graph.

As previously mentioned, we are interested in the distance matrix of a graph's boundary, a submatrix of the distance matrix. We seek to determine the realizability of these matrices and, while we have achieved characterization in the case of trees and block graphs, a similar analysis for unicyclic graphs remains elusive.

Finally, we present a pair of algorithms for reconstructing trees and unicyclic graphs from the distance matrix of their boundary. In trees, the boundary corresponds to the leaves, while in unicyclic graphs, it contains the leaves along with the vertices of the cycle with degree two.

The paper is organized as follows: this section is finished by introducing general terminology and notation. In Section 2, we explore the notion of boundary and its relation with distance matrices. Section 3 is devoted to the reconstruction of trees and 1-block graphs, completing first with the realizability of both the distance matrix and the boundary distance matrix of a tree and a block graph. In a similar way, Section 4 undertakes the characterization of distance matrices for unicyclic graphs, followed by their reconstruction from the boundary distance matrix. Finally, the paper ends with a section on conclusions and open problems.

1.1. Basic terminology

All the graphs considered are undirected, simple, finite and (unless otherwise stated) connected. If $G = (V, E)$ is a graph of order n and size m, it means that $|V| = n$ and $|E| = m$. Unless otherwise specified, $n \geq 2$ and $V = [n] = \{1, \ldots, n\}$.

Let v be a vertex of a graph G. The *open neighborhood* of v is $N(v) = \{w \in V(G) : vw \in E\}$, and the *closed neighborhood* of v is $N[v] = N(v) \cup \{v\}$. The *degree* of v is $\deg(v) = |N(v)|$. The minimum degree (respectively, maximum degree) of G is $\delta(G) = \min\{\deg(u) : u \in V(G)\}$ (respectively, $\Delta(G) = \max\{\deg(u) : u \in V(G)\}$). If $\deg(v) = 1$, then v is said to be a *leaf* of G and the set and the number of leaves of G are denoted by $\mathcal{L}(G)$ and $\ell(G)$, respectively.

Let K_n, P_n, W_n and C_n be, respectively, the complete graph, path, wheel and cycle of order n. Moreover, $K_{r,s}$ denotes the complete bipartite graph whose maximal independent sets are $\overline{K_r}$ and $\overline{K_s}$, respectively. In particular, $K_{1,n-1}$ denotes the star with $n-1$ leaves.

Given a graph $G = (V, E)$ and a subset of vertices $W \subseteq V$, the subgraph of

G induced by W, denoted by $G[W]$, has W as vertex set and $E(G[W]) = \{vw \in E : v, w \in W\}$. If $G[W]$ is a complete graph, then it is said to be a *clique* of G.

Given a pair of vertices u, v of a graph G, a $u - v$ *geodesic* lies on a $u - v$ shortest path, i.e., a path joining u and v of minimum order. Clearly, all $u - v$ geodesics have the same length, and it is called the *distance* between vertices u and v in G, denoted by $d_G(u, v)$, or simply by $d(u, v)$, when the context is clear. A set $W \subseteq V(G)$ is called *geodetic* if any vertex of the graph is in a $u-v$ geodesic for some $u, v \in W$.

The *eccentricity* $\mathrm{ecc}(v)$ of a vertex v is the distance to a farthest vertex from v. The *radius* and *diameter* of G are respectively, the minimum and maximum eccentricity of its vertices and are denoted as $\mathrm{rad}(G)$ and $\mathrm{diam}(G)$. A vertex $u \in V(G)$ is a *central* vertex of G if $\mathrm{ecc}(u) = \mathrm{rad(G)}$, and it is called a *peripheral* vertex of G if $\mathrm{ecc}(u) = \mathrm{diam(G)}$. The set of central (respectively, peripheral) vertices of G is called the *center* (respectively, *periphery*) of G.

Let $S = \{w_1, w_2, \ldots, w_k\}$ be a set of vertices of a graph G. The distance $d(v, S)$ between a vertex $v \in V(G)$ and S is the minimum of the distances between v and the vertices of S, that is, $d(v, S) = \min\{d(v, w) : w \in S\}$. The *metric representation* $r(v|S)$ of a vertex v with respect to S is defined as the k-vector $r(v|S) = (d_G(v, w_1), d_G(v, w_2), \ldots, d_G(v, w_k))$. A set of vertices S is called *resolving* if for every pair of distinct vertices $x, y \in V(G)$, there exist a vertex $u \in S$ such that $d(x, u) \neq d(y, u)$, or equivalently, if $r(x|S) \neq r(y|S)$.

Resolving sets were first introduced by Slater in [27], and since then, many other similar concepts have been defined, such as doubly resolving sets [5] and strong resolving sets [22, 25]. A set of vertices S is called *doubly resolving* if for every pair $x, y \in V(G)$, there exist $u, v \in S$ such that $d(x, u) - d(y, u) \neq d(x, v) - d(y, v)$. A set of vertices S is called *strong resolving* if for every pair $x, y \in V(G)$, either x is in a $y - v$ geodesic or y is in $x - v$ geodesic, for some vertex $v \in S$. Clearly, every doubly (respectively, strong) resolving set is also resolving, but the converse is far from being true (see Figure 1).

A *cut-vertex* is a vertex whose deletion disconnects the graph. A maximal subgraph of G without cut-vertices is a block of G. In a *block graph*, every block is a clique, or equivalently, every cycle induces a complete subgraph. A block of a block graph is called *trivial* if it is K_2. Let K_h be a non-trivial block of a block graph G such that $V(K_h) = \{x_1, \ldots, x_h\}$. For every $i \in [h]$, the connected component of $G - E(K_h)$ containing x_i is called the branching graph of x_i and its denoted by G_{x_i}. A non-trivial block K_h is called *exterior* if for some vertex $x_i \in V(K_h)$, G_{x_i} is a tree, in which case, it is called the *branching tree* of x_i and it is denoted by T_{x_i}. The tree T_{x_i} is said to be *trivial* if $V(T_{x_i}) = \{x_i\}$. A 1-block graph is a graph containing one non-trivial exterior block.

A graph G whose order and size are equal is called *unicyclic*. These graphs contain a unique cycle that is denoted as C_g, where g is the *girth* of G. The connected component of $G - E(C_g)$ containing a vertex $v \in V(C_g)$ is denoted as T_v and it is called the *branching tree* of v. The tree T_v is said to be *trivial* if $V(T_v) = \{v\}$. A vertex $v \in V(G)$ is a *branching vertex* if either $v \notin V(C_g)$ and $\deg(v) \geq 3$ or $v \in V(C_g)$ and $\deg(v) \geq 4$.

For further information on basic graph theory we refer the reader to [8].

2. The Conjecture

2.1. The boundary of a graph

In this subsection, we introduce one of the essential components of our work: the boundary of a graph, which was first studied by Chartrand *et al.* in [7]. A vertex v of a graph G is said to be a *boundary vertex* of a vertex u if no neighbor of v is further away from u than v, i.e., if for every vertex $w \in N(v)$, $d(u,w) \leq d(u,v)$. The set of boundary vertices of a vertex u is denoted by $\partial_G(u)$, or simply by $\partial(u)$, when the context is clear. Given a pair of vertices $u, v \in V(G)$ if $v \in \partial(u)$, then v is also said to be *maximally distant* from u. A pair of vertices $u, v \in V(G)$ are called *mutually maximally distant*, or simply MMD, if both $v \in \partial(u)$ and $u \in \partial(v)$.

The *boundary* of G, denoted by $\partial(G)$, is the set of all of its boundary vertices, i.e., $\partial(G) = \bigcup_{u \in V(G)} \partial(u)$. Notice that, as was pointed out in [24], the boundary of G can also be defined as the set of MMD vertices of G, i.e.,

$$\partial(G) = \{v \in V(G) : \text{there exists}\, u \in V(G)\, \text{such that}\, u, v \text{ are}\, MMD\}.$$

Theorem 1 [13, 30]**.** *Let G be a graph of order $n \geq 2$ with κ boundary vertices. Then, $\kappa = 2$ if and only if $G = P_n$. Moreover, $\kappa = 3$ if and only if either*

(1) *G is a subdivision of $K_{1,3}$; or*

(2) *G can be obtained from K_3 by attaching exactly one path* (*of arbitrary length*) *to each of its vertices.*

Also, graphs with a big κ are well-known, as the next results show.

Proposition 2. *Let G be a graph of order n with κ boundary vertices. Then,*

(1) *If* $\mathrm{rad}(G) = \mathrm{diam}(G)$*, then $\kappa = n$.*

(2) *If* $\mathrm{diam}(G) = 2$*, then $n - 1 \leq \kappa \leq n$.*
Moreover, $\kappa = n - 1$ if and only if G contains a unique central vertex.

Proof. (1) Suppose that $\mathrm{rad}(G) = \mathrm{diam}(G) = d$. Take $u \in V(G)$ and notice that $\mathrm{ecc}(u) = \mathrm{d}$. Let $v \in V(G)$ such that $d(u,v) = d$. For every vertex $w \in N(v)$, $d(u,w) \leq d = d(u,v)$. Hence, $u \in \partial(u) \subseteq \partial(G)$.

(2) If $\mathrm{rad}(G) = \mathrm{diam}(G) = 2$, then according to the previous item, $\kappa = n$. Suppose that $\mathrm{rad}(G) = 1$. Let $V(G) = U \cup W$ such that U is the set of central vertices and W is the set of peripheral vertices of G. Observe that $W \subsetneq \partial(G)$ and that if $|U| = h$, then $G[U] = K_h$. If $h \geq 2$, then every central vertex belongs to the boundary of every other vertex of G. If $h = 1$ and $U = \{u\}$, then for every vertex $w \in W$, $u \notin \partial(w)$, i.e., $\partial(G) = W$, which means that $\kappa = |W| = n - 1$. ■

Corollary 3. *Let G be a graph of order $n \geq 3$ with κ boundary vertices.*

(1) *If $G \in \{K_n, K_{r,s}, C_n\}$ and $r, s \geq 2$, then $\kappa = n$.*

(2) *If $G \in \{W_n, K_{1,n-1}\}$, then $\kappa = n - 1$.*

As previously mentioned, the boundary exhibits several intriguing properties, like being geodetic [4] and a resolving set [14]. However, for the scope of this paper, its status as a strong resolving set is particularly pertinent. Thus, we shall now develop into this concept with some detail.

That notion were first defined by Sebő and Tannier [25] in 2003, and later studied in [22]. They were interested in extending isometric embeddings of subgraphs into the whole graph and, to ensure that, they defined a *strong resolving set* of a graph G as a subset $S \subseteq V(G)$ such that for any pair $x, y \in V(G)$ there is an element $v \in S$ such that there exists either a $x - v$ geodesic that contains y or a $y - v$ geodesic containing x.

What is crucial for our goals is that, as a consequence of the definition, it only suffices to know the distances from the vertices of a strong resolving set to the rest of nodes, to uniquely determine the graph. This issue is explored in more detail in Subsection 2.2.

It was proved in [24] that the boundary of a graph is always a strong resolving set. We show next that it is also a doubly resolving set.

Proposition 4. *The boundary $\partial(G)$ of every graph G is both a strong resolving set and a doubly resolving set.*

Proof. Let $u, v \in V(G)$ such that $d(u, v) = k$ and $\{u, v\} \cap \partial(G) = \emptyset$. So, for some vertex $w_1 \in N(v)$, $d(u, w_1) = k + 1$. If $w_1 \in \partial(u)$, then we are done. Otherwise, for some vertex $w_2 \in N(w_1)$, $d(u, w_2) = k + 2$.

Thus, after iterating this procedure finitely many times, say h times, we will finally find a vertex w_h such that for every vertex $w \in N(w_h)$, $d(u, w) \leq d(u, w_h) = k + h$, i.e., a vertex $w_h \in \partial(G)$ and a $u - w_h$ geodesic containing vertex v. Thus, $\partial(G)$ is a strong resolving set of G.

Now, consider the pair $\{w_h, u\}$ and take a vertex $z_1 \in N(u)$ such that $d(w_h, z_1) = d(w_h, u) + 1$. Reasoning in the same way as before, we conclude that there is a vertex $z_\rho \in \partial(G)$ such that the pair u, v is in a $w_h - z_\rho$ geodesic. Hence, $\partial(G)$ is a doubly resolving set of G. ■

Particularly, for trees, block graphs and unicyclic graphs, the boundary is very straightforward to characterize.

Proposition 5 [30]**.** *Let T be a tree. Then, $\partial(T) = \mathcal{L}(T)$.*

Proof. If $u \in \mathcal{L}(T)$ and $N(u) = \{v\}$, then notice that $u \in \partial(v)$, and thus $u \in \partial(T)$.

Take a vertex $u \in V(T)$ such that $\deg(u) \geq 2$. If $\{v_1, v_2\} \subseteq N(u)$ then, for every vertex $w \in V(T)$, $d(w,u) < \max\{d(w,v_1), d(w,v_2)\}$. Hence, $u \notin \partial(G)$. ∎

Proposition 6. *Let G be a block graph. If $\mathcal{U}(G)$ denotes the set of vertices of the blocks of order $k \geq 3$ of degree $k-1$, then $\partial(G) = \mathcal{L}(G) \cup \mathcal{U}(G)$.*

Proof. If $u \in \mathcal{L}(G)$ and $N(u) = \{v\}$, then notice that $u \in \partial(v)$. If $u \in \mathcal{U}(G)$ and K_k is the clique of G such that $u \in V(K_k)$, then for every vertex $v \in V(K_k) - u$, $u \in \partial(v)$.

Finally, take a vertex $u \notin \mathcal{L}(G) \cup \mathcal{U}(G)$. If $u \in V(K_k)$, $\{v_1, v_2\} \subseteq N(u)$, $v_1 \in V(K_k)$ and $v_2 \notin V(K_k)$, then $d(w,u) < \max\{d(w,v_1), d(w,v_2)\}$, for every vertex $w \in V(G)$. Hence, $u \notin \partial(G)$. ∎

Proposition 7. *Let G be a unicyclic graph of girth g. If $\mathcal{U}(G)$ denotes the set of vertices of C_g of degree 2, then $\partial(G) = \mathcal{L}(G) \cup \mathcal{U}(G)$.*

Proof. If $u \in \mathcal{L}(G)$ and $N(u) = \{v\}$, then notice that $u \in \partial(v)$. If $u \in \mathcal{U}(G)$ and $v \in V(C_g)$ is a vertex such that $d(u,v) \in \left\lfloor \frac{g}{2} \right\rfloor$, then observe that $u \in \partial(v)$.

Finally, take a vertex $u \notin \mathcal{L}(G) \cup \mathcal{U}(G)$. If $u \in V(C_g)$, $N(u) \cap V(C_g) = \{v_1, v_2\}$ and $v_3 \in N(u) \cap V(T_u)$, then $d(w,u) < \max\{d(w,v_1), d(w,v_2), d(w,v_3)\}$, for every vertex $w \in V(G)$. Thus, $u \notin \partial(G)$. If $u \in V(T_v)$ for some vertex $v \in V(C_g)$, $\deg(u) \geq 2$ and $\{v_1, v_2\} \subseteq N(u)$, then $d(w,u) < \max\{d(w,v_1), d(w,v_2)\}$, for every vertex $w \in V(G)$. Hence, $u \notin \partial(G)$. ∎

2.2. The distance matrix of a graph

At this point, the other relevant element of the work is introduced: distance matrices, and, along with some notations, a complete characterization of both the distance matrix of a tree and the distance matrix of the leaves of a tree are provided. This subsection concludes by showing a conjecture, along with some related open problems.

A square matrix D is called a *dissimilarity matrix* if it is symmetric, all off-diagonal entries are (strictly) positive and the diagonal entries are zeroes. A square matrix D of order $n \geq 3$ is called a *metric dissimilarity matrix* if it satisfies, for any triplet $i, j, k \in [n]$, the *triangle inequality*: $d_{ik} \leq d_{ij} + d_{jk}$.

The *distance matrix* D_G of a graph $G = (V, E)$ with $V = [n]$ is the square matrix of order n such that, for every $i, j \in [n]$, $d_{ij} = d(i,j)$. Certainly, this matrix is a metric dissimilarity matrix. A metric dissimilarity matrix D is called a *distance matrix* if there is a graph G such that $D_G = D$.

Let S be a subset of vertices of order k of a graph $G = (V, E)$, with $V = [n]$. We denote by $D_{S,V}$ the submatrix of D_G of order $k \times n$ such that for every $i \in S$ and for every $j \in V$, $[D_{S,V}]_{ij} = d(i, j)$.

Similarly, the so-called *S-distance matrix* of G, denoted by D_S^G, or simply by D_S, when the context is clear, is the square submatrix of D_G of order k such that for every $i, j \in S$, $[D_S]_{ij} = d(i, j)$. If $S = \partial(G)$, then D_S is also denoted by $\hat{D}_G$ and it is called the *boundary distance matrix* of G.

The next result was stated and proved in [12] and constitutes a general characterization of distance matrices. We include here a (new) proof, for the sake of completeness.

Theorem 8 [12]**.** *Let D be an integer metric dissimilarity matrix of order n. Then, D is a distance matrix if and only if, for every $i, j \in [n]$, if $d_{ij} > 1$, then there exists an integer $k \in [n]$ such that*

$$d_{ik} = 1 \text{ and } d_{ij} = d_{ik} + d_{kj}. \tag{1}$$

Proof. The necessity of the above condition immediately follows from the definition of distance matrix.

To prove the sufficiency, we consider the non-negative symmetric square matrix A of order n, such that, for every pair $i, j \in [n]$, $a_{ii} \in \{0, 1\}$ being $a_{ij} = 1$ if and only if $d_{ij} = 1$. Let $G = ([n], E)$ be the graph such that its adjacency matrix is A. Next, we show that the distance matrix of G is precisely D.

If $\mathrm{diam}(G) = d$, then $d(i, j) = p \in \{1, \ldots, d\}$, for every pair of distinct vertices $i, j \in [n]$. If $p = 1$, then clearly $d(i, j) = 1$ if and only if $d_{ij} = 1$. Take $2 \leq p \leq d$ and suppose that, if $1 \leq r \leq p - 1$, then

$$d(i, j) = r \text{ if and only if } d_{ij} = r.$$

Let $i, j \in [n]$ such that $d_{ij} = p$. According to condition (1), take $k \in [n]$ such that $d(i, k) = d_{ik} = 1$ and $p = d_{ij} = d_{ik} + d_{kj} = 1 + d_{kj}$. This means that $d(i, j) \leq p$, since $d_{kj} = p - 1$ and $d(i, j) \leq d(i, k) + d(k, j) = 1 + d(k, j)$. Hence, $d(i, j) = p$ as otherwise, according to the inductive hypothesis (1), $d_{ij} = d(i, j) < p$, a contradiction.

Conversely, let $i, j \in [n]$ such that $d(i, j) = p$. Let $k \in N(i)$ such that $d(i, j) = 1 + d(k, j)$. Since A is a metric dissimilarity matrix, $d_{ij} \leq d_{ik} + d_{kj}$. This means that $d_{ij} \leq p$, since $d(k, j) = p - 1$ and $d_{ij} \leq 1 + d_{kj}$. Hence, $d_{ij} = p$ as otherwise, according to the inductive hypothesis (1), $d(i, j) = d_{ij} < p$, a contradiction. ∎

An integer metric dissimilarity matrix D of order $n \geq 3$ is called *additive* if every subset of indices $\{i, j, h, k\} \subseteq [n]$ satisfies the so-named *four-point condition*:

$$\begin{cases} d_{ij} + d_{hk} \leq \max\{d_{ih} + d_{jk}, d_{ik} + d_{jh}\} \\ d_{ih} + d_{jk} \leq \max\{d_{ij} + d_{hk}, d_{ik} + d_{jh}\} \\ d_{ik} + d_{jh} \leq \max\{d_{ij} + d_{hk}, d_{ih} + d_{jk}\}. \end{cases}$$

Notice that every metric dissimilarity matrix of order $n = 3$ is additive, which means that the four-point condition can be seen as a strengthened version of the triangle inequality (see [3]).

A graph $G = ([n], E)$ is said to satisfy the *four-point condition* if its distance matrix D_G is additive, that is, if for every 4-vertex set $\{i, j, h, k\} \subseteq [n]$:

$$\begin{cases} d(i,j) + d(h,k) \leq \max\{d(i,h) + d(j,k), d(i,k) + d(j,h)\} \\ d(i,h) + d(j,k) \leq \max\{d(i,j) + d(h,k), d(i,k) + d(j,h)\} \\ d(i,k) + d(j,h) \leq \max\{d(i,j) + d(h,k), d(i,h) + d(j,k)\}. \end{cases}$$

As was pointed out in [3], these inequalities can be characterized as follows.

Proposition 9 [3]**.** *Let $\{i, j, h, k\}$ be a 4-vertex set of a graph $G = ([n], E)$. Then, the following statements are equivalent.*

(1) *$\{i, j, h, k\}$ satisfies the four-point condition.*

(2) *Among the three sums $d(i, j) + d(h, k)$, $d(i, h) + d(j, k)$, $d(i, k) + d(j, h)$, the two largest ones are equal.*

2.3. The Conjecture

The next result was implicitly mentioned in some papers [18, 24, 25] and proved in [6]. This equivalence, along with the statement shown in Proposition 4, has served as an inspiration for the main conjecture of the paper that is presented at the end of this subsection.

Theorem 10 [6]**.** *Let S be a proper subset of vertices of a graph $G = (V, E)$. Then, the following statements are equivalent.*

(1) *S is a strong resolving set.*

(2) *G is uniquely determined by the distance matrix $D_{S,V}$.*

As was noticed in [24, 25], this result is not true if we consider resolving sets instead of strong resolving sets. For example, the pair of leaves of the graphs displayed in Figure 1 form, in both cases, a resolving set S and also for both graphs the matrix $D_{S,V}$ is the same.

As a direct consequence of both Theorem 10 and Proposition 4, the following result holds.

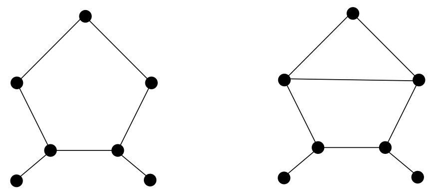


Figure 1. A pair of graphs of order 7, whose pair of leaves form a (neither doubly nor strong) resolving set.

Corollary 11 [6]**.** *Let $G = (V, E)$ be a graph. Then, G is uniquely determined by the distance matrix $D_{\partial(G),V}$.*

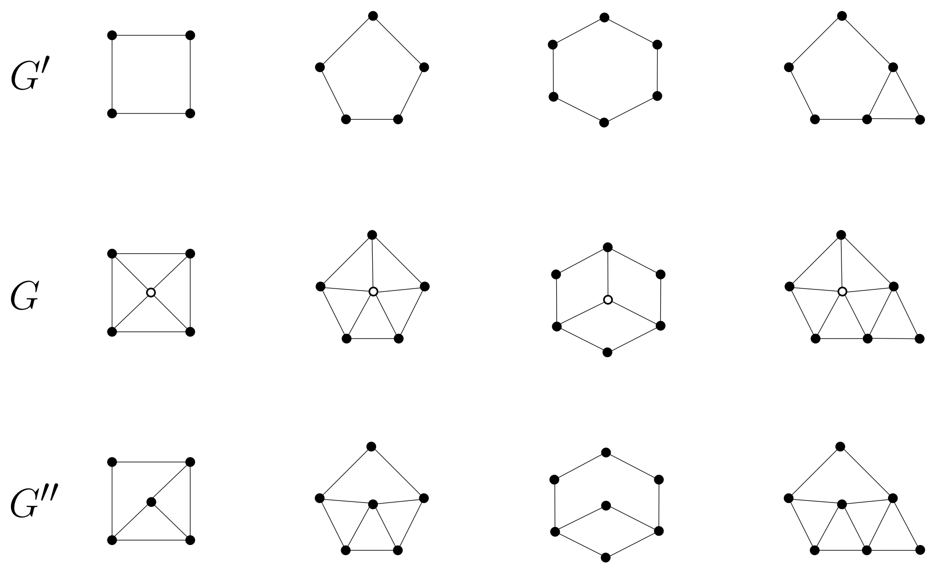


Figure 2. In each column, $\hat{D}'_G = \hat{D}_G = D^{G''}_{\partial(G)}$, G' and G have the same boundary but different order, meanwhile G and G'' have the same order but different boundary. In all cases, the boundary is the set of black vertices.

It is relatively easy to find pairs of graphs having the same boundary (that is, the same boundary distance matrix) but different order (see Figure 2, for some examples). Having in mind all of these results and particularly the one stated in Corollary 11, we present the following conjecture.

Conjecture 12. *Let $\hat{B}$ an integer metric dissimilarity matrix of order κ. Let $G = ([n], E)$ be a graph such that $\hat{D}_G = \hat{B}$. If $G' = ([n], E')$ is a graph such that $\hat{D}_{G'} = \hat{B}$, then G and G' are isomorphic.*

Equivalently, this conjecture can be restated as follows.

Conjecture 12. *Let κ, n be integers such that $2 \leq \kappa \leq n$. Let A, $\hat{B}$ be integer square matrices of order n and κ, respectively. Then, there is, at most, one graph G such that $V(G) = [n]$, $D_G = A$, $\partial(G) = [\kappa]$ and $\hat{D}_G = \hat{B}$.*

Let κ, n be integers such that $2 \leq \kappa \leq n$. Let A, $\hat{B}$ be integer square matrices of order n and κ, respectively. Let G be a graph such that $V(G) = [n]$, $\partial(G) = [\kappa]$ and $D_G = A$. We define the following graph families, denoted by $\mathcal{H}(\kappa)$, $\mathcal{H}(n)$, and $\mathcal{H}(\kappa, n)$, respectively.

- $G \in \mathcal{H}(\kappa)$ if it is the unique graph (up to isomorphism) such that $\partial(G) = [\kappa]$ and $\hat{D}_G = \hat{B}$.
- $G \in \mathcal{H}(n)$ if it is the unique graph (up to isomorphism) of order n such that $V(G) = [n]$ and $D_{[\kappa]} = \hat{B}$.
- $G \in \mathcal{H}(\kappa, n)$ if it is the unique graph (up to isomorphism) such that $V(G) = [n]$, $\partial(G) = [\kappa]$ and $D_{[\kappa]} = \hat{B}$.

Notice that Conjecture 12 can be restated as follows.

Conjecture 12. *Every graph belongs to $\mathcal{H}(\kappa, n)$.*

Although it is not difficult to find graphs not belonging neither to the graph family $\mathcal{H}(\kappa)$ nor to the graph family $\mathcal{H}(n)$ (see Figure 2, for some examples), we are persuaded that, for a wide spectrum of graph classes, it is possible to obtain the whole graph G from its boundary distance matrix. In Sections 3 and 4, we prove not only that both the block and the unicyclic families belong to $\mathcal{H}(\kappa, n)$, but also to $\mathcal{H}(\kappa) \cap \mathcal{H}(n)$.

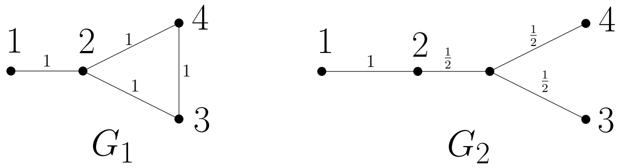
3. Block Graphs

This section is divided into three subsections: in the first one, we revise the main results regarding the characterization of the distance matrices of block graphs, and we prove the converse of the result of Graham and Pollack [10] in Theorem 19. The next subsection is devoted to determine those matrices which can be the boundary distance matrix of a block graph. Finally, in the last subsection, we describe and check the validity of an algorithm to reconstruct a 1-block graph having its boundary distance matrix as the only information.

3.1. The distance matrix of a block graph

In the seminal paper [3], Buneman noticed that trees satisfy the four-point condition and also showed that a K_3-free graph is a tree if and only if its distance matrix is additive. In the same paper, it was also proved that, for every additive matrix A of order k, there always exists a weighted tree of order $n \geq k$ containing a subset of vertices S of order k such that $D_S = A$ (see Figure 3). A different approach based on the structure of the 4×4 principal submatrices was given by Simões Pereira in [26]. In addition, it was proved in [33] that for every dissimilarity matrix D, it satisfies the four-point condition if and only if there is a unique weighted binary tree T whose $\partial(T)$-distance matrix is D.

Starting from these results, Howorka in [15] was able to characterize the family of graphs whose distance matrix is additive, i.e., satisfying the four-point condition. We include next new proofs of those results for the sake of both completeness and clarity.



$$D_{G_1} = D_{[4]} = \begin{pmatrix} 0 & 1 & 2 & 2 \\ 1 & 0 & 1 & 1 \\ 2 & 1 & 0 & 1 \\ 2 & 1 & 1 & 0 \end{pmatrix}$$

Figure 3. The distance matrix D_{G_1} of G_1 and the [4]-distance matrix of the weighted tree G_2 are the same.

Proposition 13 [15]. *Every block graph satisfies the four-point condition.*

Proof. Let S be a 4-vertex set of a block graph G, named $S = \{1, 2, 3, 4\}$. The only seven possible configurations of paths connecting the 4 vertices of S are those shown in Figure 4. We check that the four-condition holds in all cases.

(1) $d_{12} + d_{34} = d_{13} + d_{24} = d_{14} + d_{23} = a + b + c + d$,

(2) $d_{12} + d_{34} = a + b + c + d$ $d_{13} + d_{24} = d_{14} + d_{23} = a + b + c + d + 2e$,

(3) $d_{12} + d_{34} = a + b + c + d + 1$,
$d_{13} + d_{24} = d_{14} + d_{23} = a + b + c + d + 2$,

(4) $d_{12} + d_{34} = a + b + c + d + 1$,
$d_{13} + d_{24} = d_{14} + d_{23} = a + b + c + d + 2e + 2$,

(5) $d_{12} + d_{34} = a + b + c + d + 2$,
$d_{13} + d_{24} = d_{14} + d_{23} = a + b + c + d + 4$,

(6) $d_{12} + d_{34} = a + b + c + d + 2$,
$d_{13} + d_{24} = d_{14} + d_{23} = a + b + c + d + 2e + 4$,

(7) $d_{12} + d_{34} = d_{13} + d_{24} = d_{14} + d_{23} = a + b + c + d + 2$. ∎

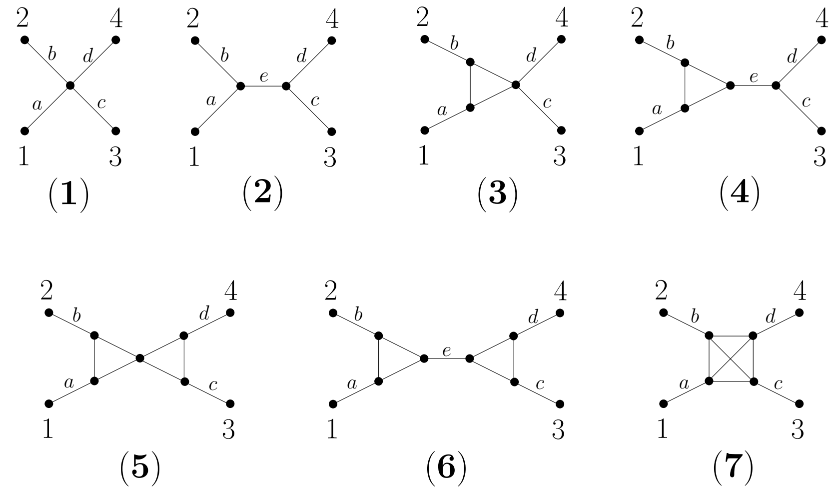


Figure 4. Seven possible configurations of paths connecting 4 vertices of a block graph.

The converse is proved in the next proposition.

Proposition 14 [15]. *If G satisfies the four-point condition, then it is a block graph.*

Proof. Let C_h be an induced cycle of G of minimum order $h \geq 4$. Then, $h = 4q + r$, with $q \geq 1$ and $0 \leq r \leq 3$. Notice that C_h is not only an induced subgraph of G but also isometric. Take a 4-vertex set $\{i, j, h, k\} \subseteq V(C_h)$ such that $\{d_{ij}, d_{jh}, d_{h,k}, d_{k,i}\} \subseteq \{q, q+1\}$. Check that $d_{ij} + d_{hk} \leq 2q + 2$, $d_{ik} + d_{jh} \leq 2q+2$ and $d_{ih}+d_{jk} \geq 4q$. Hence, this 4-vertex set violate the four-point condition, which means that either G is a tree or it is a chordal graph of girth 3, i.e., the only induced cycles have length 3.

Next, suppose that G is a chordal graph of girth 3. Take a cycle $C_p = ([p], E)$ in G of minimum order $p \geq 4$, such that $[p]$ is not a clique. Notice that $p \geq 5$, since neither the cycle C_4 nor the diamond $K_4 - e$ satisfies the four-point condition. Let $i, j \in [p]$ such that $1 \leq i < j \leq p$ and $ij \notin E(G)$. Notice that $d(i, j) = 2$, since C_p is of minimum order. W.l.o.g. we may assume that $i = 1$ and $j = 3$. Observe that for every $h \notin \{2, p\}$ and $k \notin \{2, 4\}$, $\{1h, 3k\} \cap E(G) = \emptyset$, since C_p is of minimum order.

Let h be the minimum integer between 4 and p such that $2h \in E(G)$. Then, clearly $h = 4$, since otherwise the set $\{2, \ldots, h\}$ is an induced cycle of order at least 4, a contradiction. Let k be the minimum integer between 5 and p such that $2k \in E(G)$. We distinguish cases.

Case 1. If $k = 5$, then the subgraph induced by the set $\{2, 3, 4, 5\}$ is the diamond $K_4 - e$, a contradiction.

Case 2. If $p = 5$ and $2k \in E(G)$, then the subgraph induced by the set $\{2, 4, 5, 1\}$ is the cycle C_4, a contradiction.

Case 3. If $p \geq 6$ and $k \geq 6$, then the subgraph induced by the set $\{2, 4, 5, \ldots, k\}$ is the cycle C_{k-2}, a contradiction.

Hence, we have proved that every cycle of G induces a clique, i.e., G is a block graph. ■

Once the two implications have been proved, we can establish the theorem.

Theorem 15 [15]**.** *A graph G of order n is a block graph if and only if its distance matrix D_G is additive.*

Theorem 16 [19]**.** *Let G be a block graph on n vertices and k blocks $K_{n_1}, \ldots, K_{n_k}$. Then,*

$$\det(D_G) = (-1)^{n-1} \sum_{i=1}^{k} \frac{n_i - 1}{n_i} \prod_{j=1}^{k} n_j.$$

In particular, as a straight consequence of the previous result, the following theorem, proved in [10], is obtained.

Theorem 17 [10]**.** *Let T be a tree on n vertices. Then,*

$$\det(D_T) = (-1)^{n-1}(n-1)2^{n-2}.$$

The next lemma is the crucial result that allows us to prove the characterization of distance matrices of trees by means of its determinant.

Lemma 18. *Let k and n be integers such that $n \geq 3$ and $1 \leq k \leq n-1$. Let $\{n_1, \ldots, n_k\}$ be a decreasing sequence of k integers such that $n \geq n_1 \geq \cdots \geq n_k \geq 2$ and $n_1 + \cdots + n_k = n + k - 1$. Then,*

$$\sum_{i=1}^{k} \frac{n_i - 1}{n_i} \prod_{j=1}^{k} n_j \leq (n-1)2^{n-2}$$

Moreover, the equality holds if and only if $k = n-1$ and $n_1 = \cdots = n_{n-1} = 2$.

Proof. Let $h \in [k]$ such that $n_h \geq 3$ and for every $i \in \{h+1, \ldots, k\}$, $n_i = 2$. Then,

$$\sum_{i=1}^{k} \frac{n_i - 1}{n_i} \prod_{j=1}^{k} n_j = \Big(\frac{n_1 - 1}{n_1} + \cdots + \frac{n_h - 1}{n_h} + \frac{k-h}{2}\Big) \cdot \prod_{j=1}^{h} n_j \cdot 2^{k-h}.$$

Take the $(k+1)$-sequence $\{n'_1, \ldots, n'_{k+1}\} = \{n_1, \ldots, n_{h-1}, n_h - 1, n_{h+1}, \ldots, n_k, 2\}$. Then,

$$\sum_{i=1}^{k+1} \frac{n'_i - 1}{n'_i} \prod_{j=1}^{k+1} n'_j = \Big(\frac{n_1 - 1}{n_1} + \cdots + \frac{n_{h-1} - 1}{n_{h-1}} + \frac{n_h - 2}{n_h - 1} + \frac{k-h}{2} + \frac{1}{2}\Big) \cdot \prod_{j=1}^{h-1} n_j \cdot (n_h - 1) \cdot 2^{k-h+1}.$$

Check that if $n_h \geq 3$, then both $\frac{n_h - 1}{n_h} < \frac{n_h - 2}{n_h - 1} + \frac{1}{2}$ and $n_h < (n_h - 1) \cdot 2$. Hence, $\sum_{i=1}^{k} \frac{n_i - 1}{n_i} \prod_{j=1}^{k} n_j < \sum_{i=1}^{k+1} \frac{n'_i - 1}{n'_i} \prod_{j=1}^{k+1} n'_j$.

Repeating this procedure iteratively, starting from the sequence $\{n'_1, \ldots, n'_{k+1}\}$, the inequality $\sum_{i=1}^{k} \frac{n_i - 1}{n_i} \prod_{j=1}^{k} n_j \leq (n-1)2^{n-2}$ is shown, since the last sequence is the $(n-1)$-sequence: $\{2, \ldots, 2\}$. ∎

As a direct consequence of Theorems 15, 16, 17 and Lemma 18, we are able to prove the converse of Theorem 17.

Theorem 19. *A graph of order n is a tree T if and only if its distance matrix D_T is additive and* $\det(D_T) = (-1)^{n-1}(n-1)2^{n-2}$.

3.2. The boundary distance matrix of a block graph

If, in the previous subsection, we have characterized the distance matrices of block graphs, in this one we intend to characterize the set of metric dissimilarity matrices which are the distance matrix of the boundary of these classes of graphs.

We begin by showing that no two (non-isomorphic) trees can have the same boundary distance matrix, a fact that was firstly noticed and proved in [28].

Theorem 20 [28]**.** *Let T be a tree on n vertices and κ leaves. Then, T is uniquely determined by $\hat{D}_T$, the $\mathcal{L}(T)$-distance matrix of T.*

Proof. We proceed by induction on κ. Clearly, the claim holds true when $\kappa = 2$ since the unique tree with 2 leaves of order n is the path P_n and n is uniquely determined by the distance between its leaves.

Let T_κ be a tree with κ leaves such that $\mathcal{L}(T_\kappa) = \{\ell_1, \ldots, \ell_\kappa\}$ is the set of leaves of T_κ. Assume that $\hat{D}_{T_\kappa} = \hat{D}_T$. Let $\hat{D}_{\kappa-1}$ be the submatrix of $\hat{D}_T$ obtained by deleting the last row and column of $\hat{D}_T$.

By the inductive hypothesis, there is a unique tree $T_{\kappa-1}$ with $\kappa - 1$ leaves such that $\hat{D}_{T_{\kappa-1}} = \hat{D}_{\kappa-1}$. Hence, $T_{\kappa-1}$ is the subtree of T obtained by deleting the path that joins the leaf ℓ_κ to its exterior major vertex w_κ.

According to Propositions 4 and 5, $\mathcal{L}(T_{\kappa-1}) = \{\ell_1, \dots, \ell_{\kappa-1}\}$ is a doubly resolving set of $T_{\kappa-1}$. This means that, if $d(\ell_\kappa, w_\kappa) = a$, then w_κ is the unique vertex in $T_{\kappa-1}$ such that

$$r(\ell_\kappa|\mathcal{L}(T_{\kappa-1})) = r(w_\kappa|\mathcal{L}(T_{\kappa-1})) + (a, \overset{\kappa-1}{\dots}, a)$$

Thus, T_κ and T are isomorphic. ■

In [34], the metric dissimilarity matrices which are the distance matrices of the set of leaves of a tree were characterized.

Theorem 21 [34]**.** *Let $\hat{B}_\kappa$ be an integer metric dissimilarity matrix of order $\kappa \geq 3$. Then, $\hat{B}_\kappa$ is the $\mathcal{L}(T)$-distance matrix of a tree T if and only if it is additive and, for every distinct $i, j, k \in [\kappa]$,*

(1) $\hat{b}_{ij} < \hat{b}_{ik} + \hat{b}_{jk}$,

(2) $\hat{b}_{ij} + \hat{b}_{ik} + \hat{b}_{jk}$ *is even.*

Before approaching these pair of issues for the block graph family, we show how to algorithmically reconstruct a tree T from its $\mathcal{L}(T)$-distance matrix. To this end, it is enough to notice that the proof of Theorem 20 can be turned into an algorithm which runs in the worst case in $O(\kappa n)$ times.

Algorithm 1 Reconstructing-Tree

Require: A matrix $\hat{D}_T$ of a certain tree.
Ensure: A tree $T = (V, E)$.
1: Let κ be the order of the matrix $\hat{D}_T$ and let T be initially a set of κ isolated vertices $\ell_1, \dots, \ell_\kappa$;
2: Join the vertices ℓ_1 and ℓ_2 by a path of the length determined in $\hat{D}_T$;
3: Label all the vertices $u \in V$ with $r(u|\{\ell_1, \ell_2\})$, i.e., the distances from u to $\{\ell_1, \ell_2\}$;
4: **for** $k := 3$ to κ **do**
5: Compute $r(\ell_k|\{\ell_1, \dots, \ell_{k-1}\})$ as the distances from ℓ_k to $\{\ell_1, \dots, \ell_{k-1}\}$;
6: Locate a vertex u in T and a positive integer a such that $r(u|\{\ell_1, \dots, \ell_{k-1}\}) + (a, \overset{k-1}{\dots}\, a) = r(\ell_k|\{\ell_1, \dots, \ell_{k-1}\})$;
7: Add to T a path of length a joining u and ℓ_k;
8: Relabel all the vertices in T with their distances to $\{\ell_1, \dots, \ell_k\}$;
9: **end for**
10: **return** T.

Corollary 22. *The Algorithm* 1 *runs in time $O(\kappa n)$.*

Proof. It is straightforward to check that the step dominating the computation is 6, and that step is repeated $O(\kappa n)$ times. ■

Corollary 23. *Every tree T of order n with κ leaves belongs not only to $\mathcal{H}(\kappa, n)$, but also to $\mathcal{H}(\kappa)$ and to $\mathcal{H}(n)$.*

Theorem 24. *Let G be a block graph on n vertices and $\kappa \geq 3$ boundary vertices. Then, G is uniquely determined by $\hat{D}_G$, the boundary distance matrix of G.*

Proof. We proceed by induction on κ, the number of boundary vertices of G. For $\kappa = 3$, the statement clearly holds since, according to [13], G is either a spider or a 1-block graph whose branching trees are paths, depending on whether $d(u_1, u_2) + d(u_1, u_3) + d(u_2, u_3)$ be either even or odd.

Let G_κ be a block graph of order n with $\kappa \geq 4$ boundary vertices such that $\hat{D}_{G_\kappa} = \hat{D}_G$. We distinguish cases.

Case 1. There is a pair of twin vertices $u_1, u_2 \in \partial(G_\kappa)$. Let $G_{\kappa-1}$ be the subgraph of G_κ obtained after deleting vertex u_1. Notice that, according to the induction hypothesis, $G_{\kappa-1}$ is also an induced subgraph of G, since $G_{\kappa-1}$ is a block graph with $\kappa - 1$ boundary vertices. Thus, G_κ and G must be isomorphic since u_1 is in both graphs a twin of u_2.

Case 2. Assume that $\partial(G_\kappa)$ has no twins. Let x_1 and x_2 be a pair of vertices of an exterior block of G_κ. Consider its branching trees T_{x_1} and T_{x_2}. If T_{x_1} (respectively, T_{x_2}) is neither trivial nor a path, recursively pruning from T_{x_1} (respectively, T_{x_2}) beginning always with a leaf having maximum eccentricity, in a similar way as shown in Algorithm 2, as many leaves as needed until obtaining a block graph with a pair of twins. Otherwise, delete both $T_{x_1} - x_1$ and $T_{x_2} - x_2$, obtaining thus a graph in which both x_1 and x_2 are twins. In either case, we conclude that G_κ and G must be isomorphic since both T_{x_1} and T_{x_2} are not only in G_κ but also in G. ■

Lemma 25. *Let $\hat{B}_3$ be an integer metric dissimilarity matrix of order $\kappa = 3$. Then, $\hat{B}_3$ is the boundary distance matrix of a block graph G if and only if it satisfies the following* **condition***: for every distinct $i, j, k \in [3]$, $\hat{b}_{ij} < \hat{b}_{ik} + \hat{b}_{jk}$.*

Proof. If for some block graph G, $\hat{B}_3 = \hat{D}_G$ is the boundary distance matrix of G, then it is a routine exercise to check that $\hat{B}$ satisfies the **condition**.

To prove the converse, let $\hat{B}_3$ be an integer metric dissimilarity matrix of order 3

$$\hat{B}_3 = \begin{pmatrix} 0 & a & b \\ a & 0 & c \\ b & c & 0 \end{pmatrix}.$$

We distinguish cases.

Case 1. $a+b+c$ is even. Firstly, notice that $\min\{a,b,c\} \geq 2$, since otherwise if for example $\min\{a,b,c\} = a = 1$, then, according to the **condition**: $b < 1+c$ and $c < 1+b$, which means that $b = c$, and thus $a+b+c = 1+2c$, a contradiction.

Consider the tree T of order $n = x+y+z+1$ with 3 leaves displayed in Figure 5 (left) and notice that if $\hat{B}_3 = \hat{D}_T$, then

$$(y+z, x+z, x+y) = (a,b,c) \Leftrightarrow (x,y,z) = \Big(\frac{b+c-a}{2}, \frac{a+c-b}{2}, \frac{a+b-c}{2}\Big).$$

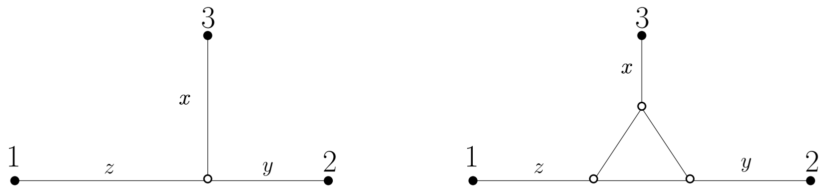


Figure 5. Left: Spider of order $n = x+y+z+1$ with 3 leaves. Right: 1-block graph of order $n = x+y+z+3$ with (at most) 3 leaves.

Clearly, x, y and z are strictly positive, since $\hat{B}_3$ satisfies the **condition**. Moreover, x, y and z are integers, since $a+b+c$ is an even integer, which means that integers $b+c-a$, $a+c-b$ and $a+b-c$ are also even. Hence, the distance matrix of the leaves of T is $\hat{B}$.

Case 2. $a+b+c$ is odd. Consider the 1-block graph G of order $n = x+y+z+3$ with (at most) 3 leaves displayed in Figure 5 (right) and notice that if $\hat{B}_3 = \hat{D}_G$, then

$$(y+z+1, x+z+1, x+y+1) = (a,b,c) \Leftrightarrow (x,y,z)$$
$$= \Big(\frac{b+c-a-1}{2}, \frac{a+c-b-1}{2}, \frac{a+b-c-1}{2}\Big).$$

Clearly, x, y and z are positive, since $\hat{B}_3$ satisfies the **condition**. Moreover, x, y and z are integers, since $a+b+c$ is an odd integer, which means that integers $b+c-a$, $a+c-b$ and $a+b-c$ are also odd. Hence, the boundary distance matrix of G is $\hat{B}_3$. ■

Theorem 26. *Let $\hat{B}_\kappa$ be an integer metric dissimilarity matrix of order $\kappa \geq 3$. Then, $\hat{B}_\kappa$ is the boundary distance matrix of a block graph G if and only if it is additive and it satisfies the following* **condition***: for every distinct $i,j,k \in [\kappa]$, $\hat{b}_{ij} < \hat{b}_{ik} + \hat{b}_{jk}$.*

Proof. If for some block graph G with κ boundary vertices, $\hat{B}_\kappa = \hat{D}_T$ is the boundary distance matrix of G, then it is a routine exercise to check that $\hat{B}$ is additive and satisfies the **condition**.

To prove the converse, take an integer additive matrix $\hat{B}_\kappa$ of order $\kappa \geq 4$ satisfying the **condition**. We proceed by induction on κ, the order of $\hat{B}_\kappa$. Case $\kappa = 3$ has been proved in Lemma 25.

Let $\hat{B}^1_{\kappa-1}$ and $\hat{B}^\kappa_{\kappa-1}$ be the matrices obtained by deleting row (and thus also column) 1 and κ of $\hat{B}_\kappa$, respectively. Let $\hat{B}_{\kappa-2}$ be the matrix obtained by deleting rows (and thus also columns) 1 and κ of $\hat{B}_\kappa$.

By the inductive hypothesis, $\hat{B}_{\kappa-2}$,$\hat{B}^1_{\kappa-1}$ and $\hat{B}^\kappa_{\kappa-1}$ are, respectively, the boundary distance matrices of three block graphs: $G_{\kappa-2}$, $G^1_{\kappa-1}$ and $G^\kappa_{\kappa-1}$. Moreover, according to Theorem 24, $G_{\kappa-2}$ is an induced subgraph of both $G^1_{\kappa-1}$ and $G^\kappa_{\kappa-1}$.

Let G_κ the block graph obtained by joining $G^1_{\kappa-1}$ and $G^\kappa_{\kappa-1}$. If $\partial(G^1_{\kappa-1}) = \{u_2, \ldots, u_\kappa\}$, $\partial(G^\kappa_{\kappa-1}) = \{u_1, \ldots, u_{\kappa-1}\}$ and $\partial(G_\kappa) = \{u_1, \ldots, u_{\kappa-1}, u_\kappa\}$, then for every $i, j \in [\kappa]$, $d(u_i, u_j) = \hat{b}_{ij}$, unless $i = 1$ and $j = \kappa$.

Suppose that, for every 4-subset $\{i, j, h, k\}$, $\hat{b}_{ij} + \hat{b}_{hk} = \hat{b}_{ih} + \hat{b}_{jk} = \hat{b}_{ik} + \hat{b}_{jh}$. In this case, according to Proposition 13 (see Cases (1) and (2)), G_κ must be either a spider with κ legs or a 1-block graph with κ branching trees, all of them being paths (see Figure 4, (1) and (7)).

Otherwise, assume w.l.o.g. that $\hat{b}_{12} + \hat{b}_{3\kappa} < \hat{b}_{13} + \hat{b}_{2\kappa} = \hat{b}_{1\kappa} + \hat{b}_{23}$. Thus, $d(\ell_1, \ell_\kappa) + d(\ell_j, \ell_h) = d(\ell_1, \ell_h) + d(\ell_j, \ell_\kappa)$, and

$$d(\ell_1, \ell_\kappa) = d(\ell_1, \ell_h) + d(\ell_j, \ell_\kappa) - d(\ell_j, \ell_h) = \hat{b}_{1h} + \hat{b}_{j\kappa} - \hat{b}_{jh} = \hat{b}_{1\kappa},$$

which means that $\hat{B}_\kappa$ is the distance matrix of G_κ. ■

3.3. Reconstructing a 1-block graph from the boundary distance matrix

At this point, we provide a procedure to obtain a 1-block graph from its boundary distance matrix. The unique previous result that we need is a way to determine the leaves of the graph.

Lemma 27. *Let G be a block graph. From the boundary distance matrix $\hat{D}_G$, it is possible to distinguish the vertices in $\mathcal{L}(G)$ from the ones in $\mathcal{U}(G)$.*

Proof. Take a vertex $u \in \partial(G)$. If $u \in \mathcal{L}(G)$, then for any two distinct vertices $w_1, w_2 \in \partial(G) - u$, $d(w_1, u) + d(u, w_2) - d(w_1, w_2) \geq 2$ (see Figure 7(1)).

If $u \in \mathcal{U}(G)$ and $N(u) = \{v_1, v_2\}$, consider the branching trees T_{v_1} and T_{v_2}. For $i = 1, 2$, let w_i be either a leaf of T_{v_i} or the vertex v_i if T_{v_i}, if it is trivial. Clearly, $d(w_1, u) + d(u, w_2) - d(w_1, w_2) = 1$ (see Figure 7(2)). ■

Finally, Theorem 28 establishes the correctness and time complexity of Algorithm 2.

Algorithm 2 Reconstructing-1Block-Recursive

Require: $(\hat{B}, G)$ where $\hat{B}$ is a boundary distance matrix and G is a graph.
if $\hat{B}$ corresponds with the distance matrix of a complete graph K_m **then**
  return $(\hat{B}, K_m)$
else
  Use Lemma 27 to distinguish the leaves in $\hat{B}$;
  Let v be the leaf with greatest eccentricity;
  if v has no siblings **then**
    Let $\hat{B}_1$ be the matrix $\hat{B}$ in which the row and column that correspond to the vertex v have been deleted and a row and a column are added corresponding with the parent of v;
    $(\hat{B}_2, G_1)$=Reconstructing-1Block-Recursive $(\hat{B}_1, G)$;
    Add v to G_1;
    return $(\hat{B}, G_1)$;
  else v has siblings $v_1, \ldots v_k$ being $v = v_0$
    Let $\hat{B}_1$ the matrix $\hat{B}$ in which the row and column that correspond to the vertex v and its siblings have been deleted and a row and a column are added corresponding with the parent of v;
    $(\hat{B}_2, G_1)$=Reconstructing-1Block-Recursive $(\hat{B}_1, G)$;
    Add $v_0, \ldots, v_k$ to G_1;
    return $(\hat{B}, G_1)$;
  end if
end if

Theorem 28. *Beginning with the boundary distance matrix $\hat{D}_G$ of a* 1*-block graph G,* Reconstructing-1Block-Recursive $(\hat{D}_G, \emptyset)$ *obtains an isomorphic graph to G in $O(n)$.*

Proof. The algorithm is recursive for simplicity and to take advantage of the recursion stack for reconstructing the graph. Two parameters are involved in this process which are the distance boundary matrix $\hat{B}$ and the graph G. The matrix $\hat{B}$ is simplified by pruning one or several leaves but ensuring that the new matrix is the distance matrix of the boundary of a new graph. The graph G plays no role in this part of the process.

The base case of the recursion occurs when $\hat{B}$ corresponds with a complete graph which is then assigned to G. In the backtracking process, $\hat{B}$ recuperate its previous state, with the originally pruned leaves and G is actualized by adding those leaves, until the algorithm reaches the last recursive call and then G is the reconstruction we are looking for.

Clearly, the algorithm pruned at least a leaf at each step, and hence the running time in the worst case is $O(n)$. ■

Corollary 29. *Every* 1*-block graph* G *of order* n *with* κ *boundary vertices belongs not only to* $\mathcal{H}(\kappa, n)$*, but also to* $\mathcal{H}(\kappa)$ *and to* $\mathcal{H}(n)$*.*

4. Unicyclic Graphs

In this section, we move from block graphs to unicyclic graphs, i.e., those graphs containing a unique cycle. It is divided into two subsections: one devoted to the procedure for knowing whether a matrix is the distance matrix of a unicyclic graph or not. A similar procedure works for recognizing the distance boundary matrix of a unicyclic graph.

The second one is dedicated to the process of reconstructing a unicyclic graph from its $\partial(G)$-distance matrix which is very similar to the analogous algorithm for 1-blocks. Incidentally, the correctness of the algorithm proves that unicyclic graphs verify Conjecture 12.

4.1. The distance matrix of a unicyclic graph

Let us focus in recognizing whether a matrix is the distance matrix of a unicyclic graph. The procedure for checking is inductive and simple. At each step, one can delete a leaf. When there are no leaves, the resulting matrix should be one of a cycle (see Figure 6).

Theorem 30. *A graph* G *is unicyclic if and only if the above procedure answers in the affirmative.*

Proof. Let D_G be the distance matrix of a graph G. Then, a row and a column with a unique one corresponds with a leaf in the graph G, and if we delete that row and column, then the new matrix D' is the distance matrix of the graph G' obtained by deleting that leaf in G (see Figure 6). Hence, if the final matrix of the above procedure is the distance matrix of a cycle, then it only remains to rebuild the graph to obtain a unicyclic graph. ■

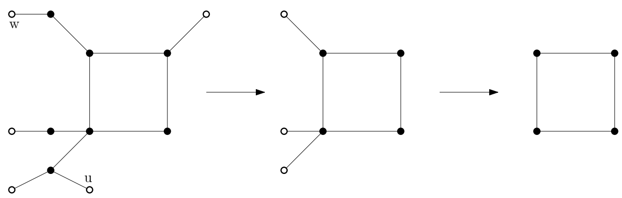


Figure 6. Procedure to recognize the distance boundary matrix of a unicyclic graph G.

It is possible to slightly modify the previous procedure to recognize $\partial(G)$-distance matrices of unicyclic graphs. This algorithm could be recursive or iterative but in any case, we have to reduce the matrix keeping in mind that the new matrix should be again a distance boundary matrix of a graph. In order to do that, it is only necessary to delete the leaves in a certain order. Thus, we will pick a leaf with maximum eccentricity. If that leaf has no siblings (case of the vertex w in Figure 6), we delete it and substitute in the matrix for its parent which undoubtedly is a boundary vertex of the reduced graph. If the vertex is part of a bunch of siblings, then all of them are deleted and changed by its common parent (vertex u in Figure 6).

It only remains a point that need to be clarify. Whereas in the distance matrix recognizing a leaf consists of determining a row or column with a unique one, in the $\partial(G)$-distance matrix, we need a different criterion for recognizing leaves which is given by the next result.

Lemma 31. *Let G be a unicyclic graph with $g \geq 3$. Given the matrix $\hat{D}_G$, it is possible to distinguish the vertices in $\mathcal{L}(G)$ from the ones in $\mathcal{U}(G)$.*

Proof. Take a vertex $u \in \partial(G)$. If $u \in \mathcal{L}(G)$, then for any two distinct vertices $w_1, w_2 \in \partial(G) - u$, $d(w_1,u) + d(u,w_2) - d(w_1,w_2) \geq 2$ (see Figure 7(1)). If $u \in \mathcal{U}(G)$ and $N(u) = \{v_1, v_2\}$, consider the branching trees T_{v_1} and T_{v_2}. For $i = 1,2$, let w_i be either a leaf of T_{v_i} or the vertex v_i if T_{v_i}, if it is trivial.

Clearly, if $g \geq 4$ then $d(w_1,w_2) = d(w_1,u) + d(u,w_2)$ (see Figure 7(3)), meanwhile that if $g = 3$, then $d(w_1,u)+d(u,w_2)-d(w_1,w_2) = 1$ (see Figure 7(2)). ■

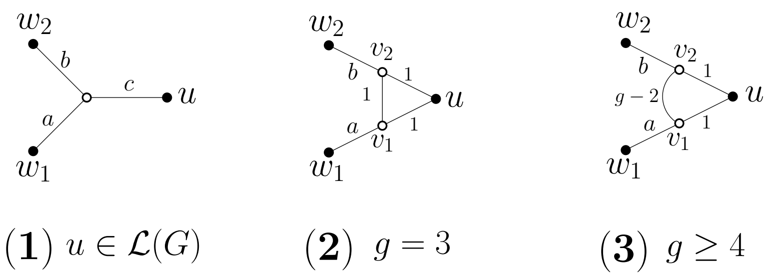


Figure 7. In all cases, $u, w_1, w_2 \in \partial(G)$.

4.2. Reconstructing a unicyclic graph from the boundary distance matrix

In this subsection, the process is described of reconstructing a unicyclic graph G from $\hat{D}_G$, the distance matrix of its boundary. The idea of the algorithm is the same as for 1-blocks: we prune all the leaves in a special order and the remaining graph should be a cycle graph in which we add again the leaves in reverse order.

The algorithm implements Proposition 7, $\partial(G) = \mathcal{L}(G) \cup \mathcal{U}(G)$, and Lemma 31 to keep track of the leaves of the graph.

Algorithm 3 Recognizing-Unicyclic-Recursive

Require: $\hat{D}_G$, the boundary distance matrix of a graph G.
Ensure: Ans=T/F depending on whether G is unicyclic or not.
  Use Lemma 31 to distinguish the leaves in $\hat{D}_G$;
  if $\hat{D}_G$ has no leaves **then**
    return Ans=True or False depending on $\hat{D}_G$ is the distance matrix of a cycle;
  else
    Let v be the leaf with greatest eccentricity;
    if v has no siblings **then**
      Let $\hat{B}$ be the matrix $\hat{D}_G$ in which the row and column that correspond to the vertex v have been deleted and a row and a column are added corresponding with the parent of v;
    else v has siblings $v_1, \ldots, v_k$ being $v = v_0$
      Let $\hat{B}$ the matrix $\hat{D}_G$ in which the row and column that correspond to the vertex v and its siblings have been deleted and a row and a column are added corresponding with the parent of v;
    end if
    Ans=Recognizing-Unicyclic-Recursive $(\hat{B})$;
  end if

The pseudocode description is given in Algorithm 4. Finally, Theorem 32 establishes the correctness and time complexity of Algorithm 4.

Theorem 32. *Beginning with the boundary distance matrix $\hat{D}_G$ of a unicyclic graph G,* Reconstructing-Unicyclic-Recursive $(\hat{D}_G, \emptyset)$ *obtains an isomorphic graph to G in $O(n)$.*

Proof. The algorithm is an evolved version of Algorithm 3 in which we added a second parameter G along with the distance boundary matrix $\hat{B}$. As in the other algorithm, the matrix $\hat{B}$ is simplified by pruning one or several leaves but ensuring that the new matrix is the distance matrix of the boundary of a new graph. The graph G plays no role in this part of the process.

The base case of the recursion occurs when $\hat{B}$ corresponds with a cycle graph which is then assigned to G. In the backtracking process, $\hat{B}$ recuperate its previous state, with the originally pruned leaves and G is actualized by adding those

Algorithm 4 Reconstructing-Unicyclic-Recursive

Require: $(\hat{B}, G)$ where $\hat{B}$ is a boundary distance matrix and G is a graph.
  if $\hat{B}$ corresponds with the distance matrix of a cycle C_g **then**
    return $(\hat{B}, C_g)$
  else
    Use Lemma 31 to distinguish the leaves in $\hat{B}$;
    Let v be the leaf with greatest eccentricity;
    if v has no siblings **then**
      Let $\hat{B}_1$ be the matrix $\hat{B}$ in which the row and column that correspond to the vertex v have been deleted and a row and a column are added corresponding with the parent of v;
      $(\hat{B}_2, G_1)$=Reconstructing-Unicyclic-Recursive $(\hat{B}_1, G)$;
      Add v to G_1;
      return $(\hat{B}, G_1)$;
    else v has siblings $v_1, \ldots, v_k$ being $v = v_0$
      Let $\hat{B}_1$ the matrix $\hat{B}$ in which the row and column that correspond to the vertex v and its siblings have been deleted and a row and a column are added corresponding with the parent of v;
      $(\hat{B}_2, G_1)$=Reconstructing-Unicyclic-Recursive $(\hat{B}_1, G)$;
      Add $v_0, \ldots, v_k$ to G_1;
      return $(\hat{B}, G_1)$;
    end if
  end if

leaves, until the algorithm reaches the last recursive call and then G is the reconstruction we are looking for.

Clearly, the algorithm pruned at least a leaf at each step, and hence the running time in the worst case is $O(n)$. ■

As a consequence, we obtain the uniqueness of the graph beginning with $\hat{D}_G$.

Corollary 33. *Let G be a unicyclic graph on n vertices and κ boundary vertices. Then, G is uniquely determined by $\hat{D}_G$, the boundary distance matrix of G. In other words, unicyclic graphs verify Conjecture* 12.

It is easy to check that, except for the cases with girth between 4 and 7 (see Figure 2, for the cases $g = 4, 5, 6$), every unicyclic graph G of order n with κ boundary vertices belongs not only to $\mathcal{H}(\kappa, n)$, but also to $\mathcal{H}(\kappa)$ and to $\mathcal{H}(n)$.

5. Conclusions and Further Work

In [25], it was firstly implicitly mentioned that a resolving set S of a graph G is strong resolving if and only if the distance matrix $D_{S,V}$ uniquely determines the graph G (see Theorem 10). On the other hand, in [24] it was proved that the boundary $\partial(G)$ of every graph G is a strong resolving set (see Proposition 4).

Mainly having in mind this pair of results, we have presented in Section 2 the following conjecture.

Conjecture 34. *Every graph belongs to $\mathcal{H}(\kappa, n)$.*

In Sections 3 and 4, we have proved that if G is either a block graph or a unicyclic graph, then it belongs to $\mathcal{H}(\kappa, n)$, and we have also provided algorithms to recognize both 1-block and unicyclic graphs.

In addition, in Section 3, we have been able to characterize, for block graphs, both the distance matrix D_G and the boundary distance matrix $\hat{D}_{GT}$ (see Theorems 15, 24 and 26).

We conclude with a list of suggested open problems.

Open Problem 1. Characterizing both the distance matrices and the boundary distance matrices of unicyclic graphs in a similar way as it has been done for trees and for block graphs.

Open Problem 2. Designing an algorithm for reconstructing block graphs, in a similar way as it has been done for trees, 1-block graphs and unicyclic graphs.

Open Problem 3. Checking whether every cactus graph belongs to $\mathcal{H}(\kappa)$, to $\mathcal{H}(\kappa)$, or at least to $\mathcal{H}(\kappa, n)$.

Open Problem 4. Checking whether every split graph belongs to $\mathcal{H}(\kappa)$, to $\mathcal{H}(\kappa)$, or at least to $\mathcal{H}(\kappa, n)$.

Open Problem 5. Checking whether every Ptolemaic graph belongs to $\mathcal{H}(\kappa)$, to $\mathcal{H}(\kappa)$, or at least to $\mathcal{H}(\kappa, n)$.

Open Problem 6. Checking whether every graph of order n with $n-1$ boundary vertices belongs to $\mathcal{H}(\kappa)$, to $\mathcal{H}(\kappa)$, or at least to $\mathcal{H}(\kappa, n)$.

Open Problem 7. Checking whether every graph of diameter 3 belongs to $\mathcal{H}(\kappa, n)$, and characterizing the set of graphs of diameter 3 belonging to $\mathcal{H}(n)$ (respectively, to $\mathcal{H}(\kappa)$).

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