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Total Outer-Independent Domination Number: Bounds and Algorithms

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Abstract: In graph theory, the study of domination sets has garnered significant interest due to its applications in network design and analysis. Consider a graph $G(V, E)$; a subset of its vertices is a total dominating set (TDS) if, for each $x \in V(G)$, there exists an edge in $E(G)$ connecting x to at least one vertex within this subset. If the subgraph induced by the vertices outside the TDS has no edges, the set is called a total outer-independent dominating set (TOIDS). The total outer-independent domination number, denoted as $\gamma_t^{oi}(G)$, represents the smallest cardinality of such a set. Deciding if a given graph has a TOIDS with at most r vertices is an NP-complete problem. This study introduces new lower and upper bounds for $\gamma_t^{oi}(G)$ and presents an exact solution approach using integer linear programming (ILP). Additionally, we develop a heuristic and a procedure to efficiently obtain minimal TOIDS.

Keywords: graph theory; total outer-independent dominating set; integer linear program; heuristic algorithm; time complexity



Academic Editor: Massimiliano Caramia

Received: 16 January 2025

Revised: 28 February 2025

Accepted: 6 March 2025

Published: 10 March 2025

Citation: Bosch, P.; Parra Inza, E.; Rios Villamar, I.; Sánchez-Santesteban, J.L. Total Outer-Independent Domination Number: Bounds and Algorithms. *Algorithms* **2025**, *18*, 159. <https://doi.org/10.3390/a18030159>

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1. Introduction

The study of domination problems constitutes a fundamental line of research within graph theory, offering both deep theoretical insights and practical applications. Over recent decades, attention in this field has grown significantly due to its wide range of applications across various scientific disciplines, including social sciences, linear algebra, computational complexity, communication networks, algorithm design, optimization problems, and complex ecosystems (see [1,2]). In this context, several domination parameters have been introduced in previous studies, often involving the combination of multiple parameters [1,3–5]. This paper examines a particular parameter that combines the well-known notions of independence and total domination. Furthermore, we investigate the properties of this parameter from both computational and combinatorial perspectives.

In this paper, we consider simple graphs $G(V, E)$ with size $m = |E(G)|$ and order $n = |V(G)|$, where A is a subset of $V(G)$ and $x \in V(G)$ is a vertex. The subgraph induced by A is represented as $G[A]$. The symbol $N_A(x)$ denotes the set of neighbors of x contained within A , formally defined as $N_A(x) = \{v \in A : (v, x) \in E(G)\}$. Furthermore, $N_A[x]$ represents the closed neighborhood of x within A , defined as $N_A(x) \cup \{x\}$. We also define $\delta_A(x)$ as the cardinality of $N_A(x)$, i.e., $\delta_A(x) = |N_A(x)|$. The degree of x is denoted as

$\delta(x) = \delta_{V(G)}(x) = |N_{V(G)}(x)|$. For ease of notation, we will often use $N(x)$ and $N[x]$ to refer to $N_{V(G)}(x)$ and $N_{V(G)}[x]$, respectively. The *maximum degree* of $G(V, E)$ is defined as $\Delta(G) = \max_{x \in V(G)} \delta(x)$, and the *minimum degree* as $\delta(G) = \min_{x \in V(G)} \delta(x)$. Vertices $x \in V(G)$ are *leaf vertices* if $|N(x)| = 1$, while *support vertices* are any vertices adjacent to leaf vertices. $S(G)$ and $L(G)$ denote the sets of support and leaf vertices, respectively.

A set $I \subset V(G)$ is an independent set of $G(V, E)$ if $G[I]$ is an edgeless graph, and $\alpha(G)$, the independence number, is the size of the largest independent set in $G(V, E)$ [6–8].

A nonempty set T is called a *total dominating set* (TDS) if, for every $x \in V(G)$, there exists an edge $(x, y) \in E(G)$ such that $y \in T$. The *total domination number*, denoted by $\gamma_t(G)$, is the smallest number of elements in any TDS of $G(V, E)$. A TDS containing exactly $\gamma_t(G)$ vertices is referred to as a $\gamma_t(G)$ -set. Since total domination cannot be defined for graphs containing isolated vertices, all graphs considered in this paper are assumed to have no isolated vertices. Please note that by the previous definitions, $2 \leq \gamma_t(G) \leq n$. For additional details on total domination, refer to [3,8–11].

If T is a TDS such that the subgraph induced by $V(G) \setminus T$ forms an independent set, then T is called a *total outer-independent dominating set* (TOIDS). The *total outer-independent domination number*, represented as $\gamma_t^{oi}(G)$, refers to the smallest cardinality of any TOIDS. A TOIDS with cardinality $\gamma_t^{oi}(G)$ is called a $\gamma_t^{oi}(G)$ -set. This concept was first presented in [12] and was briefly studied in [13], where it was referred to as the total co-independent domination number. Please note that by the previous definitions, $\delta(G) \leq \gamma_t^{oi}(G) \leq n - 1$, for $n \geq 3$.

If $H_1, H_2, \dots, H_k$ with $k \geq 2$ are the connected components of a graph $G(V, E)$ with $\delta(G) \geq 1$, then any TOIDS of $G(V, E)$ is the union of TOIDSs from each connected component H_i , for $i = 1, \dots, k$. This is expressed in the following simple result.

Remark 1. Let $H_1, H_2, \dots, H_k$ with $k \geq 2$ be the components of a non-connected graph $G(V, E)$ that has no isolated vertices. Then

$$\gamma_t^{oi}(G) = \sum_{i=1}^k \gamma_t^{oi}(H_i).$$

Aligned with the previous remark, we will henceforth restrict our analysis to TOIDS in nontrivial connected graphs.

The study of TOIDS has gained considerable attention in recent years, owing to their valuable practical applications and extensive theoretical properties [4,12–15]. The objective is to identify a TOIDS with the smallest cardinality, which is an *optimal* total outer-independent dominating set. However, as demonstrated in [4], this problem has been proven to be NP-complete. A problem is considered NP-complete if it is part of the NP class (nondeterministic polynomial time), and every other NP problem can be reduced to it in polynomial time. In simpler terms, an NP-complete problem is as hard as any other problem within NP. If a polynomial-time solution is discovered for any NP-complete problem, then all problems in NP would be solvable in polynomial time. Since no polynomial-time algorithm is currently known for NP-complete problems, research often focuses on approximation algorithms, heuristics, and integer programming formulations to obtain efficient solutions for practical instances.

In [5], a polynomial-time algorithm is proposed to compute $\gamma_t^{oi}(G)$ for trees. In addition, refs. [4,14–16] have presented various upper and lower bounds for the problem. As far as we know, no further results have been reported concerning this issue. In particular, to the best of our knowledge, no exact or approximation algorithms have been previously suggested for the TOIDS problem in general graph classes.

This paper presents new lower and upper bounds for $\gamma_t^{oi}(G)$. We also propose an exact solution approach using an integer linear programming (ILP) formulation alongside

a heuristic method and a purification procedure to reduce the size of the total outer-independent dominating set produced by the heuristic. Additionally, we provide experimental results and computational analyses to assess the performance of both the ILP and heuristic methods across 500 graph instances. Our ILP approach successfully found optimal solutions for graphs with up to 9100 vertices. Specifically, we computed $\gamma_t^{oi}(G)$ for the 500 graph with $50 \leq |V(G)| \leq 9100$, which were randomly generated and can now be used as benchmarks for future research. These $\gamma_t^{oi}(G)$ values and the corresponding instances are publicly available in [17]. Interestingly, in about 28.69% of the cases where the exact algorithm produced an optimal solution, the heuristic also yielded an optimal result. For the remaining instances, the average absolute error was roughly 1.012 vertices, with an average approximation ratio of 1.0032.

In summary, our work contributes to the understanding and advancement of the total outer-independent dominating set problem, offering insights into its structural properties and providing a practical algorithm for its computation. Section 2 explores new upper and lower bounds for $\gamma_t^{oi}(G)$ and establishes relationships with other domination and independence parameters, along with an ILP formulation. Section 3 presents our heuristic, defines several graph families for which it provides an optimal solution, and outlines a purification process. Finally, Section 4 provides a detailed overview of our experimental results.

2. Bounds and Exact Results for $\gamma_t^{oi}(G)$

2.1. Bounds

A subset $S \subseteq V(G)$ is a defensive k -alliance, with $k \in \{-\Delta(G), \dots, \Delta(G)\}$, if $\delta_S(x) \geq \delta_{V(G) \setminus S}(x) + k$ for every $x \in S$. The boundary of $S \subseteq V(G)$ is the set $\partial(S) = N(S) \setminus S$. A subset $S \subseteq V(G)$ is a offensive k -alliance, with $k \in \{2 - \Delta(G), \dots, \Delta(G)\}$, if $\delta_S(x) \geq \delta_{V(G) \setminus S}(x) + k$ for every $x \in \partial(S)$. A global offensive k -alliance is an offensive k -alliance S such that $\partial(S) = V(G) \setminus S$. The global offensive k -alliance number of G , represented by $\gamma_k^o(G)$, is the smallest size of any global offensive k -alliance in the graph G . A subset $S \subseteq V(G)$ is called a powerful k -alliance if it acts as both a defensive k -alliance and an offensive $(k + 2)$ -alliance. The powerful k -alliance number of G , represented by $a_k^p(G)$, is the minimum size of any powerful k -alliance in the graph G . A $a_k^p(G)$ -set is a set S of cardinality $a_k^p(G)$ such that S is a powerful k -alliance of G . Alliances in graphs have been studied extensively by many researchers. Some important results can be found in [6,18–21].

Theorem 1. For any nontrivial graph G of order n ,

$$\gamma_{\delta(G)}^o(G) \leq \gamma_t^{oi}(G) \leq a_{\Delta(G)-2}^p(G).$$

Proof. We now prove the lower bound. Let T be a $\gamma_t^{oi}(G)$ -set. Observe that $N(T) = V(G)$ since T is a TDS. This fact, along with the definition of T , leads to $\partial(T) = N(T) \setminus T = V(G) \setminus T$, which is an independent set in G . It follows that $\delta_T(v) \geq \delta(G) = \delta_{V(G) \setminus T}(v) + \delta(G)$ for every $v \in V(G) \setminus T$. Hence, T is a global offensive $\delta(G)$ -alliance of G . Thus, $\gamma_{\delta(G)}^o(G) \leq |T| = \gamma_t^{oi}(G)$, as desired.

Next, we establish the upper bound. Let S be a $a_{\Delta(G)-2}^p$ -set. Since $\Delta(G) \geq \delta_S(v) \geq \delta_{V(G) \setminus T}(v) + \Delta(G)$ for every $v \in \partial(S)$, we deduce that $\delta_{V(G) \setminus T}(v) = 0$. Hence, $\partial(S)$ is an independent set of G . In addition, since G is a connected graph, we obtain that $V(G) \setminus (S \cup \partial(S)) = \emptyset$. Therefore, $\partial(S) = V(G) \setminus T$ is an independent set. Finally, from the fact that $\delta_S(v) \geq \delta_{V(G) \setminus T}(v) + \Delta(G) - 2$ for any $v \in S$, we deduce that S is a total dominating set of G . Thus, S is a TOIDS of G . Therefore, $a_{\Delta(G)-2}^p(G) \geq \gamma_t^{oi}(G)$. $\square$

The bounds in Theorem 1 are tight. For example, the lower bound is attained in complete graphs and wheel graphs. On the other hand, the upper bound is attained in

complete graphs and graphs belonging to $\mathcal{G}$, where $\mathcal{G}$ is the family of graphs formed as follows. Let $k \geq 2$ be an integer. $G \in \mathcal{G}$ if is formed by a cycle C_{3k} and k vertices adjacent to only three vertices in the cycle C_{3k} .

Theorem 2. For any nontrivial graph G of size m ,

$$\gamma_t^{oi}(G) \geq \max \left\{ \left\lceil \frac{2m + \delta(G)}{2\Delta(G)} \right\rceil, \left\lceil \frac{2m}{2\Delta(G) - 1} \right\rceil \right\}.$$

Proof. Let T be a $\gamma_t^{oi}(G)$ -set. Since $G[V(G) \setminus T]$ is an edgeless graph and T is a TDS of G , we deduce that

$$\begin{aligned} 2m &= \sum_{v \in T} \delta(v) + |E(T, V(G) \setminus T)| \\ &\leq |T|\Delta(G) + |T|(\Delta(G) - 1) \\ &= |T|(2\Delta(G) - 1). \end{aligned}$$

Which implies that $\gamma_t^{oi}(G) = |T| \geq 2m / (2\Delta(G) - 1)$. In addition, we observe that $|T| \geq \delta(G)$. Therefore, $2\Delta(G)|T| \geq 2m + |T| \geq 2m + \delta(G)$. Therefore, $\gamma_t^{oi}(G) = |T| \geq (2m + \delta(G)) / 2\Delta(G)$, as desired. $\square$

The corona product of two graphs G_1 and G_2 , denoted as $G_1 \circ G_2$, is constructed by taking one instance of G_1 and $|V(G_1)|$ replicas of G_2 , and then connecting each vertex in the i^{th} replica of G_2 to the i^{th} vertex of G_1 with an edge [22,23]. The bound in Theorem 2 is attained in the corona product of $C_3 \circ N_k$, where k is a positive integer and N_k is the empty graph of k vertices.

A subset $P \subseteq V(G)$ is called a 2-packing of G if $N[x] \cap N[y] = \emptyset$ for all distinct vertices $x, y \in P$. The 2-packing number of G , represented by $\rho(G)$, is the largest size of any 2-packing in G . A $\rho(G)$ -set is a 2-packing of cardinality $\rho(G)$. This parameter has been studied in [24–26].

Theorem 3. For any nontrivial graph G of order n ,

$$\left\lceil \frac{\delta(G)(n+1)}{\Delta(G) + \delta(G)} \right\rceil \leq \gamma_t^{oi}(G) \leq n - \rho(G).$$

Proof. Let P be a $\rho(G)$ -set such that $|P \cap L(G)|$ is minimum among all $\rho(G)$ -sets. We claim that $V(G) \setminus P$ is a TOIDS. Since P is a packing set of G , we have that P is an independent set. In addition, $|N_G(v) \cap P| \leq 1$ for any $v \in V(G) \setminus P$. Therefore, we only need to prove that $G[V(G) \setminus P]$ has no isolated vertex. Let $v \in V(G) \setminus P$. If $\delta(v) \geq 2$, then we deduce that $|N_G(v) \cap V(G) \setminus P| \geq 1$, as desired. Now suppose that $\delta(v) = 1$. If $N_G(v) \cap P = \{u\}$, then the set $P' = (P \setminus \{u\}) \cup \{v\}$ is a $\rho(G)$ -set such that $|P' \cap L(G)| < |P \cap L(G)|$, a contradiction. Hence, $|N_G(v) \cap V(G) \setminus P| = 1$, as desired. Therefore, $\gamma_t^{oi}(G) \leq |V(G) \setminus P| = n - |P| = n - \rho(G)$.

Next, we establish the upper bound. Observe that

$$\delta(G)(n - |P|) \leq |E(P, V(G) \setminus P)| \leq |P|(\Delta(G) - 1).$$

From this inequality and the fact that $|P| \geq \delta(G)$ we deduce that $|P|(\Delta(G) + \delta(G)) \geq n\delta(G) + |P| \geq n\delta(G) + \delta(G) = \delta(G)(n + 1)$. It follows that $\gamma_t^{oi}(G) = |P| \geq \delta(G)(n + 1) / (\Delta(G) + \delta(G))$. $\square$

The bounds in Theorem 3 are tight. For example, the upper bound is attained in the double-star graphs. In addition, the lower bound is attained in the corona product of $C_3 \circ N_r$, where r is a positive integer and N_r is the empty graph of r vertices.

Proposition 1. Let G be a nontrivial graph of order $n \geq 5$. If G is a triangle-free graph that is different from C_5 , then $\alpha(G) \geq 3$.

Proof. We consider two cases.

Case 1. G is a graph with a connected structure. Suppose that G is a tree. If $|L(G)| = 2$, then $G = P_n$. Hence, $\alpha(G) \geq 3$. If $|L(G)| \geq 3$, then $\alpha(G) \geq |L(G)| \geq 3$, as desired. From now on, suppose that G has a cycle of minimum length $C = c_1c_2 \cdots c_kc_1$. If $k \geq 6$, then $\{v_1, v_3, v_5\}$ is an independent set. Thus, $\alpha(G) \geq 3$. Now, suppose $k \in \{4, 5\}$. Since $n \geq 5$ and $G \neq C_5$, it follows that $V(G) \setminus V(C) \neq \emptyset$. In addition, by minimality of C and since G is triangle-free, there exists $v \notin V(C)$ such that v is adjacent to at most two nonadjacent vertices of $V(C)$. We assume that $N(v) \cap V(C) = \{v_1, v_3\}$ without loss of generality. The set $\{v, v_2, v_4\}$ is an independent set of G . Thus, we obtain that $\alpha(G) \geq 3$, as desired.

Case 2. G is a disconnected graph. If it consists of more than two connected components, then it is evident that $\alpha(G) \geq 3$. Therefore, suppose that G has two connected components, H_1 and H_2 . If $\alpha(H_1) = \alpha(H_2) = 1$, then H_1 and H_2 are complete graphs. Since $n \geq 5$, we deduce that $|V(H_1)| \geq 3$ or $|V(H_2)| \geq 3$. As a consequence, G has a triangle, a contradiction. Hence $\alpha(H_1) \geq 2$ or $\alpha(H_2) \geq 2$, which implies that $\alpha(G) \geq 3$, as desired. $\square$

Consider a graph G with $|V(G)| = n$, and let $\overline{G}$ denote its complement. For every $v \in V(G)$, we denote by v' the vertex corresponding to v in $\overline{G}$. The complementary prism, denote by $G\overline{G}$, is the graph with vertex set $V(G\overline{G}) = V(G) \cup V(\overline{G})$ and edge set $E(G\overline{G}) = E(G) \cup E(\overline{G}) \cup \{vv' : v \in V(G)\}$. Various domination parameters have been analyzed in the context of complementary prisms. For example, in [27–29]. Figure 1 shows a graph G and $G\overline{G}$. The set of black colored vertices describes a $\gamma_t^{oi}(G\overline{G})$ -set.

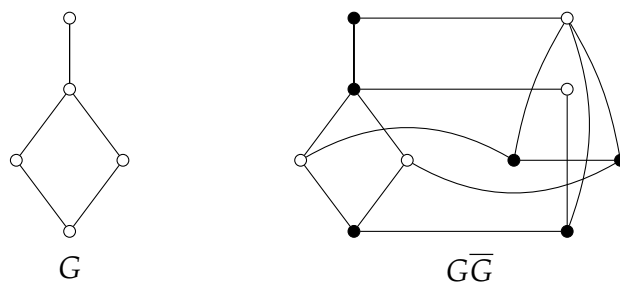


Figure 1. Graph G and $G\overline{G}$.

The following theorem provides the exact value for $\gamma_t^{oi}(G\overline{G})$. For this purpose, we introduce the following family of graphs. For any integer $k \geq 2$, let $\mathcal{F}_k$ denote the family consisting of complete graphs K_k and graphs G of order k in which any two minimum independent sets D_1 and D_2 of G and $\overline{G}$, respectively, satisfy $|D_1 \cap D_2| > 0$. Please note that any two minimum independent sets D_1 and D_2 of G and $\overline{G}$, respectively, satisfy $|D_1 \cap D_2| \leq 1$.

Theorem 4. For any nontrivial graph G with $n \geq 5$,

$$\gamma_t^{oi}(G\overline{G}) = \begin{cases} 2n - \alpha(G) - \alpha(\overline{G}) + 1 & \text{if } G \in \mathcal{F}_n, \\ 2n - \alpha(G) - \alpha(\overline{G}) & \text{otherwise.} \end{cases}$$

Proof. First, observe that $\gamma_t^{oi}(K_n \overline{K_n}) = n = 2n - \alpha(G) - \alpha(\overline{G}) + 1$ and $\gamma_t^{oi}(C_5 \overline{C_5}) = 6 = 2n - \alpha(G) - \alpha(\overline{G})$. Therefore, from now on we suppose that $G \notin \{C_5, \overline{C_5}, K_n, \overline{K_n}\}$. Now, we proceed to prove that

$$\gamma_t^{oi}(G\overline{G}) \geq \begin{cases} 2n - \alpha(G) - \alpha(\overline{G}) + 1 & \text{if } G \in \mathcal{F}_n, \\ 2n - \alpha(G) - \alpha(\overline{G}) & \text{otherwise.} \end{cases}$$

Let D be a $\gamma_t^{oi}(G\overline{G})$ -set and let $D_1 = D \cap V(G)$ and $D_2 = D \cap V(\overline{G})$. Observe that $V(G) \setminus D_1$ and $V(\overline{G}) \setminus D_2$ are independent sets of G and $\overline{G}$, respectively. As a consequence,

$$2n - |D_1| - |D_2| = |V(G) \setminus D_1| + |V(\overline{G}) \setminus D_2| \leq \alpha(G) + \alpha(\overline{G}). \quad (1)$$

Furthermore, if $G \in \mathcal{F}_n$, then $V(G) \setminus D_1$ and $V(\overline{G}) \setminus D_2$ cannot both be independent sets of minimum cardinality of G and $\overline{G}$, respectively. Hence, $|V(G) \setminus D_1| \leq \alpha(G) - 1$ or $|V(\overline{G}) \setminus D_2| \leq \alpha(\overline{G}) - 1$. In any case, we obtain that

$$2n - |D_1| - |D_2| = |V(G) \setminus D_1| + |V(\overline{G}) \setminus D_2| \leq \alpha(G) + \alpha(\overline{G}) - 1. \quad (2)$$

Using Equations (1) and (2), we derive that

$$\gamma_t^{oi}(G\overline{G}) = |D_1| + |D_2| \geq \begin{cases} 2n - \alpha(G) - \alpha(\overline{G}) + 1 & \text{if } G \in \mathcal{F}_n, \\ 2n - \alpha(G) - \alpha(\overline{G}) & \text{otherwise.} \end{cases}$$

Now we proceed to prove that

$$\gamma_t^{oi}(G\overline{G}) \leq \begin{cases} 2n - \alpha(G) - \alpha(\overline{G}) + 1 & \text{if } G \in \mathcal{F}_n, \\ 2n - \alpha(G) - \alpha(\overline{G}) & \text{otherwise.} \end{cases}$$

Let S_1 and S_2 be independent sets of minimum cardinality of G and $\overline{G}$ (respectively) such that $|S_1 \cap S_2|$ is minimum. Let $S'_1 = \{v' \in V(\overline{G}) : v \in S_1\}$ and let $S'_2 = \{v \in V(G) : v' \in S_2\}$. We consider the set

$$S = \begin{cases} (V(G) \setminus S_1) \cup (V(\overline{G}) \setminus S_2) & \text{if } G \notin \mathcal{F}_n, \\ (V(G) \setminus S_1) \cup (V(\overline{G}) \setminus S_2) \cup (S'_1 \cap S'_2) & \text{if } G \in \mathcal{F}_n \text{ and } \alpha(G) = 2, \\ (V(G) \setminus S_1) \cup (V(\overline{G}) \setminus S_2) \cup (S_1 \cap S'_2) & \text{otherwise.} \end{cases}$$

We claim that S is a TOIDS of $G\overline{G}$. Observe that $V(G\overline{G}) \setminus S$ is an independent set of $G\overline{G}$. Therefore, we only need to prove that $G\overline{G}[S]$ has no isolated vertex. Let $v \in S \cap V(G)$. If $v' \notin S_2$, then v is dominated by v' . Now suppose that $v' \in S_2$. If $G \notin \mathcal{F}_n$ or $\alpha(\overline{G}) \geq 3$, then there exists $u' \in S_2$ such that $u' \neq v'$ and $u' \notin S'_1 \cap S'_2$. As a consequence, v is dominated by $u \in V(G) \setminus S_1$. On the other hand, suppose that $G \in \mathcal{F}_n$ and $\alpha(\overline{G}) = 2$. By Proposition 1 we have that $\alpha(G) \geq 3$, which leads to $S = (V(G) \setminus S_1) \cup (V(\overline{G}) \setminus S_2) \cup (S_1 \cap S'_2)$. Hence, there exists $u' \in S_2$ such that $u' \neq v'$. In addition, we observe that $u \in (V(G) \setminus S_1) \cup (S_1 \cap S'_2)$. Thus, v is dominated by u , as desired. Analogously, we deduce that every $v' \in S \cap V(\overline{G})$ is dominated by S . Therefore, S is a TOIDS of $G\overline{G}$, which implies that

$$\gamma_t^{oi}(G\overline{G}) \leq |S| = \begin{cases} 2n - \alpha(G) - \alpha(\overline{G}) + 1 & \text{if } G \in \mathcal{F}_n, \\ 2n - \alpha(G) - \alpha(\overline{G}) & \text{otherwise.} \end{cases}$$

□

A *split graph* is a type of graph in which the vertex set is divided into a maximal clique K and an independent set I [30].

Proposition 2. For any nontrivial connected split graph such that $|K| \geq 3$, the following statements hold.

- (i) I is a maximal independent set of G if and only if $\gamma_t^{oi}(G) = |K|$.
- (ii) I is not a maximal independent set of G if and only if $\gamma_t^{oi}(G) = |K| - 1$.

Proof. First, we observe that K is a TOIDS of G , which implies that $\gamma_t^{oi}(G) \leq |K|$. Let T be a $\gamma_t^{oi}(G)$ -set such that $T \cap K$ is maximum among all $\gamma_t^{oi}(G)$ -sets. If $K \subseteq T$, then $\gamma_t^{oi}(G) = |T| \geq |K|$. If $K \setminus T \neq \emptyset$, then there exists $v \in K \setminus T$. This implies that $(K \setminus \{v\}) \cup N_I(v) \subseteq T$. It follows that

$$|T| \geq |K \setminus \{v\}| + |N_I(v)| = |K| - 1 + |N_I(v)|. \quad (3)$$

Thus,

$$|K| - 1 \leq \gamma_t^{oi}(G) \leq |K| \quad (4)$$

We now move on to proving (i). Suppose that I is a maximal independent set of G . By Equation (4) we only need to prove that $\gamma_t^{oi}(G) \geq |K|$. Since I is a maximal independent set, every $v \in K$ satisfies $|N_I(v)| \geq 1$. This fact together with (3) lead to $\gamma_t^{oi}(G) = |T| \geq |K|$, as desired. Now, suppose that $\gamma_t^{oi}(G) = |K|$. If I is not a maximal independent set of G , then there exists $v \in K$ such that $N_I(v) = \emptyset$. As a consequence, $K \setminus \{v\}$ is a TOIDS of G . It follows that $\gamma_t^{oi}(G) \leq |K| - 1$, a contradiction. Therefore, I is a maximal independent set of G , which completes the proof of (i). Finally, observe that (ii) is a consequence of (i) and Equation (4). $\square$

If we remove the vertices x_1 and x_2 in the graph from Figure 2, then $N_I(u_4) = \emptyset$, and the vertex u_4 can be removed from the $\gamma_t^{oi}(G)$ -set. Then, $\gamma_t^{oi}(G) = |K| - 1$.

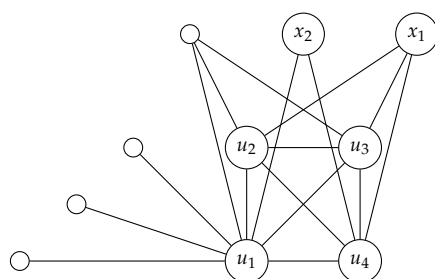


Figure 2. A split graph with $K = \{u_1, u_2, u_3, u_4\}$ and $\gamma_t^{oi}(G) = |K| = 4$.

A set $S \subseteq V(G)$ is an independent dominating set of G if every vertex in $V(G) \setminus S$ has a neighbor in S , and S is an independent set. The independent domination number of G , represented by $i(G)$, is the smallest size of any independent dominating set in G . Detailed information can be found in the survey [31].

Proposition 3. Let G be a nontrivial graph of order n and let S be a $\gamma_t^{oi}(G)$ -set. The following statements hold.

- (i) If $V(G) \setminus S$ is a maximal independent set of G , then $\gamma_t^{oi}(G) \leq n - i(G)$.
- (ii) If $V(G) \setminus S$ is not a maximal independent set of G , then $\gamma_t^{oi}(G) \geq n - \alpha(G) + 1$.

Proof. First, we proceed to prove (i). Suppose that $V(G) \setminus S$ is a maximal independent set. Please note that any vertex of S has a neighbor in $V(G) \setminus S$. Hence, $V(G) \setminus S$ is an independent dominating set of G . Thus, $i(G) \leq |V(G) \setminus S| = n - \gamma_t^{oi}(G)$, as desired.

Now, we proceed to prove (ii). Suppose that $V(G) \setminus S$ is not a maximal independent set of G . Therefore, there exists $v \in S$ such that $N(v) \cap (V(G) \setminus S) = \emptyset$. Hence, $(V(G) \setminus S) \cup \{v\}$ is an independent set of G . Thus, $\alpha(G) \geq |(V(G) \setminus S) \cup \{v\}| = n - \gamma_t^{oi}(G) + 1$, as desired. $\square$

Now, we present the exact results for several well-known graph families, as proposed in [12,13]. These results provide valuable insights into the behavior of $\gamma_t^{oi}(G)$ for specific graph structures. Furthermore, in the next subsection, we propose an ILP formulation to find a $\gamma_t^{oi}(G)$ -set.

Proposition 4. *The following statements hold for any integer $n \geq 3$.*

- (i) $\gamma_t^{oi}(K_n) = n - 1$.
- (ii) $\gamma_t^{oi}(C_n) = \lceil 2n/3 \rceil$.
- (iii) $\gamma_t^{oi}(P_n) = \lfloor 2n/3 \rfloor$.
- (iv) $\gamma_t^{oi}(W_n) = \lfloor n/2 \rfloor + 1$.
- (v) *If r is a positive integer, then $\gamma_t^{oi}(K_{r,n-r}) = \min\{r, n - r\} + 1$.*

These results contribute to a better understanding of the total outer-independent domination number in various graph families, including complete graphs, cycles, paths, and wheel graphs.

2.2. ILP Formulation

In this subsection, we propose the following ILP formulation for the problem we are studying (TOIDS). Consider a graph $G = (V, E)$ with order n , and its adjacency matrix $A = (a_{ij})_{n \times n}$ is given by: $a_{ij} = a_{ji} = 1$ if $(i, j) \in E(G)$, and $a_{ij} = a_{ji} = 0$ in the other case. Given a TOIDS T of cardinality $\gamma_t^{oi}(G)$ and $i \in V(G)$, our decision variables are defined in the following way:

$$x_i = \begin{cases} 1, & \text{if } i \in T \\ 0, & \text{otherwise,} \end{cases} \quad (5)$$

The TOIDS problem can now be expressed as follows:

$$\min \sum_{i=1}^n x_i, \quad (6)$$

$$\text{subject to : } \sum_{j=1}^n a_{ij}x_j \geq 1, \quad \forall i \in V(G), \quad (7)$$

$$\sum_{j=1}^n a_{ij}(1 - x_i) - \sum_{j=1}^n a_{ij}x_j \leq 0, \quad \forall i \in V(G), \quad (8)$$

$$\sum_{i=1}^n x_i \geq L, \quad (9)$$

$$\sum_{i=1}^n x_i \leq U, \quad (10)$$

$$x_i \in \{0, 1\}. \quad (11)$$

We have $2n + 2$ constraints: the n constraints of type (7) ensure that for each $j \in V(G)$, at least one vertex in T is adjacent to j , while the n constraints of type (8) ensure that no vertex in $V(G) \setminus T$ has a neighbor in $V(G) \setminus T$. Please note that in the adjacency matrix A , we define $a_{ii} = 0$ for all i . As a result, when $j = i$, the term $a_{ij} \cdot x_j$ evaluates to zero, ensuring that self-loops do not affect constraints of type (7), i.e., vertices do not dominate themselves. Additionally, constraints (9) and (10) limit the search space (feasible region), ensuring that

the cardinality of the generated solutions is between the lower bound L and the upper bound U . We can use the lower and upper bounds proposed in Section 2 to determine L and U . It should be noted that, in practice, the heuristic proposed in Section 3 provided a better upper bound U than the theoretical bounds for the instances analyzed.

3. Heuristic Algorithm

Now, we present our heuristic for approximating a total outer-independent dominating set. This heuristic is divided into two stages: Stage 1 follows a greedy methodology to find a TOIDS, and Stage 2 consists of a purification procedure that delivers a minimal TOIDS. Stage 1 is further divided into two fundamental parts: the first part constructs a total dominating set, and the second part updates this set to ensure that its complement is independent.

We need a few definitions to describe our heuristic. We denote by T_h the TOIDS formed by the heuristic in iteration h . The dominated set in iteration h is denoted by I_h ; this vertex set is formed by the vertices that have at least one neighbor in T_h . Please note that in the final iteration of Stage 1, the set I_h is an independent set. Finally, A_h denotes the vertex set that has no neighbors in T_h in iteration h , i.e., $N(A_h) \cap T_h = \emptyset$.

In general, our heuristic is a greedy algorithm that runs over several iterations. The iterative process in Stage 1 is guaranteed to converge, as in each iteration, a vertex is selected from I_h and added to T_h , reducing the size of A_h or I_h . Since these sets are subsets of $V(G)$, the number of iterations is at most n , ensuring termination in a finite number of steps. Below, we provide a detailed description of our heuristic.

First, we select two vertices $\{u, v\}$ where u is the vertex with the highest degree in $V(G)$ and v is its neighbor with the highest number of neighbors not dominated by u . Thus, initially $T_0 = \{u, v\}$, $I_0 = (N(u) \cup N(v)) \setminus \{u, v\}$ and $A_0 = V \setminus (T_0 \cup I_0)$. Notice that these are disjoint sets and $A_0 \cup I_0 \cup T_0 = V$.

Remark 2. The sets A_h , I_h and T_h are disjoint and $A_h \cup I_h \cup T_h = V$.

Lemma 1. If $A_0 = \emptyset$ then $N[u] \cup N[v] = V(G)$ and $T_0 = \{u, v\}$ is a minimum total dominating set.

Proof. By Remark 2 and $A_0 = \emptyset$, it follows immediately that $I_0 = V \setminus T_0$. This implies that all vertices in $V(G)$ have a neighbor in T_0 . Please note that by the construction of the algorithm, $(u, v) \in E(G)$. Since $|T_0| = 2$, then T_0 is minimum, a TDS cannot contain fewer than two vertices. $\square$

A direct consequence of the previous lemma is the following observation.

Remark 3. If $A_0 = \emptyset$ and I_0 is an independent set, then $T_0 = \{u, v\}$ is a minimum TOIDS.

The initial sets are updated iteratively at each iteration $h > 0$, resulting in the current sets of vertices T_h , I_h , and A_h , where T_h is the partial total outer-independent dominating set. Each iteration $h > 0$ begins if $A_h \neq \emptyset$ or I_h is not an independent set. In the first iterative part of Stage 1, for each iteration, we choose a vertex $v \in I_{h-1}$ such that $N_{A_{h-1}}[v]$ is as large as possible. Then, we add v to T_h , i.e., $T_h = T_{h-1} \cup \{v\}$. Please note that v is chosen to maximize the number of adjacent vertices among those that do not yet have neighbors in T_{h-1} . At this point, the sets A_h and I_h are updated accordingly.

In the second iterative part of Stage 1, each iteration runs if the set I_{h-1} is not yet an independent set. Thus, we choose a vertex $u \in I_{h-1}$ such that $N_{I_{h-1}}[u]$ is as large as possible, then we add u to T_h , i.e., $T_h = T_{h-1} \cup u$. Please note that u is the vertex that has the most neighbors in I_{h-1} . At this point, the sets A_h and I_h are updated accordingly.

At the end of Stage 1, we obtain a TOIDS of the graph G in T_h . Up to this point, the algorithm may have included redundant vertices in T_h . Therefore, in Stage 2, we proceed to apply a purification procedure that yields a minimal TOIDS of G . The purification procedure is described in Section 3. The pseudo-code for the heuristic is shown as follows (see Algorithm 1).

Algorithm 1 Heuristic TOID

Input: A graph $G(V, E)$.
 Output: A minimal total outer-independent dominating set T^* .
 $h := 0$;
 $u :=$ is the vertex with the maximum degree in $V(G)$;
 $v :=$ is a vertex in $N(u)$ such that $|N(v) \setminus N(u)|$ be maximum;
 $T_0 := \{u, v\}$;
 $I_0 := (N(u) \cup N(v)) \setminus \{u, v\}$;
 $A_0 := V \setminus (T_0 \cup I_0)$;
 {first iterative part of Stage 1}
while $A_h \neq \emptyset$ **do**
 $h := h + 1$;
 $v_h :=$ a vertex $v \in I_{h-1}$ such that $N_{A_{h-1}}[v]$ be maximum;
 $T_h := T_{h-1} \cup \{v_h\}$;
 $I_h = N(T_h) \setminus T_h$;
 $A_h := V(G) \setminus (T_h \cup I_h)$;
end while
 {second iterative part of Stage 1}
while I_h is not an independent set **do**
 $h := h + 1$;
 $u_h :=$ a vertex $u \in I_{h-1}$ such that $N_{I_{h-1}}[u]$ be maximum;
 $T_h := T_{h-1} \cup \{u_h\}$;
 $I_h = I_{h-1} \setminus \{u_h\}$;
end while
 {Stage 2}
 $T^* := \text{Purify}(G, T_h)$;

Theorem 5. Stage 1 of the Heuristic TOID runs in at most $n - 3$ iterations, taking $O(n^3)$ time.

Proof. The total number of iterations in the loops of Stage 1 is bounded by $|A_0| + |I_0| \leq n - 2$. Please note that the bound is reached for the graph K_n and $\alpha(K_n) = 1$. Then, Stage 1 performs $n - 3$ iterations.

In iteration $h = 0$, for each vertex $u \in V(G)$, the neighborhood $N(u)$ is determined by summing all the entries equal to 1 in the row associated with vertex u . The selection of the maximum takes $O(n^2)$ time. Similarly, for each vertex $v \in N(u)$, the value $|N(v) \setminus N(u)|$ is computed by summing all the entries equal to 1 in the row corresponding to vertex v , provided that the entries for vertex u are not both 1.

In each iteration, $h \geq 1$, $N_{A_{h-1}}(v) + 1$ is calculated for every vertex $v \in I_{h-1}$ by counting all the 1 entries in the row corresponding to that vertex, if the entries are simultaneously 1 in $N_{A_{h-1}}$. Similarly, $N_{I_{h-1}}(u) + 1$ is calculated for every vertex $u \in I_{h-1}$. Given that each row consists of n entries and there are fewer than n rows to check, the computation of $N_{A_{h-1}}(v) + 1$ or $N_{I_{h-1}}(u) + 1$, along with the selection of the maximum, requires $O(n^2)$ time. Following the same idea, we can determine if the set I_h is independent if, for every vertex $u \in I_h$, it holds that $N_{I_h}(u) = \emptyset$.

Please note that $|A_0| < n$ and $|I_0| < n$. Therefore, the total number of iterations in the loops of Stage 1 is bounded by n . Hence, Stage 1 finds a total outer-independent dominating set in $O(n^3)$ time. $\square$

Proposition 5. Let G be a connected split graph with maximum clique K and independent set I . Then, the Heuristic TOID finds an optimal solution for the graph G if, in iteration i of the second iterative part of Stage 1, there is no vertex $v \in I$ such that $N_{I_{h+i-1}}(v) = K \setminus T_{h+i-1}$.

Proof. Clearly, every vertex in K has a higher degree than the vertices in $V \setminus K$. Then, in iteration $h = 0$, Heuristic TOID will select the vertices $u, v \in K$ such that $N(u) \cup N(v)$ is maximized, forming the set $T_0 = \{u, v\}$. Since T_0 dominates all the vertices in K , and $V \setminus K$ is an independent set, in every iteration $h \geq 1$ of the first iterative part of Stage 1, v_h is a vertex in $K \setminus T_{h-1}$ with the largest number of undominated neighbors in $V \setminus K$, and T_h is updated as $T_h = T_{h-1} \cup v_h$. The first iterative part stops when all the vertices in $V \setminus K$ are dominated.

If $T_h = K$, then $V \setminus K$ is an independent set, and the second iterative part of Stage 1 is skipped, proceeding directly to Stage 2. If there exists a vertex $v \in K$ such that $N_{V \setminus K}(v) = \emptyset$, the procedure *Purify*(G, T_h) removes this vertex from the set T_h and returns a set T^* with $|K| - 1$ vertices. Otherwise, the cardinality of T_h cannot be reduced, and $T^* = T_h$. In either case, by the proof of Proposition 2, this is an optimal solution.

If $|T_h| < |K|$, then $I_h = V \setminus T_h$ is not an independent set and has $r = |K| - |T_h|$ vertices from K in I_h . Please note that these r vertices form a K_r graph. Therefore, in the second iterative part of Stage 1, since in every iteration $i < r$, there is no vertex $v \in I$ such that $N_{I_{h+i-1}}(v) = K \setminus T_{h+i-1}$, $r - 1$ vertices from the set $K \setminus T_h$ are removed from I_h and added to T_h to ensure that I_h becomes an independent set. Then, $|T_{h+r-1}| = |K| - 1$. The current set T_{h+r-1} does not allow purification by the proof of Proposition 2, and $T^* = T_{h+r-1}$ is an optimal solution. $\square$

Purify Procedure

In Theorem 2.3 of [13], Soner et al. demonstrate that:

Lemma 2. Let T be a TOIDS. T is a minimal set if and only if, for each vertex $x \in T$, one of the following conditions holds:

- (i) There exists a vertex $y \in V(G)$ such that $N(y) \cap T = \{x\}$.
- (ii) There exists a vertex $w \in V \setminus T$ that is adjacent to x .

Following these ideas, the objective of this subsection is to propose a purification procedure that yields a minimal total outer-independent domination set (see Algorithm 2). Below are two definitions that we will use in the purification procedure. The *private neighborhood* of a vertex $x \in T \subseteq V(G)$, denoted by $pn(x, T, G)$, is given by

$$pn(x, T, G) = \{y \in V \mid N(y) \cap T = \{x\}\}.$$

A vertex in $pn(x, T, G)$ is referred to as a *private neighbor* of x . These definitions are equivalent to condition (i) in Lemma 2.

Please note that all vertices in the set D^* formed in this way satisfy one of the conditions proposed in Lemma 2, making it a minimal total outer-independent dominating set for the graph G . Using similar reasoning as in the proof of Theorem 5, it follows that the purification procedure can be executed in time $O(kn^2) = O(n^3)$.

Theorem 6. *Purify* runs in at most k iterations, and its time complexity is $O(n^3)$.

Algorithm 2 Purify

Input: A TOIDS T_h and a graph $G(V, E)$.
Output: A minimal TOIDS T^* .
 $T^* = \{v_1, \dots, v_k\}$; {vertices of T_h in the sequence in which they were included by Stage 1}
 $h := k$;
while $h > 0$ **do**
 if $pn(v_h, T^*, G) = \emptyset \wedge N_{V \setminus T^*}(v_h) = \emptyset$ **then**
 $T^* := T^* \setminus \{v_h\}$; {we purify vertex v_h }
 end if
 $h := h - 1$;
end while

4. Experimental Results

This section provides an overview of our computational analysis. We implemented the ILP formulation and Heuristic TOID in C++ using the CPLEX library, both running on a Windows 11 operating system for 64-bit architecture. The experiments were conducted on a personal computer equipped with an Intel Core i7-9750H processor (2.6 GHz) and 16 GB of DDR4 RAM. Our algorithm was tested on a set of 500 benchmark instances from [17,32,33].

Since no benchmark instances for the TOIDS problem previously existed, we used optimal values from CPLEX alongside established upper and lower bounds to evaluate heuristic performance. While our computational experiments provide valuable insights into the performance of the proposed heuristic and ILP formulation, some limitations should be considered. First, since no standard benchmark instances existed for this problem, the generated dataset may not fully represent the characteristics of real-world graphs. Second, computational constraints limited the exact resolution of larger instances using CPLEX, which may affect the evaluation of the heuristic's performance in such cases. Finally, further experiments on graphs from real-world applications would be necessary to assess the generalizability of our approach beyond the tested instances.

Table 1 presents the values of $\gamma_t^{oi}(G)$ for 39 instances out of the 500 analyzed using CPLEX. These instances were randomly selected from the full dataset. Additionally, T and T^* represent the solutions provided by our heuristic in Stages 1 and 2, respectively. The values of $\gamma_t^{oi}(G)$ shown in Table 1 can be compared with the solutions obtained by the heuristic. This comparison enables an assessment of the accuracy and effectiveness of the heuristic in estimating $\gamma_t^{oi}(G)$ for the analyzed instances.

Table 1. Comparison of $\gamma_t^{oi}(G)$ with heuristic solutions.

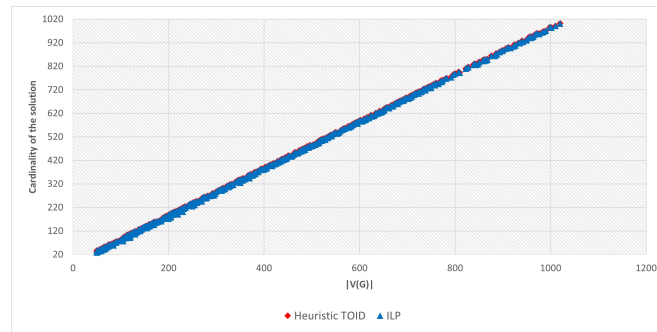
Graph	V	E	ILP Formulation		Heuristic TOID			
					Stage 1		Stage 2 (Purify)	
			$\gamma_t^{oi}(G)$	Time (s)	Time (s)	T	Time (s)	T*
BD0_1	50	306	37	0.230068	0.0002706	38	4.91×10^{-5}	37
BD3_21	150	4946	133	2.95812	0.0084127	135	0.0004906	134
BD6_77	252	26,482	241	2.60138	0.035878	243	0.0010007	242
BD6_135	368	57,889	356	15.5367	0.110472	358	0.0021302	357
BD6_176	450	87,361	438	31.7399	0.209045	441	0.0026331	440
BD6_233	564	123,045	550	423.17	0.44251	553	0.0040765	552
BD6_281	660	185,227	642	215.011	0.600134	645	0.0159938	643
BD6_324	746	244,124	734	286.535	0.887851	737	0.0072333	735
BD6_380	858	324,010	846	471.777	1.11367	848	0.0126979	847
BD6_436	970	415,180	958	927.578	1.65739	960	0.0109188	959
BD5_3	1150	1185	545	0.0510396	0.168395	584	0.115	546
BD5_11	1550	1570	709	0.0860892	0.572558	773	0.445647	711

Table 1. Cont.

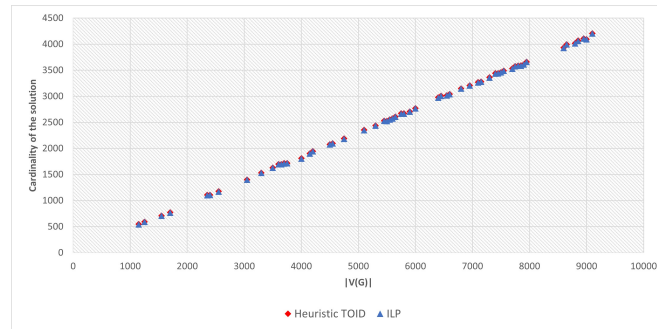
Graph	V	E	ILP Formulation		Heuristic TOID			
					Stage 1		Stage 2 (Purify)	
			$\gamma_t^{oi}(G)$	Time (s)	Time (s)	T	Time (s)	T*
BD5_14	1700	1740	769	0.0795056	0.476713	834	0.364287	771
BD5_27	2350	2391	1104	0.121842	1.27066	1183	0.960436	1106
BD5_28	2400	2422	1110	0.12279	1.34126	1203	1.06798	1110
BD5_31	2550	2583	1171	0.164572	2.05084	1260	1.22465	1174
BD5_41	3050	3064	1401	0.191348	2.72543	1497	2.09337	1401
BD5_46	3300	3342	1532	0.228255	3.48528	1647	2.82267	1533
BD5_50	3500	3530	1629	0.232505	4.16378	1743	3.5349	1629
BD5_63	4150	4160	1902	0.327835	6.93315	2043	6.13336	1902
BD5_64	4200	4202	1945	0.341413	7.30855	2081	6.15451	1945
BD5_71	4550	4589	2097	0.487072	9.37915	2248	8.46375	2097
BD5_89	5450	5489	2528	0.573985	16.1085	2707	17.6451	2528
BD5_90	5500	5531	2526	0.622945	17.0035	2712	18.6134	2527
BD5_92	5600	5610	2575	0.733355	17.1854	2773	19.9931	2575
BD5_95	5750	5781	2667	0.810157	19.0429	2868	22.4188	2669
BD5_100	6000	6010	2770	0.704363	21.6481	2972	26.2418	2770
BD5_111	6550	6586	3018	2.73775	28.0874	3240	34.0218	3018
BD5_112	6600	6610	3041	1.11453	28.6423	3258	36.958	3041
BD5_123	7150	7165	3279	1.22675	37.6569	3527	53.2459	3279
BD5_128	7400	7474	3436	1.35171	42.432	3693	61.6927	3439
BD5_130	7500	7535	3458	1.75227	43.2636	3686	62.1309	3458
BD5_136	7800	7804	3585	1.50382	49.4515	3837	73.3572	3585
BD5_138	7900	7932	3613	1.80407	51.9771	3899	80.5513	3613
BD5_153	8650	8700	3995	2.01012	68.8654	4272	108.539	3997
BD5_156	8800	8815	4016	3.16192	73.0794	4321	121.301	4016
BD5_159	8950	9009	4106	14.8081	77.9773	4404	127.993	4108
BD5_160	9000	9026	4093	9.27611	78.4205	4401	131.768	4093
BD5_162	9100	9106	4203	10.6997	85.3615	4519	139.437	4203
BD4_80	13,800	47,544,483	—	—	6316.35	13780	12.9821	13777
BD4_83	13,950	48,521,695	—	—	6348.22	13925	25.7166	13921
BD4_85	14,050	49,283,921	—	—	6513.36	14032	13.5854	14026
BD4_86	14,100	49,635,558	—	—	6604.26	14083	15.044	14075

Figure 3 presents a comparison between the solutions produced by our Heuristic TOID and the optimal values obtained by CPLEX for instances with up to 9100 vertices. Our heuristic successfully found the optimal solution in 28.69% of the instances. For the cases where the optimal solution was not achieved, the average absolute error was approximately 1.012 vertices.

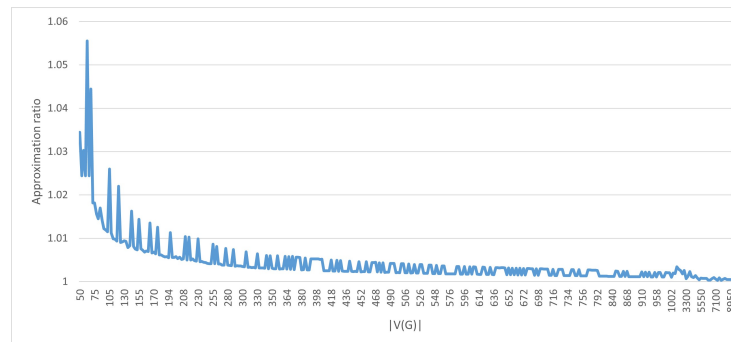
Figure 4 shows the approximation ratio of our heuristic in those instances where the optimal solution was not found. For these instances, the minimum approximation ratio was 1.00028, the maximum was 1.05555, and the average was 1.0032. Figure 4 also reveals a clear trend toward reducing the approximation ratio as the number of vertices increases. This result highlights the strong performance of our heuristic in terms of approximation ratio for instances with a larger number of vertices. The low approximation ratios demonstrate the high quality of our heuristic in efficiently providing near-optimal solutions.



(a) Instances with fewer than 1000 vertices

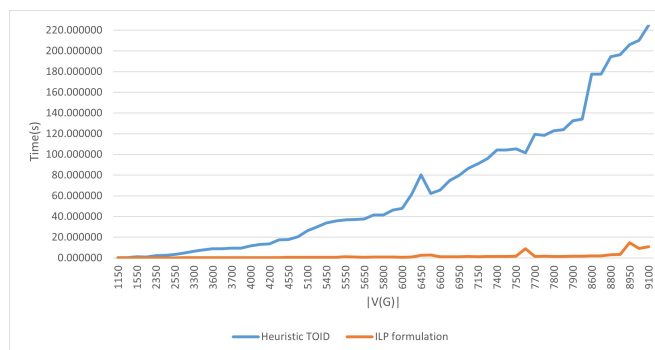


(b) Instances with more than 1000 vertices

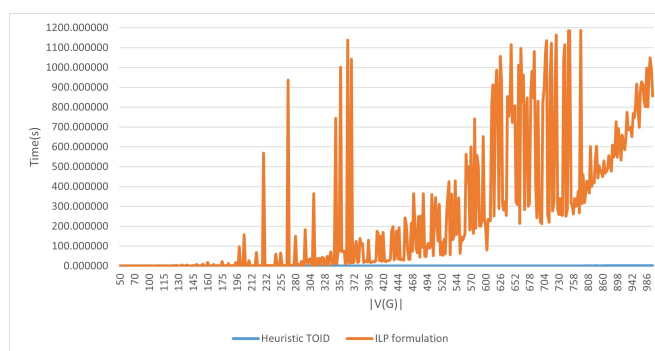
Figure 3. Approximation results vs. $\gamma_t^{oi}(G)$.**Figure 4.** Approximation Ratio.

The execution time of CPLEX and the heuristic varies depending on the density of the analyzed instances. In our analysis, graph density is defined as $\frac{2m}{n(n-1)}$. Figure 5a,b compare the time taken by CPLEX to find $\gamma_t^{oi}(G)$ with the time taken by the heuristic to find a feasible solution, considering graph density. Figure 5a shows the execution time for instances with a density of less than 0.1. For these instances, CPLEX performed better; on average, it was approximately 48.15 times faster than the heuristic. CPLEX successfully solved instances of this type with up to 9100 vertices. However, for instances with more than 9100 vertices, CPLEX ran out of available memory on the system and failed to find the optimal solution. Whereas the heuristic was not constrained by memory capacity, successfully solving instances with more than 14,000 vertices. Figure 5b shows the execution time for instances with a density greater than 0.1. For these instances, the heuristic outperformed CPLEX, being approximately 650.32 times faster on average. CPLEX was able to solve instances of this type with up to 1100 vertices, while the heuristic successfully solved instances with up to 14,100 vertices in less than two hours without reaching the memory limit (see BD4_xx instances in Table 1). In instances where the heuristic identified the optimal solution, i.e., a $\gamma_t^{oi}(G)$ -set, regardless of the instance density, the heuristic

was, on average, 594 times faster than CPLEX. These findings, along with the excellent approximation ratios shown in Figure 4, emphasize the critical role of heuristics in solving large-scale problems that are computationally infeasible for exact methods.



(a) Instances with density less than 0.1



(b) Instances with density greater than 0.1

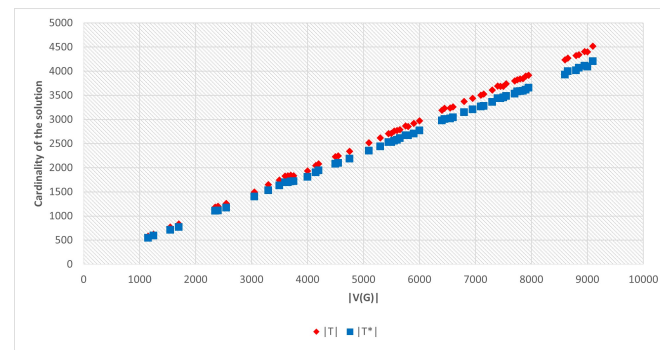
Figure 5. Time ILP formulation vs. Heuristic TOID.

The results reported for our heuristic include the purification stage (Stage 2). The purification process proved effective in practice, as illustrated in Figure 6. In this figure, $|T|$ and $|T^*|$ represent the number of vertices in the TOIDS before and after purification, respectively. In 99.59% of the analyzed instances, Stage 1 did not yield minimal TOIDS, i.e., Stage 1 produced TOIDS with redundant vertices. The purification process in Stage 2 of our heuristic exhibited different behaviors depending on the graph density. For graphs with a density lower than 0.1, an average of 191.68 vertices were removed, with a minimum of 28 and a maximum of 316. In these instances, on average, 6.81% of the vertices provided by Stage 1 were eliminated. In contrast, for graphs with a density greater than 0.1, the purification process had a significantly smaller impact. The average number of vertices removed was only 2.80, with a minimum of 0 and a maximum of 5. In these cases, the purification step reduced, on average, only 1.09% of the vertices provided by Stage 1. These results highlight that the purification procedure is notably more effective in sparse graphs, where a larger proportion of vertices can be removed, while in denser graphs, the final solution remains almost unchanged after Stage 2.

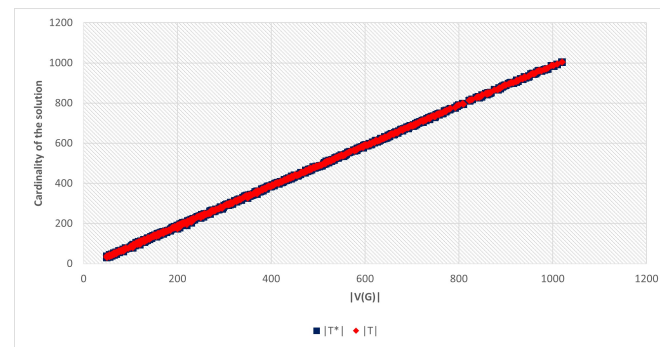
Figures 7a,b display boxplots illustrating the distribution of purified vertices in graphs with varying densities. The box represents the interquartile range (IQR), encompassing the central 50% of the data. The line within the box marks the median, which is the middle value. The whiskers represent the range of data that is not considered outliers, while any points outside this range are considered outliers. In Figure 7a, which corresponds to graphs with a density of 0.1 or higher, we observe that the purified vertices are concentrated between 0 and 3. This suggests that the number of purified vertices is generally low in high-

density graphs, indicating a better quality of the solution delivered by Stage 1. However, Stage 2 is still needed to guarantee a minimal TOIDS.

In contrast, Figure 7b, representing graphs with very low density (almost trees), shows a much wider spread in the values. The number of purified vertices is significantly higher, ranging from 28 to 316 vertices. This indicates that in low-density graphs, where the structure is more dispersed and less connected, the purification process has a much more significant impact. In these cases, it is more likely that many redundant or non-essential vertices can be removed. In summary, Stage 1 of our heuristic tends to be more effective in higher-density graphs, while it faces greater challenges in very low-density graphs.

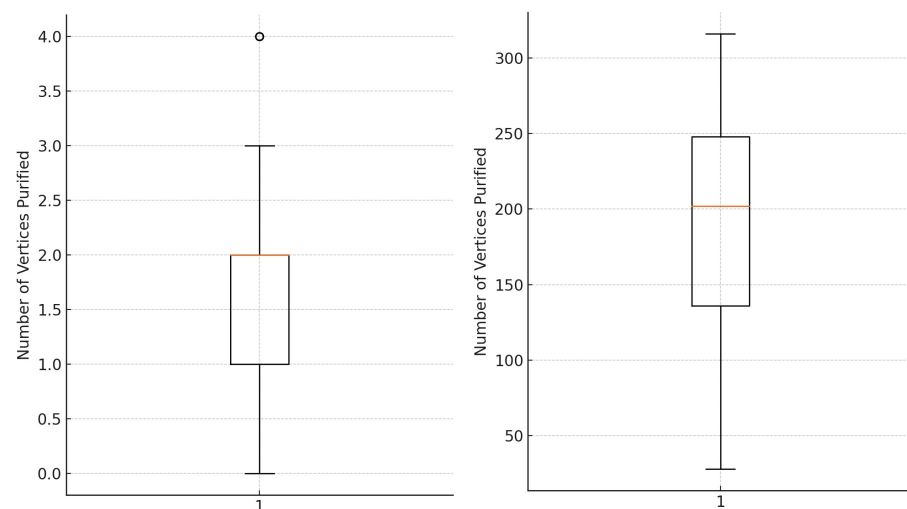


(a) Instances with density less than 0.1



(b) Instances with density greater than 0.1

Figure 6. Stage 1 vs. Stage 2 of Heuristic TOID.



(a) Instances with a $density \geq 0.1$

(b) Instances with a $density < 0.1$

Figure 7. Distribution of the number of purified vertices.

5. Conclusions

In this work, we introduced new lower and upper bounds for $\gamma_t^{oi}(G)$ and presented both an ILP formulation and a heuristic algorithm for addressing the total outer-independent domination problem. As no prior algorithm had been developed for this specific problem, we utilized the optimal solutions generated by CPLEX for our ILP model as a basis for evaluating the performance of our heuristic. Our experiments employed well-established benchmark instances originally designed for the classical domination problem. CPLEX successfully solved 500 of these instances, which included graphs with up to 9100 vertices. In addition, our heuristic consistently produced high-quality solutions for the same benchmarks, achieving an average error of 1.012 vertices across all tested instances. We also identified certain families of graphs where our heuristic guarantees optimal solutions. Looking ahead, we believe this research can be extended to tackle more complex variants of domination problems, such as k-tuple domination, secure domination, alliance domination, and total outer k-independent domination, opening new lines of research.

In addition to the results presented in this paper, several open problems remain related to $\gamma_t^{oi}(G)$. One significant direction for future research is the study of this parameter in the context of various graph operators and transformations. Specifically, the behavior of $\gamma_t^{oi}(G)$ under graph product operators (e.g., corona product, lexicographic product) and graph transformations (e.g., edge contractions, vertex deletions) remains largely unexplored. Investigating these operators could provide valuable insights and inspire further research in domination theory. Moreover, a comparative analysis with existing domination parameters across various graph families would offer deeper insights into the advantages and limitations of $\gamma_t^{oi}(G)$. Such comparisons could highlight the applicability of $\gamma_t^{oi}(G)$ in relation to well-established parameters, including the powerful k-alliance number, 2-packing number, global offensive k-alliance number, independence number, and independent domination number. Exploring these areas will not only expand our understanding of $\gamma_t^{oi}(G)$ but could also reveal new relationships between domination parameters in different graph families. We believe that addressing these open problems will significantly contribute to the theory of domination in graphs and inspire future research in this area.

Author Contributions: Conceptualization, P.B., E.P.I. and J.L.S.-S.; methodology, E.P.I., I.R.V. and J.L.S.-S.; software, E.P.I.; validation, E.P.I. and I.R.V.; formal analysis, P.B., E.P.I. and J.L.S.-S.; investigation, E.P.I., I.R.V. and J.L.S.-S.; data curation, E.P.I.; writing—original draft preparation, E.P.I., I.R.V. and J.L.S.-S.; writing—review and editing, P.B., E.P.I. and J.L.S.-S.; visualization, E.P.I. and J.L.S.-S.; supervision, P.B. and J.L.S.-S. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Data Availability Statement: Data are available at DOI: <https://doi.org/10.17632/rr5bkj6dw5.9>.

Conflicts of Interest: The authors declare no conflicts of interest.

Abbreviations

The following abbreviations are used in this manuscript:

TDS	Total Dominating Set
TOIDS	Total Outer-Independent Dominating Set
ILP	Integer Linear Programming
RAM	Random Access Memory

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