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The difference between the metric dimension and the determining number of a graph

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A B S T R A C T

We study the maximum value of the difference between the metric dimension and the determining number of a graph as a function of its order. We develop a technique that uses functions related to locating-dominating sets to obtain lower and upper bounds on that maximum, and exact computations when restricting to some specific families of graphs. Our approach requires very diverse tools and connections with well-known objects in graph theory; among them: a classical result in graph domination by Ore, a Ramsey-type result by Erdős and Szekeres, a polynomial time algorithm to compute distinguishing sets and determining sets of twin-free graphs, k-dominating sets, and matchings.

1. Introduction and preliminaries

Roughly speaking a *resolving set* is a subset of the vertices of a graph such that all other vertices are uniquely determined by their distances to those vertices. This concept was introduced in the 1970s by Harary and Melter [21], and independently by Slater [31]. Since one obtains a labeling process for all the vertices, resolving sets can be used to store the position of a mobile object in a scenario modeled by a graph, and design effective algorithms to robot navigation. This is not the only area where this type of sets can be used; we refer the reader to [6] and the survey of Bailey and Cameron [2] for more references on applications to coin weighing problems, strategies for Mastermind game, and pattern recognition, among others.

Obviously, in order to design effective algorithms, resolving sets are required to have a cardinality as small as possible but it is also important to consider the following property related to symmetries: the only automorphism of the graph fixing a resolving set is the identity. In general, it is possible to find subsets of vertices with this property (of "destroying" all the automorphisms) and with smaller cardinality than all the resolving sets in the graph; these are cases of *determining sets*, which were introduced in the 1970s by Sims [30] in the context of computational group theory as specific types of *bases*. Much later, Boutin [4] and Erwin and Harary [17] used respectively the terms determining set and *fixing set* to refer to the same concept.

In order to analyze how different resolving sets and determining sets can be, Boutin in [4] asked the following question on the parameters minimizing their cardinalities, which are formally defined below together with resolving sets and determining sets.

Problem 1. Can the difference between the determining number and the metric dimension of a graph be arbitrarily large?

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One of the main contributions of this paper is the technique that we have developed to approach this problem, which has interest by its own, since it combines very diverse tools that go from a classical result by Ore and a Ramsey-type result of Erdős and Szekeres to matchings and the design of a polynomial time algorithm to compute sets with some specific properties. To be more precise, we first provide some definitions and notations.

Let $G = (V(G), E(G))$ be a finite, simple, undirected, and connected graph of order $n = |V(G)|$. As usual, $\overline{G}$ denotes the complement of G. We write $N_G(u)$ and $N_G[u]$, respectively, for the open and the closed neighbourhood of a vertex $u \in V(G)$. The degree of vertex u is denoted by $\delta_G(u)$, and $\delta(G)$ is the minimum degree of G. The subscript G will be dropped from these notations when no confusion may arise.

An *automorphism* of G is a bijective mapping of $V(G)$ onto itself such that $f(u)f(v) \in E(G)$ if and only if $uv \in E(G)$. The *automorphism group* of G is denoted by $\mathrm{Aut}(G)$, and its identity element is id_G. The *stabilizer* of a set $S \subseteq V(G)$ is $\mathrm{Stab}(S) = \{\phi \in \mathrm{Aut}(G) | \phi(u) = u, \forall u \in S\}$, and S is a *determining set* of G if $\mathrm{Stab}(S) = \{id_G\}$. The minimum cardinality of a determining set is the *determining number* of G, written as $\mathrm{Det}(G)$.

The *distance* $d(u, v)$ between two vertices $u, v \in V(G)$ is the length of a shortest u-v path. A vertex $u \in V(G)$ *resolves* a pair $\{x, y\} \subseteq V(G)$ if $d(u, x) \neq d(u, y)$. When every pair of vertices of G is resolved by some vertex in S, it is said that S is a *resolving set* of G. The minimum cardinality of a resolving set is the *metric dimension* of G, denoted by $\dim(G)$, and a resolving set of cardinality $\dim(G)$ is called a *metric basis* of G.

Problem 1 arises naturally since, as it was said before, every resolving set of a graph G is also a determining set, and so $\mathrm{Det}(G) \leqslant \dim(G)$ (see [4,17]). Further, the difference between both parameters is either zero or very small in many families of graphs; among them: paths, cycles, complete graphs, and 2-dimensional grids [17,27]. To approach the question we first define the function $(\dim - \mathrm{Det})(n)$ as the maximum value of $\dim(G) - \mathrm{Det}(G)$ over all graphs G of order n (note that its computation would give the answer to the problem). Then, we develop a technique based mainly on the study of two functions (which are introduced below) related to locating-dominating sets: $(\lambda - \mathrm{Det})(n)$ and $\lambda_{|_{\mathcal{C}^*}}(n)$. Besides its independent interest, this technique lets us improve significantly the best result known to date on Problem 1 which, in terms of our function $(\dim - \mathrm{Det})(n)$, is the following.

Proposition 1.1 [5]. *For every $n \geqslant 8$,*

$$\left\lfloor \frac{2}{5}n \right\rfloor - 2 \leqslant (\dim - \mathrm{Det})(n) \leqslant n - 2.$$

A vertex $u \in V(G)$ *distinguishes* a pair $\{x, y\} \subseteq V(G)$ if either $u \in \{x, y\}$ or precisely one of x, y is adjacent to u, and a set $D \subseteq V(G)$ is a *distinguishing set* of G if every pair of vertices of G is distinguished by some vertex in D. When D is also a *dominating set* (i.e., $N(x) \cap D \neq \emptyset$ for every $x \in V(G) \setminus D$) it is said that D is a *locating-dominating set*. The minimum cardinality of a locating-dominating set is the *locating-domination number* of G, denoted by $\lambda(G)$. Note that $\lambda(G) \leqslant n - 1$ since every subset of $n - 1$ vertices is a locating-dominating set of G.

Although distinguishing sets and locating-dominating sets were introduced in different contexts (see [1,32]) they are in essence the same concept: given a distinguishing set $D \subseteq V(G)$, by definition there is at most one vertex $x \in V(G) \setminus D$ so that $N(x) \cap D = \emptyset$. Thus $D \cup \{x\}$ is a locating-dominating set. This yields the following.

Observation 1.2. Let D be a distinguishing set of a graph G. Then, $\lambda(G) \leqslant |D| + 1$.

Every locating-dominating set $D \subseteq V(G)$ is clearly a resolving set since each pair $\{x, y\} \subseteq V(G) \setminus D$ is distinguished by some vertex $u \in D$ and so either $d(u, x) = 1 < d(u, y)$ or $d(u, y) = 1 < d(u, x)$. Thus, $\mathrm{Det}(G) \leqslant \dim(G) \leqslant \lambda(G)$ for every graph G.

Let $(\lambda - \mathrm{Det})(n)$ and $\lambda(n)$ be the maximum values of, respectively, $\lambda(G) - \mathrm{Det}(G)$ and $\lambda(G)$ over all graphs G of order n. Note that the function $\lambda(n)$ equals $n - 1$ (attained by the complete graph K_n) but the non-trivial restriction of this function to the class $\mathcal{C}^*$ of *twin-free* graphs (i.e., graphs that do not contain *twin* vertices, which are formally defined in SubSection 3.1), denoted by $\lambda_{|_{\mathcal{C}^*}}(n)$, will play an important role throughout the paper. Thus,

$$(\dim - \mathrm{Det})(n) \leqslant (\lambda - \mathrm{Det})(n) \leqslant \lambda(n) = n - 1. \tag{1}$$

In Section 2, we find lower bounds on the functions $(\dim - \mathrm{Det})(n)$ and $(\lambda - \mathrm{Det})(n)$ by constructing appropriate families of graphs. In particular, we improve the lower bound of Proposition 1.1 and conjecture that these new bounds are precisely the exact expressions of those functions.

Section 3 develops a method to prove that $\lambda_{|_{\mathcal{C}^*}}(n)$ is an upper bound on $(\dim - \mathrm{Det})(n)$ and $(\lambda - \mathrm{Det})(n)$, which is a key result in our study. Moreover, we conjecture a formula for the function $\lambda_{|_{\mathcal{C}^*}}(n)$.

Sections 4 and 5 contain two explicit upper bounds on $\lambda_{|_{\mathcal{C}^*}}(n)$. Although the one in Section 5 gives a better approach, we believe that the technique used to obtain the bound in Section 4 has interest by its own and so it is worth to be included in this paper. This technique uses a variant of a classical theorem in domination theory due to Ore [28], which lets us relate, for twin-free graphs, the locating-domination number with a series of classical graph parameters (following the same spirit as the relationships existing among different domination parameters; see [23] for a number of examples). The desired bound is then obtained by using those relations and a Ramsey-type result of Erdős and Szekeres [16].

Our second upper bound on $\lambda_{|_{C^*}}(n)$ appears in Section 5 and is, as far as we know, the best approach to the function $(\dim - \mathrm{Det})(n)$. It is obtained by a greedy algorithm which produces distinguishing sets and determining sets of bounded size. This algorithm also gives an upper bound on the determining number of a twin-free graph.

In Section 6, we obtain exact expressions and bounds on the restrictions of the functions $(\dim - \mathrm{Det})(n)$ and $(\lambda - \mathrm{Det})(n)$ to the family of graphs not containing the cycle C_4 as a subgraph, and the subfamily of trees. To do this, we design tools of independent interest related to k-dominating sets and matchings. Our results on trees close the study initiated by Cáceres et al. [5] on the difference between the metric dimension and the determining number in this class of graphs.

We conclude the paper in Section 7 with some remarks and open problems.

2. Lower bounds on $(\dim - \mathrm{Det})(n)$ and $(\lambda - \mathrm{Det})(n)$

Let T_m with $m \geqslant 6$ be a tree that consists of a path $(u_1, \ldots, u_m)$ and a pendant vertex u_0 adjacent to u_3, and let G_m be the corona product $T_m \circ K_1$, i.e., the graph with vertex set $V(G_m) = V(T_m) \cup \{v_0, v_1, \ldots, v_m\}$ and edge set $E(G_m) = E(T_m) \cup \{u_i v_i | 0 \leqslant i \leqslant m\}$. By adding another pendant vertex $v_{0'}$ to u_0 in G_m we obtain the graph H_m. Both graphs are shown in Fig. 1. By definition, $V(H_m) = V(G_m) \cup \{v'_0\}$ and $E(H_m) = E(G_m) \cup \{u_0 v'_0\}$.

The following lemma is the key tool to obtain lower bounds on the functions $(\dim - \mathrm{Det})(n)$ and $(\lambda - \mathrm{Det})(n)$.

Lemma 2.1. *For every $m \geqslant 6$, the following statements hold.*

(i) $\mathrm{Det}(G_m) = 0$ *and* $\mathrm{Det}(H_m) = 1$.
(ii) $\dim(\overline{G}_m) = m$ *and* $\dim(\overline{H}_m) = m + 1$.
(iii) $\lambda(G_m) = m + 1$ *and* $\lambda(H_m) = m + 2$.

Proof. Since $m \geqslant 6, \mathrm{Aut}(G_m)$ is trivial and there is only one non-trivial automorphism of H_m which maps v_0 onto v'_0. Thus, Statement (i) easily follows.

Every resolving set S of $\overline{G}_m$ contains, for every $0 \leqslant i \leqslant m$ but at most one, either vertex u_i or vertex v_i (note that, in $\overline{G}_m, d(u_j, v_\ell) = d(v_j, v_\ell) = 1$ for all $j \neq \ell$ and so the pair $\{u_j, u_\ell\}$ is only distinguished by vertices u_j, u_ℓ, v_j and v_ℓ). Hence $\dim(\overline{G}_m) \geqslant m$, and the set $S = \{u_0, u_1, \ldots, u_{m-2}, u_m\}$ attains the bound. An analogous argument proves that $S \cup \{v'_0\}$ is a metric basis of $\overline{H}_m$. Therefore, Statement (ii) holds.

To prove Statement (iii), consider a locating-dominating set D of G_m. Clearly, for every $0 \leqslant i \leqslant m$, either vertex u_i or vertex v_i belongs to D. Thus $\lambda(G_m) \geqslant m + 1$, and the set $D = \{u_0, \ldots, u_m\}$ gives the equality. By a similar argument one obtains $\lambda(H_m) = m + 1$. $\square$

Observation 2.2. Since $\mathrm{Aut}(G) = \mathrm{Aut}(\overline{G})$ then $\mathrm{Det}(G) = \mathrm{Det}(\overline{G})$ and so the preceding lemma gives $\mathrm{Det}(\overline{G}_m) = 0$ and $\mathrm{Det}(\overline{H}_m) = 1$.

Cáceres et al. [5] used the wheel graph $W_{1,n}$ to obtain the lower bound of Proposition 1.1. Our graphs $\overline{G}_m$ and $\overline{H}_m$ (for appropriate m) improve that bound, and moreover, we also obtain a lower bound on $(\lambda - \mathrm{Det})(n)$ by using the graphs G_m and H_m.

Theorem 2.3. *For every $n \geqslant 14$,*

$$(\dim - \mathrm{Det})(n) \geqslant \left\lfloor \frac{n}{2} \right\rfloor - 1 \quad \text{and} \quad (\lambda - \mathrm{Det})(n) \geqslant \left\lfloor \frac{n}{2} \right\rfloor.$$

Proof. For each function, it suffices to give a graph of order $n \geqslant 14$ such that the difference between its corresponding parameters equals the bound of the statement. By Lemma 2.1, we can take the graphs $\overline{G}_{\frac{n}{2}-1}$ (n even) and $\overline{H}_{\frac{n-1}{2}-1}$ (n odd) for the function $(\dim - \mathrm{Det})(n)$; the graphs $G_{\frac{n}{2}-1}$ (n even) and $H_{\frac{n-1}{2}-1}$ (n odd) yield the bound for $(\lambda - \mathrm{Det})(n)$. Note that $n \geqslant 14$ since the graphs $G_m, H_m, \overline{G}_m$ and $\overline{H}_m$ are defined for $m \geqslant 6$. $\square$

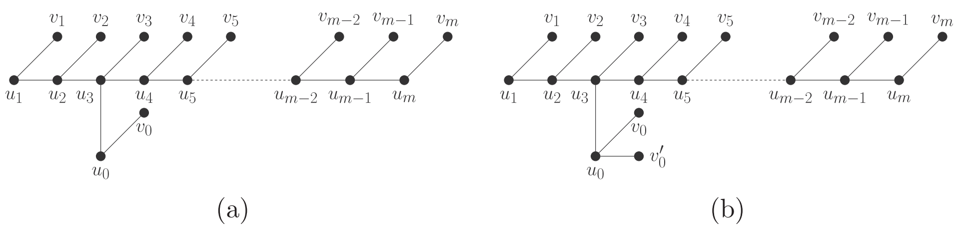

Fig. 1. The graphs (a) G_m and (b) H_m.

We shall exhibit large classes of graphs $\mathcal{C}$ such that the maximum values of, respectively, $\dim(G) - \mathrm{Det}(G)$ and $\lambda(G) - \mathrm{Det}(G)$ over all graphs $G \in \mathcal{C}$ of order n do not exceed $\lfloor \frac{n}{2} \rfloor$. Thus, we believe that the preceding bounds are in fact the exact expressions of our functions.

Conjecture 1. There exists a positive integer n_0 such that, for every $n \geqslant n_0$,

$$(\dim - \mathrm{Det})(n) = \left\lfloor \frac{n}{2} \right\rfloor - 1 \quad \text{and} \quad (\lambda - \mathrm{Det})(n) = \left\lfloor \frac{n}{2} \right\rfloor.$$

3. An upper bound on $(\dim - \mathrm{Det})(n)$ and $(\lambda - \mathrm{Det})(n)$

This section is devoted to the proof of one of our main results: the functions $(\dim - \mathrm{Det})(n)$ and $(\lambda - \mathrm{Det})(n)$ are bounded above by $\lambda_{|_{\mathcal{C}^*}}(n)$. The main idea of this proof is that from every graph G one can obtain an adequate twin-free graph $\widetilde{G}$ such that $\lambda(G)$ is bounded above by $\lambda(\widetilde{G})$ plus some constant depending on the graphs.

3.1. The twin graph G^* and the graph $\widetilde{G}$

The construction of our twin-free graph $\widetilde{G}$ is based on the so called *twin graph* G^*, which is obtained from a given graph G by identifying vertices with the same neighbourhood. This graph and its variations (depending on the choice of closed and/or open neighbourhoods) have been used to solve many problems in graph theory (see for instance [22,29]) since they completely characterize the original graph G. We begin by recalling its formal definition.

Two different vertices $u, v \in V(G)$ are *twins* if $N(u) = N(v)$ or $N[u] = N[v]$, i.e., no vertex of $V(G) \setminus \{u, v\}$ distinguishes the pair $\{u, v\}$. This definition induces the following equivalence relation on $V(G) : u \equiv v$ if and only if either $u = v$ or u and v are twins; see [26]. Let $u^* = \{v \in V(G) | u \equiv v\}$ and consider the partition $u_1^*, \ldots, u_r^*$ of $V(G)$ induced by the relation $\equiv$, where $r \geqslant 1$ and every u_i is a representative of u_i^*. The *twin graph* of G, denoted by G^*, has vertex set $V(G^*) = \{u_1^*, \ldots, u_r^*\}$ and edge set $E(G^*) = \{u_i^* u_j^* | u_i u_j \in E(G)\}$ (which is well-defined as Statement (i) of Lemma 3.1 below shows). Note that, for every $u \in V(G)$, we shall consider u^* as a class in $V(G)$ as well as a vertex of G^* (see the graphs G and G^* in Fig. 2 for an example).

Lemma 3.1 [26]. *For every graph G, the following statements hold.*

(i) *The graph G^* is independent of the choice of the representatives u_i, i.e.,*

$u_i^* u_j^* \in E(G^*) \iff xy \in E(G) \forall x \in u_i^*, y \in u_j^*$.

(ii) *Every class u_i^* either induces a complete subgraph or is an independent set in G.*

A vertex $u_i^* \in V(G^*)$ is said to be of *type* (1) if $|u_i^*| = 1$; otherwise, according to Statement (ii) of Lemma 3.1, vertex u_i^* is either of *type* (K) or of type (N), depending on whether u_i^* induces a complete subgraph or is an independent set in G. When u_i^* is of type (K) or (N), it is said to be of *type* (KN). Considering vertex u_i^* as a class in $V(G)$ and $x, y \in u_i^*$, one has that $N[x] = N[y]$ whenever u_i^* is of type (K), and $N(x) = N(y)$ if u_i^* is of type (N) (see the graph G^* in Fig. 2). For more properties of G^* we refer the reader to [26].

Let $\widetilde{G}$ be the graph obtained from G^* by adding a pendant vertex to every vertex $u_i^* \in V(G^*)$ of type (KN) that has a twin in G^* (note that G^* is not necessarily twin-free). Let $V(\widetilde{G}) = V(G^*) \cup \mathcal{P}$ where $\mathcal{P}$ denotes the set of pendant vertices adjacent to the u_i^*'s. Fig. 2 shows an example of this construction. Observe that now the notation u^* represents a class in $V(G)$, a vertex of G^*, and a vertex of $\widetilde{G}$.

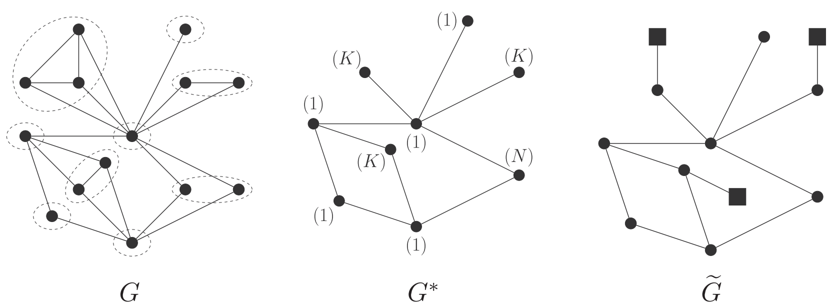

Fig. 2. The dotted ellipses in G indicate the different classes in $V(G)$. Informally, the vertices of G^* are obtained by replacing each class in $V(G)$ by one vertex; the labels indicate the type of vertex. The squared vertices in $\widetilde{G}$ form the set $\mathcal{P}$.

3.2. Using locating-dominating sets of twin-free graphs

In this section, we obtain the desired upper bound on the functions $(\dim - \mathrm{Det})(n)$ and $(\lambda - \mathrm{Det})(n)$ by using the locating-domination number of our graph $\widetilde{G}$, which is proved to be twin-free in Lemma 3.4 below. Twin-free graphs are important for their own sake and also for their multiple applications (see for example [7,22]); here, their properties are fundamental for reaching Theorem 3.7 which is one of our main results. We begin with an observation and a series of lemmas.

Observation 3.2. For every graph G, no two different vertices $u_i^*, u_j^* \in V(G^*)$ of type (1) are twins in G^*; otherwise, by construction of G^*, u_i and u_j would be twins in G but $u_i^* \neq u_j^*$.

Let $\Omega_G = \bigcup_{1 \leqslant i \leqslant r}(u_i^* \setminus \{u_i\})$ where $r = |V(G^*)|$. This set consists of all but one vertex of every class of type (KN) since $u_i^* \setminus \{u_i\}$ is empty for classes u_i^* of type (1). Thus $|\Omega_G| = n - r$ and moreover, by definition of equivalence classes, no two vertices of $V(G) \setminus \Omega_G$ are twins in G.

Lemma 3.3. *Let G be a graph of order n such that G^* has order r. Then,*

$$\mathrm{Det}(G) \geqslant n - r.$$

In particular, $\lambda(G) - \mathrm{Det}(G) \leqslant r - 1$.

Proof. Given a class u_i^* of type (KN) in $V(G)$ and $x, y \in u_i^*$, there is a non-trivial automorphism which maps x onto y and fixes the remaining vertices. Hence, every determining set S of G contains either vertex x or vertex y. Thus, one can deduce that S contains all but one vertex of each class of type (KN), i.e., $|\Omega_G| = n - r$ vertices. Therefore $\mathrm{Det}(G) \geqslant n - r$, and combining this with $\lambda(G) \leqslant n - 1$ yields $\lambda(G) - \mathrm{Det}(G) \leqslant r - 1$. $\square$

Lemma 3.4. *Let G be a graph of order n such that G^* is not isomorphic to K_2. Then, the graph $\widetilde{G}$ has order $\widetilde{n} \leqslant n$ and is twin-free.*

Proof. When obtaining G^* from G, we "lose" at least one vertex per each class of type (KN). Further, to construct $\widetilde{G}$ from G^* we only have to add the set $\mathcal{P}$ whose cardinality is at most the number of vertices of type (KN). Hence, $\widetilde{n} \leqslant n$.

Suppose now on the contrary that $\widetilde{G}$ has a pair of twin vertices. Since by construction each vertex in $\mathcal{P}$ has a single distinct neighbour in $V(G^*)$, those twin vertices are not both contained in $\mathcal{P}$. If both belong to $V(G^*)$, one can easily check that they are also twins in G^* and, by Observation 3.2, at least one of them is of type (KN). Thus, they are distinguished in $\widetilde{G}$ by the corresponding pendant vertex of $\mathcal{P}$; a contradiction. Suppose now that just one of the twin vertices is in $V(G^*)$; let $u_i^* \in V(G^*)$ (for some $1 \leqslant i \leqslant r$) and $v \in \mathcal{P}$ be those twin vertices.

Let $N_{\widetilde{G}}(v) = \{u_j^*\}$ where $u_j^* \in V(G^*)$. If $N_{\widetilde{G}}[u_i^*] = N_{\widetilde{G}}[v] = \{v, u_j^*\}$ then $u_i^* = u_j^*$ and $\widetilde{G} \cong K_2$. Moreover, since $v \in \mathcal{P}$ we have $G^* \cong K_1$ but then $\widetilde{G}$ would also be isomorphic to K_1; a contradiction. Hence, $N_{\widetilde{G}}(u_i^*) = N_{\widetilde{G}}(v) = \{u_j^*\}$ and $u_i^* \neq u_j^*$. Note that $N_{G^*}(u_i^*) = N_{\widetilde{G}}(u_i^*) = \{u_j^*\}$. Further, by construction of $\widetilde{G}$, vertex u_j^* has a twin u_ℓ^* in G^* which cannot be vertex u_i^* (otherwise u_i^* and u_j^* would be twins in G^* and so G^* would be isomorphic to K_2). This implies that $u_\ell^* \in N_{G^*}(u_i^*) = \{u_j^*\}$, which leads to a contradiction. $\square$

We now relate the locating-domination numbers of the graph G and its associated twin-free graph $\widetilde{G}$.

Lemma 3.5. *Let G be a graph of order n such that G^* has order r. Then,*

$$\lambda(G) \leqslant \lambda(\widetilde{G}) + n - r.$$

In particular, $\lambda(G) - \mathrm{Det}(G) \leqslant \lambda(\widetilde{G})$.

Proof. Let $\widetilde{S}$ be a minimum locating-dominating set of $\widetilde{G}$, and let $\widetilde{u} \in V(\widetilde{G}) = V(G^*) \cup \mathcal{P}$. If $\widetilde{u} \in V(G^*)$ then there exists a unique vertex $u_i^* \in V(G^*)$ such that $\widetilde{u} = u_i^*$, and if $\widetilde{u} \in \mathcal{P}$ then there is a unique vertex $u_i^* \in V(G^*)$ so that $N_{\widetilde{G}}(\widetilde{u}) = \{u_i^*\}$. For each case, consider the representative $u_i \in V(G)$ of that class u_i^*, and the mapping $\pi : V(\widetilde{G}) \longrightarrow V(G)$ given by $\pi(\widetilde{u}) = u_i$.

Clearly, the set $\pi(\widetilde{S}) = \{\pi(\widetilde{u}) | \widetilde{u} \in \widetilde{S}\}$ satisfies that $|\pi(\widetilde{S})| \leqslant |\widetilde{S}| = \lambda(\widetilde{G})$ (it might be $\pi(\widetilde{u}) = \pi(\widetilde{v})$ for $\widetilde{u} \in \mathcal{P}$ and $\widetilde{v} \in N_{\widetilde{G}}(\widetilde{u})$). Thus, to obtain the desired bound it suffices to prove that $S = \pi(\widetilde{S}) \cup \Omega_G$ is a locating-dominating set of G (recall that $\Omega_G = \bigcup_{1 \leqslant i \leqslant r}(u_i^* \setminus \{u_i\})$ and so $|\Omega_G| = n - r$). We next show that S is a distinguishing set of G; a similar analysis (omitted for the sake of brevity) proves that S is also a dominating set.

Observe first that $(\pi(\widetilde{u}))^* \subseteq S$ for every $\widetilde{u} \in \widetilde{S}$. Now, let $x, y \in V(G) \setminus S$. Since $x, y \notin \Omega_G$ then $x^* \neq y^*$ and thus $x^*, y^* \in V(G^*) \subseteq V(\widetilde{G})$. Hence, there is a vertex $\widetilde{u} \in \widetilde{S}$ distinguishing $\{x^*, y^*\}$ in $\widetilde{G}$, and such that $\widetilde{u} \neq x^* \neq y^*$ (if, say, $\widetilde{u} = x^*$ then $x^* = (\pi(\widetilde{u}))^* \subseteq S$ but $x \notin S$).

We have $\widetilde{u} \in V(G^*)$ since if $\widetilde{u} \in \mathcal{P}$ then one can assume, without loss of generality, that $N_{\widetilde{G}}(\widetilde{u}) = \{x^*\}$ and so $(\pi(\widetilde{u}))^* = x^* \subseteq S$ which contradicts $x \notin S$. Therefore, $\widetilde{u}$ is distinguishing $\{x^*, y^*\}$ in G^*. If $x^* \in N_{G^*}(\widetilde{u})$ and $y^* \notin N_{G^*}(\widetilde{u})$ then, by Lemma 3.1, $x \in N_G(\pi(\widetilde{u}))$ and $y \notin N_G(\pi(\widetilde{u}))$ (the opposite case is similar). This implies that S is a distinguishing set of G.

Finally, by Lemma 3.3, $\mathrm{Det}(G) \geqslant n - r$ and so $\lambda(G) - \mathrm{Det}(G) \leqslant \lambda(\widetilde{G})$. $\square$

Let $(\dim - \mathrm{Det})_{|_\mathcal{C}}(n), (\lambda - \mathrm{Det})_{|_\mathcal{C}}(n)$ and $\lambda_{|_\mathcal{C}}(n)$ denote the restrictions of our functions to a class of graphs $\mathcal{C}$. Recall that $\mathcal{C}^*$ is the class of twin-free graphs, and note that for that class, the functions can be considered for $n \geqslant 4$ since P_4 is the smallest twin-free graph.

Lemma 3.6. $\lambda_{|_{\mathcal{C}^*}}(n) \leqslant \lambda_{|_{\mathcal{C}^*}}(n+1)$.

Proof. We first prove that $\lambda(G) \leqslant \lambda(H)$ for every graph H obtained by adding a pendant edge to a given graph G. Indeed, consider a minimum locating-dominating set S of H, and let $uv \in E(H)$ denote the pendant edge with $u \in V(H) \setminus V(G)$. If $u \notin S$ then $S \subseteq V(G)$ is also a locating-dominating set of G, and so $\lambda(G) \leqslant \lambda(H)$. Otherwise $u \in S$, and $S' = (S \setminus \{u\}) \cup \{v\}$ is a locating-dominating set of G. Therefore, $\lambda(G) \leqslant |S'| \leqslant |S| = \lambda(H)$.

Consider now a twin-free graph G of order n such that $\lambda(G) = \lambda_{|_{\mathcal{C}^*}}(n)$. Set H to be the graph obtained from G by adding a pendant vertex u to a vertex $v \in V(G)$ whose neighbours in G have degree at least 2. Note that to find such a vertex is possible since G is not the disjoint union of copies of K_1 or K_2, which is neither connected nor twin-free. Hence, H has order $n+1$ and is twin-free. Moreover, $\lambda(G) \leqslant \lambda(H)$ since H is obtained by adding a pendant edge to G. Therefore, $\lambda_{|_{\mathcal{C}^*}}(n) \leqslant \lambda_{|_{\mathcal{C}^*}}(n+1)$. $\square$

We thus reach the main result of this section which, in particular, improves significantly Expression (1) in Section 1.

Theorem 3.7. *For every* $n \geqslant 4$,

$$(\dim - \mathrm{Det})(n) \leqslant (\lambda - \mathrm{Det})(n) \leqslant \lambda_{|_{\mathcal{C}^*}}(n).$$

Proof. Let G be a graph of order n such that $\lambda(G) - \mathrm{Det}(G) = (\lambda - \mathrm{Det})(n)$. Observe first that $G^* \ncong K_2$; otherwise, by Lemma 3.3, $(\lambda - \mathrm{Det})(n) = \lambda(G) - \mathrm{Det}(G) \leqslant 1 < \lfloor \frac{n}{2} \rfloor$ which contradicts Theorem 2.3. Thus, by Lemma 3.4, the graph $\widetilde{G}$ is twin-free and $\widetilde{n} = |V(\widetilde{G})| \leqslant n$. Hence,

$$\lambda(\widetilde{G}) \leqslant \lambda_{|_{\mathcal{C}^*}}(\widetilde{n}) \leqslant \lambda_{|_{\mathcal{C}^*}}(n), \tag{2}$$

the last inequality being a consequence of Lemma 3.6. Further, Lemma 3.5 yields

$$(\lambda - \mathrm{Det})(n) = \lambda(G) - \mathrm{Det}(G) \leqslant \lambda(\widetilde{G}). \tag{3}$$

The result follows combining Expressions (2) and (3). $\square$

Theorems 2.3 and 3.7 give $\lambda_{|_{\mathcal{C}^*}}(n) \geqslant \lfloor \frac{n}{2} \rfloor$ and, throughout this paper, we shall find numerous conditions for a twin-free graph to satisfy $\lambda(G) \leqslant \lfloor \frac{n}{2} \rfloor$. Thus, we believe that the following conjecture, which implies most of Conjecture 1, is true.

Conjecture 2. There exists a positive integer n_1 such that, for every $n \geqslant n_1$,

$$\lambda_{|_{\mathcal{C}^*}}(n) = \left\lfloor \frac{n}{2} \right\rfloor.$$

Theorem 3.7 implies that bounding the function $\lambda_{|_{\mathcal{C}^*}}(n)$ yields bounds on $(\dim - \mathrm{Det})(n)$ and $(\lambda - \mathrm{Det})(n)$. Thus, the following two sections are mainly concerned with the locating-domination number of twin-free graphs.

4. From minimal dominating sets to locating-dominating sets

In this section we present a variant of one of the first results in the field of domination theory due to Ore [28] (see [23] for an extensive bibliography on this very active area of graph theory) which lets us relate the locating-domination number of a twin-free graph G with the upper domination numbers and chromatic numbers of G and $\overline{G}$, and the independence number and clique number of G. On the one hand, these relations produce sufficient conditions for G to verify $\lambda(G) \geqslant \lfloor \frac{n}{2} \rfloor$, giving thus support to Conjecture 2. On the other hand, by means of the last-mentioned relation and a classical result due to Erdős and Szekeres [16], we reach our first upper bound on the function $\lambda_{|_{\mathcal{C}^*}}(n)$.

A set $D \subseteq V(G)$ is a *minimal dominating set* if no proper subset of D is a dominating set of G; *minimal locating-dominating sets* are defined analogously. The *domination number* $\gamma(G)$ is the minimum cardinality of a dominating set of G.

Theorem 4.1 [28]. *A set $D \subseteq V(G)$ is a minimal dominating set if and only if each vertex $u \in D$ satisfies that either $N(u) \subseteq V(G) \setminus D$ or $N(x) \cap D = \{u\}$ for some $x \in V(G) \setminus D$.*

Theorem 4.2 [28]. *Let G be a graph without isolated vertices and let $D \subseteq V(G)$ be a minimal dominating set of G. Then, $V(G) \setminus D$ is a dominating set of G. Consequently, $\gamma(G) \leqslant \lfloor \frac{n}{2} \rfloor$.*

Observe that if one could prove that the complement of every minimal locating-dominating set of a twin-free graph is a locating-dominating set then $\lambda_{|_{\mathcal{C}^*}}(n) \leqslant \lfloor \frac{n}{2} \rfloor$, and by Theorems 2.3 and 3.7, $\lambda_{|_{\mathcal{C}^*}}(n) \geqslant \lfloor \frac{n}{2} \rfloor$. Thus, Conjecture 2 would be proved in the affirmative. Unfortunately, Fig. 3 shows that this property is not true in general for minimal locating-dominating sets of twin-free graphs. However, we can establish a similar relation between minimal dominating sets and locating-dominating sets.

Theorem 4.3. *Let G be a twin-free graph and let $D \subseteq V(G)$ be a minimal dominating set of G. Then, $V(G) \setminus D$ is a locating-dominating set of G.*

Proof. Let D be a minimal dominating set of G. Since G is connected, by Theorem 4.2, it suffices to prove that $V(G) \setminus D$ is a distinguishing set of G. To do this, we show that every pair of vertices $x, y \in D$ is distinguished by some vertex in $V(G) \setminus D$. If $N(x), N(y) \subseteq V(G) \setminus D$ then the result easily follows since G is twin-free. Otherwise, say that $N(x) \cap D \neq \emptyset$. By Theorem 4.1, there is a vertex $u \in V(G) \setminus D$ such that $N(u) \cap D = \{x\}$. Hence, vertex u distinguishes the pair $\{x, y\}$. □

One of the most studied invariants in domination theory is the *upper domination number* $\Gamma(G)$ which is the maximum cardinality of a minimal dominating set of G. We refer the reader to [23] for a number of results involving this parameter.

Corollary 4.4. *Let G be a twin-free graph. Then,*

$$\lambda(G) \leqslant n - \max\{\Gamma(G), \Gamma(\overline{G}) - 1\}.$$

In particular, $\lambda(G) \leqslant \lfloor \frac{n}{2} \rfloor$ when either $\Gamma(G) \geqslant \frac{n}{2}$ or $\Gamma(\overline{G}) \geqslant \frac{n}{2} + 1$.

Proof. By Theorem 4.3, $\lambda(G) \leqslant n - \Gamma(G)$ for every twin-free graph G. Further, Theorem 7 of [25] gives $|\lambda(G) - \lambda(\overline{G})| \leqslant 1$ and so $\lambda(G) \leqslant \lambda(\overline{G}) + 1 \leqslant n - \Gamma(\overline{G}) + 1$ since $\overline{G}$ is also twin-free. Therefore, $\lambda(G) \leqslant \min\{n - \Gamma(G), n - \Gamma(\overline{G}) + 1\}$. □

Recall that the *independence number* $\alpha(G)$ and the *clique number* $\omega(G)$ are the maximum cardinality of an independent set and the maximum order of a complete subgraph of G, respectively.

Corollary 4.5. *Let G be a twin-free graph. Then,*

$$\lambda(G) \leqslant n - \max\{\alpha(G), \omega(G) - 1\}.$$

In particular, $\lambda(G) \leqslant \lfloor \frac{n}{2} \rfloor$ when either $\alpha(G) \geqslant \frac{n}{2}$ or $\omega(G) \geqslant \frac{n}{2} + 1$.

Proof. Every vertex in an independent set I of maximum cardinality $\alpha(G)$ has a neighbour in $V(G) \setminus I$ and so I is a dominating set of G. Moreover, by Theorem 4.1, the dominating set I is minimal since $N(u) \subseteq V(G) \setminus I$ for every $u \in I$. Hence $\alpha(G) \leqslant \Gamma(G)$, and analogously $\Gamma(\overline{G}) \geqslant \alpha(\overline{G}) = \omega(G)$. Combining these inequalities with Corollary 4.4, one obtains the desired bound since G is twin-free and so is $\overline{G}$. □

The *chromatic number* of G, denoted by $\chi(G)$, is the smallest number of classes needed to partition $V(G)$ such that no two adjacent vertices belong to the same class. A classical result in graph theory establishes that $\omega(G) \geqslant 2\chi(G) - n$ for every graph G (see for instance [9]). Thus, $\alpha(G) = \omega(\overline{G}) \geqslant 2\chi(\overline{G}) - n$ and we can deduce the following result from Corollary 4.5.

Corollary 4.6. *Let G be a twin-free graph. Then,*

$$\lambda(G) \leqslant 2n - \max\{2\chi(G), 2\chi(\overline{G}) - 1\}.$$

Consequently, $\lambda(G) \leqslant \lfloor \frac{n}{2} \rfloor$ when either $\chi(G) \geqslant \frac{3}{4}n$ or $\chi(\overline{G}) \geqslant \frac{3}{4}n + \frac{1}{2}$.

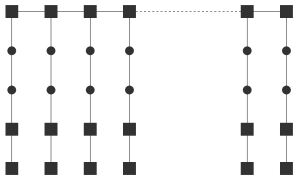

Fig. 3. A twin-free graph of order $5k$ that consists of k paths of length 4, each hanging from a vertex of a path on $k \geqslant 1$ vertices. This graph has a minimal locating-dominating set (depicted as squared vertices) of cardinality $3k$, whose complement is not a locating-dominating set.

Erdős and Szekeres [16] proved that every graph of order n contains either an independent set or a complete subgraph with at least $\lceil \frac{\log_2 n}{2} \rceil$ vertices. This and Corollary 4.5 give our first upper bound on $\lambda_{|_{\mathcal{C}^*}}(n)$ which, by Theorem 3.7, is also a bound on the functions $(\dim - \mathrm{Det})(n)$ and $(\lambda - \mathrm{Det})(n)$.

Corollary 4.7. *For every $n \geqslant 4$,*

$$(\dim - \mathrm{Det})(n) \leqslant (\lambda - \mathrm{Det})(n) \leqslant \lambda_{|_{\mathcal{C}^*}}(n) \leqslant n - \left\lceil \frac{\log_2 n}{2} \right\rceil + 1.$$

Observe that the preceding bound improves significantly the upper bound of Proposition 1.1, due to Cáceres et al. [5].

5. A greedy algorithm to compute distinguishing sets and determining sets of twin-free graphs

Babai [1] introduced distinguishing sets to study the graph isomorphism problem; he proved that deciding whether a graph G of order n is isomorphic to any other graph can be done in $o(n^{d+3})$ time whenever G has a distinguishing set of size d. As a consequence of one of his results, concretely the following lemma, we obtain Observation 5.2 below, which also supports Conjecture 2.

Lemma 5.1 [1]. *Let G be a graph of order n and let M be such that $|N(x)\Delta N(y)| \geqslant M$ for any $x, y \in V(G)$. Then, G has a distinguishing set of cardinality at most $\left\lceil \frac{2n\log n}{M+2} \right\rceil$ provided that $M > 4\log n$.*

Note that the condition of Lemma 5.1 on the symmetric difference $N(x)\Delta N(y)$ implies, in particular, that the graph G is twin-free (as those of Conjecture 2). Further, when $n \geqslant 32$ and $M > 4\log n$, Lemma 5.1 and Observation 1.2 give $\lambda(G) \leqslant \left\lceil \frac{2n\log n}{M+2} \right\rceil + 1 \leqslant \lfloor \frac{n}{2} \rfloor$.

Observation 5.2. A graph G of order $n \geqslant 32$ satisfies that $\lambda(G) \leqslant \lfloor \frac{n}{2} \rfloor$ whenever $|N(x)\Delta N(y)| > 4\log n$ for every $x, y \in V(G)$.

By Procedure Greedy-Partition below, we can also obtain distinguishing sets of bounded size but (unlike in Lemma 5.1) imposing no restriction on the twin-free graph G. This is a polynomial time algorithm that, in addition, produces determining sets of bounded size. Its restriction to a specific family of graphs (concretely twin-free graphs) is natural since Colbourn et al. [13] showed that computing the locating-domination number of an arbitrary graph is NP-hard. We first require some notation.

Given $D \subseteq V(G)$, there is an equivalence relation on $V(G)$ given by $u \sim_D v$ if and only if either $u = v$ or $\{u, v\}$ is distinguished by no vertex of D. Denote by $[u]_D$ the set of vertices $v \in V(G)$ such that $u \sim_D v$. Note that a set D is a distinguishing set of G if the partition of $V(G)$ induced by $\sim_D$ consists of unitary classes. Let D^1 be the set of vertices of $V(G) \setminus D$ whose class is unitary, and let $D^{>1} = V(G) \setminus (D \cup D^1)$. Observe that $D, D^1, D^{>1}$ form a partition of $V(G)$, where any of these sets may be empty.

Procedure: Greedy-Partition

Input: A twin-free graph G.

Output: A partition of $V(G)$ into three subsets A, B, C.

1. Take a vertex $u_0 \in V(G)$. Let $A = \{u_0\}, B = A^1$, and $C = A^{>1}$;
2. **While** there exist $u, x, y \in C$ such that $[x]_A = [y]_A$ and $[x]_{A\cup\{u\}} \neq [y]_{A\cup\{u\}}$ **do**
   (a) Add vertex u to A, and rename $A := A \cup \{u\}$;
   (b) Take $B := A^1$ and $C := A^{>1}$;

The following lemma says that combining the sets A, B, C properly, one obtains, as it was mentioned before, distinguishing sets and determining sets of bounded size.

Lemma 5.3. *Let A, B, C be the sets obtained by application of Procedure Greedy-Partition to a twin-free graph G. Then, the following statements hold.*

(i) *$A \cup B, A \cup C$ and $B \cup C$ are distinguishing sets of G.*
(ii) *A and $B \cup C$ are determining sets of G.*

Proof. To prove Statement (i), observe first that Procedure Greedy-Partition returns a partition of $V(G)$ into three subsets A, B, C such that $B = A^1, C = A^{>1}$ and no pair $\{x, y\} \subseteq C$ with $[x]_A = [y]_A$ is distinguished by any $u \in C \setminus \{x, y\}$ (if it exists).

Since $[x]_{A\cup C} \subseteq [x]_A$ and the class $[x]_A$ is unitary for every $x \in (V(G) \setminus (A \cup C)) = B = A^1$, then the partition of $V(G)$ induced by $\sim_{A\cup C}$ consists of unitary classes. Hence, $A \cup C$ is a distinguishing set of G.

That $A \cup B$ is a distinguishing set follows from the fact that G is twin-free and so, in particular, every pair $\{x, y\} \subseteq (V(G) \setminus (A \cup B)) = C$ is distinguished by some vertex $u \in V(G) \setminus \{x, y\}$. Further, vertex u either belongs to A (if $[x]_A \neq [y]_A$) or belongs to B (if $[x]_A = [y]_A$).

It remains to prove that $B \cup C$ is a distinguishing set. To do this, let $A = \{x_1, \ldots, x_{|A|}\}$ whose elements are ordered as they appear in Procedure Greedy-Partition; we next show that every pair $\{x_i, x_j\}$ with $i < j$ is distinguished by some vertex in $B \cup C$.

Vertex x_j comes from a vertex $u \in C$ that is added to A (at Step 2(a) of Procedure Greedy-Partition) when a class $[x]_{\{x_1,\ldots,x_{j-1}\}} = [y]_{\{x_1,\ldots,x_{j-1}\}}$ (for some $x, y \in C$) can be split into two distinct classes $[x]_{\{x_1,\ldots,x_{j-1},x_j\}}$ and $[y]_{\{x_1,\ldots,x_{j-1},x_j\}}$. Hence, every pair $\{z, t\}$ with $z \in [x]_{\{x_1,\ldots,x_j\}}$ and $t \in [y]_{\{x_1,\ldots,x_j\}}$ is distinguished by x_j and not by $x_1, \ldots, x_{j-1}$. Thus, $\{z, t\}$ is not contained in $\{x_1, \ldots, x_j\}$, and moreover the pair $\{x_i, x_j\}$ with $i < j$ is distinguished by either z or t. In the following steps of the procedure, it might happen that $z = x_\ell$ with $\ell > j$ (analogous for vertex t) and so, at the end of the process, vertex z would not belong to $B \cup C$ but to A. In this case, z can be replaced by another vertex $z' \in B \cup C$ that plays the same role than z. This comes from the fact that when a vertex in C goes to A (at Step 2(a) of the process), the remaining vertices of its class (which has cardinality at least 2) either go to the corresponding set B or stay in the corresponding set C; one of those vertices can be taken as z'. Therefore, at the end of the process, we obtain two sets B, C such that $B \cup C$ is a distinguishing set of G, and so Statement (i) follows.

Observe now that every distinguishing set is a resolving set and so also a determining set. Thus, Statement (i) implies Statement (ii) for $B \cup C$. To prove that A is a determining set of G, it suffices to show that $\mathrm{Stab}(A) = \mathrm{Stab}(A \cup B)$ since one can deduce from Statement (i) that $A \cup B$ is a determining set, i.e., $\mathrm{Stab}(A \cup B) = \{id_G\}$.

By definition, $\mathrm{Stab}(A \cup B) \subseteq \mathrm{Stab}(A)$. Further, given $x \in B = A^1$ there does not exist $y \in B \cup C$ such that $N(y) \cap A = N(x) \cap A$. Hence, an automorphism of G that fixes every vertex in A has to fix vertex x. Therefore, $\mathrm{Stab}(A) \subseteq \mathrm{Stab}(A \cup \{x\})$. Extending this argument to every vertex in B it follows that $\mathrm{Stab}(A) \subseteq \mathrm{Stab}(A \cup B)$. $\square$

5.1. The best approach to $(\dim - \mathrm{Det})(n)$ and an upper bound on $\mathrm{Det}(G)$ for twin-free graphs G

The pigeonhole principle ensures that one set among the A, B, C of Procedure Greedy-Partition has cardinality at least $\lceil \frac{n}{3} \rceil$ and so one of $A \cup B, A \cup C, B \cup C$ has cardinality at most $\lfloor \frac{2}{3} n \rfloor$. Thus, by Statement (i) of Lemma 5.3 and Observation 1.2, we reach our second upper bound on the function $\lambda_{|_{C^*}}(n)$.

Theorem 5.4. *Let G be a twin-free graph of order $n \geqslant 4$. Then, there exists a locating-dominating set of G of cardinality at most $\lfloor \frac{2}{3} n \rfloor + 1$, which can be computed in polynomial time. In particular,*

$$\lambda_{|_{C^*}}(n) \leqslant \left\lfloor \frac{2}{3} n \right\rfloor + 1.$$

The following corollary combines Theorems 2.3, 3.7 and 5.4 providing, as far as we know, the best approach to Problem 1.

Corollary 5.5. *For every $n \geqslant 14$,*

$$\left\lfloor \frac{n}{2} \right\rfloor - 1 \leqslant (\dim - \mathrm{Det})(n) \leqslant (\lambda - \mathrm{Det})(n) \leqslant \lambda_{|_{C^*}}(n) \leqslant \left\lfloor \frac{2}{3} n \right\rfloor + 1.$$

Again, by the pigeonhole principle, it follows that either A or $B \cup C$ has cardinality at most $\lfloor \frac{n}{2} \rfloor$. Hence, by Statement (ii) of Lemma 5.3, we obtain the following.

Theorem 5.6. *Let G be a twin-free graph of order $n \geqslant 4$. Then, there exists a determining set of G of cardinality at most $\lfloor \frac{n}{2} \rfloor$, which can be computed in polynomial time. In particular,*

$$\mathrm{Det}(G) \leqslant \left\lfloor \frac{n}{2} \right\rfloor.$$

We conclude this section with two remarks on the bound of Theorem 5.6. On the one hand, we do not know if that bound is tight although we have already found a tree that has determining number $\lfloor \frac{n}{2} \rfloor - 1$ (see Fig. 4). On the other hand, the bound is explicit; this is important since Gibbons and Laison [20] gave an algorithm that for an arbitrary graph G of order n, returns a determining set of cardinality $O(\mathrm{Det}(G) \log \log n)$.

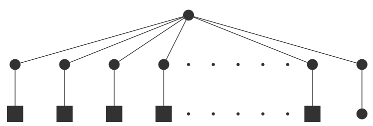

Fig. 4. A tree of order n that consists of $\lfloor \frac{n}{2} \rfloor$ paths of length 2 with a common endpoint. Its determining number is $\lfloor \frac{n}{2} \rfloor - 1$ since the squared vertices form a minimum determining set.

6. Restriction to specific families of graphs

In this section we study the functions $(\dim - \mathrm{Det})(n)$ and $(\lambda - \mathrm{Det})(n)$ restricted to the class $\mathcal{C}_4$ of graphs not containing the cycle C_4 as a subgraph, and also to the subclass $\mathcal{T}$ of trees. Concretely, we compute $(\lambda - \mathrm{Det})_{|_{\mathcal{C}_4}}(n)$, and both functions restricted to $\mathcal{T}$; we also obtain bounds on $(\dim - \mathrm{Det})_{|_{\mathcal{C}_4}}(n)$. The main tool used for our approach is a study relating k-dominating sets and matchings to locating-dominating sets, which contains results of independent interest. Theorem 6.11 below closes the study initiated by Cáceres et al. [5] on the difference between the metric dimension and the determining number of trees.

6.1. Tools: k-domination and matchings

Given a set $D \subseteq V(G)$ and a positive integer k, a vertex $x \in V(G) \setminus D$ is *k-dominated* by D if $|N(x) \cap D| \geqslant k$. The set D is a *k-dominating set* of G if every vertex in $V(G) \setminus D$ is k-dominated by D. The minimum cardinality of a k-dominating set is the *k-domination number* $\gamma_k(G)$. By definition, $\gamma_1(G) = \gamma(G)$ and $\gamma_k(G) \leqslant \gamma_{k'}(G)$ for every $k \leqslant k'$.

The concept of k-dominating set was introduced by Fink and Jacobson [19] as a natural generalization of dominating sets, and has since been intensively studied (see [10] for references on this type of domination). In particular, the k-domination number $\gamma_k(G)$ has been related to many graph parameters; among them, the path covering number [14], the order and the minimum degree [18], and the j-dependence number [19]. Here, we prove that $\lambda(G) \leqslant \gamma_k(G)$ for $k \geqslant 2$ and G in the class $\mathcal{K}_{2,k}$ of graphs not containing the complete bipartite graph $K_{2,k}$ as a subgraph. Observe that, by definition, $\gamma_1(G) = \gamma(G) \leqslant \lambda(G)$ for every graph G.

Lemma 6.1. *Let $G \in \mathcal{K}_{2,k}$ with $k \geqslant 2, D \subseteq V(G)$, and $x \in V(G) \setminus D$. If vertex x is k-dominated by D then for all $y \in V(G) \setminus D$, the pair $\{x, y\}$ is distinguished by some vertex in D.*

Proof. Let $y \in V(G) \setminus D$ and $A \subseteq N(x) \cap D$ such that $|A| = k$. Clearly, some vertex in A distinguishes $\{x, y\}$; otherwise $A \subseteq N(y)$ and so the induced subgraph by $A \cup \{x, y\}$ would contain a copy of $K_{2,k}$. $\square$

As a consequence of Lemma 6.1, if $G \in \mathcal{K}_{2,k}$ then every k-dominating set of G is a locating-dominating set and so $\lambda(G) \leqslant \gamma_k(G)$ for $k \geqslant 2$; Fig. 5 shows that the converse is not true. Further, as it was mentioned before, $\gamma(G) \leqslant \lambda(G)$, and it is proved in [11] that $\gamma_k(G) \leqslant \frac{k}{k+1} n$ for every graph G such that $k \leqslant \delta(G)$. Thus, we obtain the following.

Proposition 6.2. *For every $G \in \mathcal{K}_{2,k}$ with $k \geqslant 2$ it holds that*

$$\gamma(G) \leqslant \lambda(G) \leqslant \gamma_k(G).$$

In particular, $\lambda(G) \leqslant \lfloor \frac{k}{k+1} n \rfloor$ whenever $k \leqslant \delta(G)$.

Our next aim is to relate the locating-domination number $\lambda(G)$ of a twin-free graph $G \in \mathcal{K}_{2,2} = \mathcal{C}_4$ to its *matching number* $\alpha'(G)$, which is the cardinality of a maximum matching in G. Thus, we follow the same spirit of other relationships that have been established between the matching number and domination parameters (see for instance [3,12,24]). We begin with some notation and two lemmas.

Edges of a graph G will now be considered as 2-subsets of $V(G)$ and so we shall write $\{u, v\}$ for an edge, $N(x) \subseteq e \in E(G)$ to indicate that the neighbours of a vertex x are either one or the two endpoints of the edge e, etc. Let M be a matching in G, and let $\overline{M}$ denote the set of vertices of G which are endpoints of no edge in M. By definition, if M is maximum then $\overline{M}$ is an independent set (which may be empty).

Lemma 6.3. *Let M be a maximum matching in a graph G. For every $\{u, v\} \in M$, exactly one of the following statements holds.*

(i) $N(u) \cap \overline{M} = N(v) \cap \overline{M} = \emptyset$.
(ii) *Either* $N(u) \cap \overline{M} \neq \emptyset$ *or* $N(v) \cap \overline{M} \neq \emptyset$, *but not both.*
(iii) $N(u) \cap \overline{M} = N(v) \cap \overline{M} = \{x\}$ *for some* $x \in \overline{M}$.

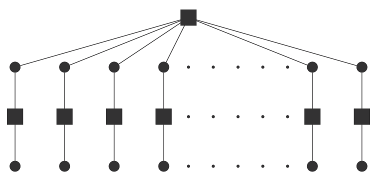

Fig. 5. A tree of order n that consists of $\lfloor \frac{n}{3} \rfloor$ paths of length 3 with a common endpoint. It belongs to the class $\mathcal{K}_{2,2}$, and has a locating-dominating set (illustrated with squared vertices) which is not a 2-dominating set.

Proof. It suffices to prove that there is no edge $\{u, v\} \in M$ and distinct vertices $x, y \in \overline{M}$ such that $x \in N(u)$ and $y \in N(v)$. Indeed, if it would be the case that there exist such an edge $\{u, v\} \in M$ and vertices $x, y \in \overline{M}$, the matching $(M \setminus \{u, v\}) \cup \{\{u, x\}, \{v, y\}\}$ would have more edges than M which is maximum; a contradiction. □

Let $U_M = \{x \in \overline{M} | N(x) \subseteq e \text{ for some } e \in M\}$. When M is a maximum matching, all vertices $x \in \overline{M}$ with $\delta(x) = 1$ belong to the set U_M.

Lemma 6.4. *For every twin-free graph G, there exists a polynomial-time computable maximum matching M in G such that* $U_M = \emptyset$.

Proof. Consider a maximum matching M in G, and its associated set U_M. Observe first that no two distinct vertices $x, y \in U_M$ satisfy that $N(x), N(y) \subseteq e$ for any edge $e \in M$ (otherwise Lemma 6.3 yields $N(x) = N(y)$, which contradicts the fact that G is twin-free). Thus, when M is maximum, two distinct vertices $x, y \in U_M$ have different associated edges $e, f \in M$.

If $U_M \neq \emptyset$ then there exist a vertex $x \in \overline{M}$ and an edge $e = \{u, v\} \in M$ such that $N(x) \subseteq e$. Assume, without loss of generality, that $u \in N(x)$. We next prove that the maximum matching $M' = (M \setminus \{e\}) \cup \{\{u, x\}\}$ verifies that $U_{M'} = U_M \setminus \{x\}$.

Let $y \in U_M \setminus \{x\}$. Since $y \in \overline{M} \setminus \{x\} \subseteq \overline{M'}$ has an associated edge f in M (i.e., $N(y) \subseteq f \in M$) which is not edge e, then $f \in M'$ and so $y \in U_{M'}$. Thus, $U_M \setminus \{x\} \subseteq U_{M'}$. To prove that $U_{M'} \subseteq U_M \setminus \{x\}$, consider a vertex $y \in U_{M'}$ and let $f \in M'$ such that $N(y) \subseteq f$.

Suppose first that $f = \{u, x\}$ and $y \neq v$. Then, $y \notin N(x) \subseteq e$ and so $N(y) = \{u\}$. Further $x \notin N(v)$; otherwise the intersections $N(u) \cap \overline{M}$ and $N(v) \cap \overline{M}$ contradict Lemma 6.3. Hence $N(x) = N(y) = \{u\}$, which is a contradiction since G is twin-free.

Assume now that $f = \{u, x\}$ and $y = v$. Since $N(x) \subseteq e$ and $N(y) \subseteq f$ then either $N(v) = N(x) = \{u\}$ or $N[v] = N[x] = \{u, v, x\}$; again a contradiction. Therefore, $f \in M \setminus \{e\}$ and $y \in U_M \setminus \{x\}$ (note that $y \neq v$ since $e, f \in M$).

We have constructed a maximum matching M' such that $U_{M'} = U_M \setminus \{x\}$. Iterating this process, the result follows. The time complexity comes from the construction of the maximum matching M in G (see [15]) and the above iteration process. □

We now reach the desired relationship between the locating-domination number $\lambda(G)$ and the matching number $\alpha'(G)$ for twin-free graphs $G \in \mathcal{C}_4$.

Proposition 6.5. *Let $G \in \mathcal{C}_4$ be a twin-free graph of order $n \geqslant 4$. Then, there exists a locating-dominating set of G of cardinality $\alpha'(G)$ which can be computed in polynomial time. Consequently,*

$$\lambda(G) \leqslant \alpha'(G).$$

In particular, $\lambda(G) \leqslant \lfloor \frac{n}{2} \rfloor$.

Proof. Let M be a maximum matching in G obtained from Lemma 6.4, i.e., $U_M = \emptyset$. Consider a partition of $V(G)$ into three subsets, the already defined set $\overline{M}$ (recall that this set may be empty), and sets V_1 and V_2 that consist of the endpoints of the edges in M: one endpoint of each edge in V_1 and the other in V_2. We can assume, without loss of generality, that if $x \in \overline{M}$ and $e = \{u, v\} \in M$ such that $N(x) \cap e = \{u\}$ then $u \in V_1$ and $v \in V_2$. Thus, if $e = \{u, v\} \in M$ verifies that $N(u) \cap \overline{M} \neq \emptyset$ and $N(v) \cap \overline{M} = \emptyset$ then $u \in V_1$ and $v \in V_2$ (recall the different possibilities of intersection between $\overline{M}$ and the edges in M given in Lemma 6.3). We now prove that V_1 is a locating-dominating set of G and so the result follows since $|V_1| = \alpha'(G) \leqslant \lfloor \frac{n}{2} \rfloor$.

By construction, V_1 is a dominating set of G. Moreover, every vertex $x \in \overline{M}$ is 2-dominated by V_1 since $U_M = \emptyset$ and so $N(x)$ intersects at least two distinct edges in M; each intersection is one vertex that belongs to V_1.

To prove that V_1 is a distinguishing set, it suffices to show that every pair $\{x, y\} \subseteq V_2 \cup \overline{M}$ is distinguished by some vertex in V_1. If either vertex x or vertex y is in $\overline{M}$ then, by Lemma 6.1, the result follows since $G \in \mathcal{C}_4 = K_{2,2}$ and every vertex of $\overline{M}$ is 2-dominated by V_1. Assume now that $x, y \in V_2$, and let $u, v \in V_1$ such that $\{u, x\}, \{v, y\} \in M$. Since $G \in \mathcal{C}_4$ then either vertex u or vertex v distinguishes $\{x, y\}$; otherwise G would contain the cycle (u, x, v, y). □

6.2. Graphs not containing C_4 as a subgraph

As a consequence of Proposition 6.2 (setting $k = 2$), the function $(\lambda - \text{Det})(n)$ restricted to the set of graphs in $\mathcal{C}_4$ with minimum degree at least 2 can be bounded above by $\lfloor \frac{2}{3} n \rfloor$; essentially the same upper bound on $(\lambda - \text{Det})(n)$ (and so on $(\dim - \text{Det})(n)$) of Corollary 5.5. However, we can improve this bound, and even more: compute the function $(\lambda - \text{Det})_{|_{\mathcal{C}_4}}(n)$ and give better bounds on $(\dim - \text{Det})_{|_{\mathcal{C}_4}}(n)$; these results support Conjecture 1.

Theorem 6.6. *For every $n \geqslant 14$, it holds that*

$$(\lambda - \text{Det})_{|_{\mathcal{C}_4}}(n) = \left\lfloor \frac{n}{2} \right\rfloor.$$

Proof. Mimicking the proof of Theorem 2.3 on $(\lambda - \text{Det})(n)$ yields $(\lambda - \text{Det})_{|_{\mathcal{C}_4}}(n) \geqslant \lfloor \frac{n}{2} \rfloor$ since the graphs considered belong to $\mathcal{C}_4$ (the condition $n \geqslant 14$ comes from the constructions used in that proof). To prove the reverse inequality, it suffices to show that every graph $G \in \mathcal{C}_4$ of order $n \geqslant 14$ satisfies that $\lambda(G) - \text{Det}(G) \leqslant \lfloor \frac{n}{2} \rfloor$.

If the twin graph G^* (defined together with $\widetilde{G}$ in SubSection 3.1) is isomorphic to K_2 then Lemma 3.3 gives $\lambda(G) - \text{Det}(G) \leqslant 1 < \lfloor \frac{n}{2} \rfloor$. Assume now that $G^* \ncong K_2$. By Lemma 3.4, the graph $\widetilde{G}$ is twin-free and has order $\widetilde{n} \leqslant n$. Further, by construction, $\widetilde{G} \in \mathcal{C}_4$ since $G \in \mathcal{C}_4$. Hence, by Proposition 6.5, we have $\lambda(\widetilde{G}) \leqslant \lfloor \frac{\widetilde{n}}{2} \rfloor \leqslant \lfloor \frac{n}{2} \rfloor$ and so Lemma 3.5 gives the desired inequality. □

Theorem 6.7. *For every $n \geqslant 49$, it holds that*

$$\left\lfloor \frac{2}{7} n \right\rfloor \leqslant (\dim - \text{Det})_{|_{\mathcal{C}_4}}(n) \leqslant \left\lfloor \frac{n}{2} \right\rfloor.$$

Proof. The upper bound follows immediately from Expression (1) (in Section 1) and Theorem 6.6. To obtain the lower bound, it suffices to construct a graph G of order $n \geqslant 49$ not containing C_4 as a subgraph, and such that $\dim(G) - \text{Det}(G) = \lfloor \frac{2}{7} n \rfloor$. We next construct not only a graph but a family of graphs satisfying those conditions.

Let $n = 7q + s$ for integers $q \geqslant 7$ and $0 \leqslant s < 7$ (and so $n \geqslant 49$). Let $T_{q,0}$ be the tree shown in Fig. 6(a), which results from attaching a copy of T_6 to every vertex of T_{q-1} (recall that the tree $T_m, m \geqslant 6$, is described in Section 2). Now, for $s \in \{1,2,3\}$ we define $T_{q,s}$ to be the tree obtained from $T_{q,0}$ by replacing the edge u_1u_2 by a path of length $s+1$ (see Fig. 6(b)). Finally, for $s \in \{4,5,6\}$, the tree $T_{q,s}$ results from attaching a path of length s to vertex u_1 in $T_{q,0}$ (see Fig. 6(c)).

Clearly, $\text{Aut}(T_{q,s}) = id_{T_{q,s}}$ and so $\text{Det}(T_{q,s}) = 0$. Further, Fig. 6 shows metric bases for the family of trees $T_{q,s}$ which give

$$\dim(T_{q,s}) = \begin{cases} 2q & \text{if} \quad s \in \{0,1,2,3\}. \\ 2q+1 & \text{if} \quad s \in \{4,5,6\}. \end{cases}$$

Since $|V(T_{q,s})| = n = 7q + s$ then $\dim(T_{q,s}) = \lfloor \frac{2}{7} n \rfloor$. Thus, $\dim(T_{q,s}) - \text{Det}(T_{q,s}) = \lfloor \frac{2}{7} n \rfloor$. □

6.3. Trees

Cáceres et al. [5] constructed a family of trees for which the difference between the metric dimension and the determining number is $O(\sqrt{n})$. Here, we show that the trees $T_{q,s}$ of the proof of Theorem 6.7 attain the maximum value of that difference restricted to trees, thus closing Problem 1 for this class of graphs. We also compute the function $(\lambda - \text{Det})_{|_{\mathcal{T}}}(n)$. First, let us recall some terminology from [8].

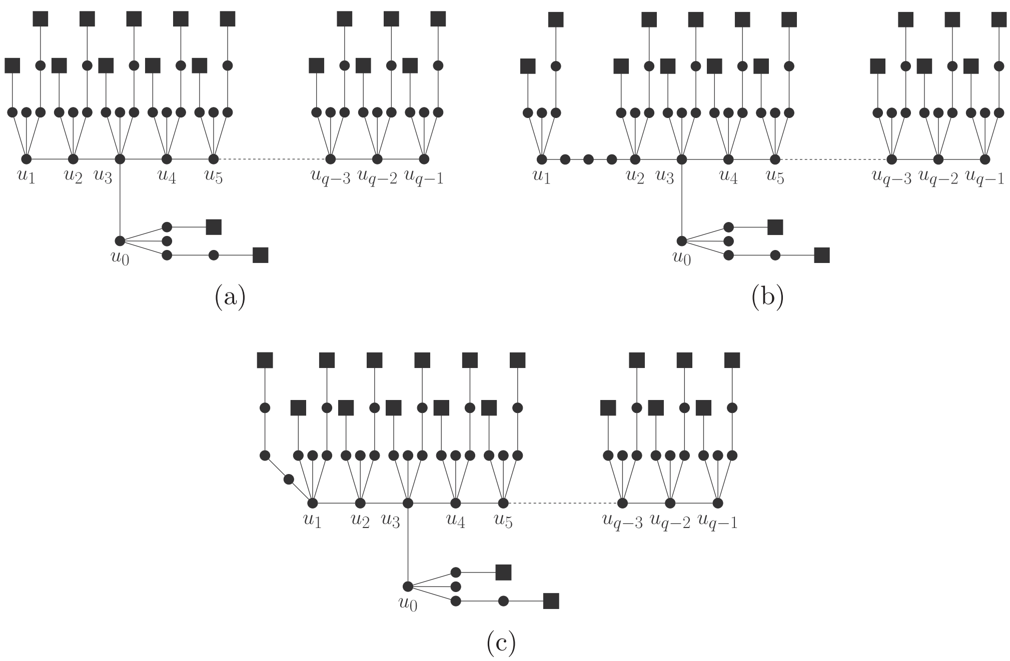

Fig. 6. Metric bases (depicted as squared vertices) of the graphs (a) $T_{q,0}$, (b) $T_{q,3}$ and (c) $T_{q,5}$.

Given a tree T, a vertex of degree at least 3 is called a *major vertex* of T. A pendant vertex v is a *terminal vertex* of a major vertex u if the major vertex closest to v in T is u. The *terminal degree* of a major vertex u, denoted by $\mathrm{ter}(u)$, is the number of terminal vertices of u. A major vertex u is an *exterior major vertex* of T if it has positive terminal degree in T. The set of exterior major vertices of T is denoted by $\mathrm{Ex}(T)$.

The following proposition shows a well-known formula to compute the metric dimension of a tree, that together with the two lemmas below will be used to prove Theorem 6.11, which is one of the main results in this section.

Proposition 6.8 [27]. *If T is a tree that is not a path, then*

$$\dim(T) = \sum_{u \in \mathrm{Ex}(T)} (\mathrm{ter}(u) - 1).$$

Let $\mathrm{ter}'(u)$ be the number of different distances between an exterior mayor vertex u and its terminal vertices. For every $u \in \mathrm{Ex}(T)$, we write n_u for the number of vertices of the simple paths between u and its terminal vertices.

Lemma 6.9. *Let T be a tree and $u \in \mathrm{Ex}(T)$. Then, $\mathrm{ter}'(u) \leqslant \lfloor \frac{2}{7} n_u \rfloor + 1$.*

Proof. Let $d_1, d_2, \ldots, d_{\mathrm{ter}'(u)}$ with $d_1 < d_2 < \ldots < d_{\mathrm{ter}'(u)}$ be the different distances between u and its terminal vertices. One can easily check that

$$n_u \geqslant \left(\sum_{i=1}^{\mathrm{ter}'(u)} d_i \right) + 1 \geqslant \left(\sum_{i=1}^{\mathrm{ter}'(u)} i \right) + 1 = \frac{\mathrm{ter}'(u)(\mathrm{ter}'(u)+1)}{2} + 1.$$

Hence, $\mathrm{ter}'(u) \leqslant \frac{\sqrt{8n_u - 7} - 1}{2} \leqslant \lfloor \frac{2}{7} n_u \rfloor + 1$. □

Lemma 6.10. *Let T be a tree that is not a path. Then,*

$$\mathrm{Det}(T) \geqslant \sum_{u \in \mathrm{Ex}(T)} (\mathrm{ter}(u) - \mathrm{ter}'(u)).$$

Proof. Let S be a minimum determining set of T, which can be assumed to consist of pendant vertices [17]. Consider a vertex $u \in \mathrm{Ex}(T)$ and two of its terminal vertices, say v and v'. If $d(u, v) = d(u, v')$ then either vertex v or vertex v' belongs to S; otherwise there would be an automorphism mapping the u-v shortest path onto the u-v' shortest path, and fixing the remaining vertices of T. Therefore, there are at least $ter(u) - ter'(u)$ terminal vertices of u in S. By extending this argument to all vertices in $\mathrm{Ex}(T)$, we obtain the desired bound. □

We are now ready for computing the function $(\dim - \mathrm{Det})(n)$ restricted to trees.

Theorem 6.11. *For every $n \geqslant 49$, it holds that*

$$(\dim - \mathrm{Det})_{|_{\mathcal{T}}}(n) = \left\lfloor \frac{2}{7} n \right\rfloor.$$

Proof. We first prove that $\dim(T) - \mathrm{Det}(T) \leqslant \lfloor \frac{2}{7} n \rfloor$ for every tree T of order $n \geqslant 49$. We can assume that T is not a path since that difference is zero for all paths with at least 2 vertices. By Proposition 6.8,

$$\begin{aligned} \dim(T) &= \sum_{u \in \mathrm{Ex}(T)} (\mathrm{ter}(u) - 1) \\ &= \sum_{u \in \mathrm{Ex}(T)} (\mathrm{ter}(u) - \mathrm{ter}'(u)) + \sum_{u \in \mathrm{Ex}(T)} (\mathrm{ter}'(u) - 1). \end{aligned}$$

Hence, according to Lemma 6.10, we obtain

$$\dim(T) - \mathrm{Det}(T) \leqslant \sum_{u \in \mathrm{Ex}(T)} (\mathrm{ter}'(u) - 1) \leqslant \left\lfloor \frac{2}{7} n \right\rfloor,$$

the last inequality being a consequence of Lemma 6.9. This shows that $(\dim - \mathrm{Det})_{|_{\mathcal{T}}}(n) \leqslant \lfloor \frac{2}{7} n \rfloor$ and equality is given by the graphs $T_{q,s}$ constructed in the proof of Theorem 6.7, which are trees. □

Since trees do not contain C_4 as a subgraph then, by Theorem 6.6, $(\lambda - \mathrm{Det})_{|_{\mathcal{T}}}(n) \leqslant (\lambda - \mathrm{Det})_{|_{C_4}}(n) = \lfloor \frac{n}{2} \rfloor$. Further, the graphs in the proof of Theorem 2.3 are trees and so we obtain the following.

Theorem 6.12. *For every $n \geqslant 14$, it holds that*

$$(\lambda - \mathrm{Det})_{|_{\mathcal{T}}}(n) = \left\lfloor \frac{n}{2} \right\rfloor.$$

7. Concluding remarks

We have used locating-dominating sets to study the function $(\dim - \mathrm{Det})(n)$, and thus approach Problem 1 posed by Boutin [4]. Our technique involves a study on the functions $(\lambda - \mathrm{Det})(n)$ and $\lambda_{|_{\mathcal{C}^*}}(n)$, for which we require a remarkable number of tools that go from results by Ore, and Erdős and Szekeres to matchings, k-domination, and the design of a polynomial time algorithm to obtain distinguishing sets and determining sets of twin-free graphs. We want to stress that many of the results obtained in this paper and used here as tools, are of independent interest.

Our approach produces a series of lower and upper bounds on the different functions handled in the paper, which for $(\dim - \mathrm{Det})(n)$, improve significantly the best result known to date regarding Problem 1, due to Cáceres et al. [5]. We also note the interesting upper bound on the determining number of a twin-free graph. Further, we study the restriction of our functions to specific families of graphs obtaining, in particular, exact computations for trees. This closes the study initiated by Cáceres et al. [5] on the difference between the metric dimension and the determining number of this family of graphs.

It would be interesting to settle Conjectures 1 and 2, which deal with the exact expressions of our functions. Also, it remains open the computation of $(\dim - \mathrm{Det})_{|_{\mathcal{C}_4}}(n)$. Further, it would be of interest to find specific families of graphs $\mathcal{F}$ where the functions $(\dim - \mathrm{Det})_{|_{\mathcal{F}}}(n)$ and $(\lambda - \mathrm{Det})_{|_{\mathcal{F}}}(n)$ may be computed. Finally, the maximum value of the difference between the locating-domination number and the metric dimension is still unknown and a study on this function may be proposed.

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