Efficient Maximum Defective Clique Search in Massive Graphs

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ABSTRACT

The study of k-defective cliques, defined as induced subgraphs that differ from cliques by at most k missing edges, has garnered much attention in graph analysis due to their relevance in various applications, including social network analysis and implicit interaction predictions. However, determining the maximum k-defective clique in graphs has been proven to be an NP-hard problem, presenting significant challenges in finding an efficient solution. To address this problem, we develop a theoretically sound and practically efficient algorithm that leverages newly-designed branch reduction rules and a pivot-based branching rule. Our analysis establishes that the time complexity of the proposed algorithm is bounded by $O(m\gamma_k^n)$, where γ_k is a real value strictly less than 2. To our knowledge, this algorithm achieves the best worst-case time complexity to date compared to existing state-of-the-art approaches. Furthermore, to minimize unnecessary branches, we introduce a time-efficient upper bound-based pruning algorithm, which is obtained by utilizing information such as the number of distinct colors assigned to vertices and the presence of non-neighbors among them. Additionally, to further enhance computational efficiency, we improve our algorithm by employing an ordering-based heuristic approach as a preprocessing step. Finally, we conduct extensive experiments on massive graphs to evaluate the efficiency of the proposed solutions. The results demonstrate that our algorithm achieves at least 3 orders of magnitude faster than the state-of-the-art solutions on the majority of large graphs.

PVLDB Artifact Availability:
The source code, data, and/or other artifacts have been made available at https://anonymous.4open.science/r/xxxxxxx.

1 INTRODUCTION

Graph has emerged as a versatile model for representing diverse real-world networks, including social networks [2], web networks [25], biological networks [47], and others. The task of identifying cohesive subgraphs from these networks is a fundamental problem in graph analysis, with broad applications in various domains. For instance, community detection in social networks [5, 15, 26], identification of protein complexes in protein-protein interaction (PPI) networks [61, 64], and statistical analysis in financial networks [6, 7] all can be formulated as cohesive subgraph mining problems. Perhaps, the classical clique [35], which requires every pair of vertices associated with an edge, is a commonly used cohesive subgraph model, as extensively advanced solutions have been investigated in literature [9, 16, 41, 57].

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In real-world applications, it is often too restrictive to mandate the presence of all possible relationships within a community. This is due to the fact that a subgraph missing certain edges can still effectively represent a community [46]. Moreover, real-world networks often involve noise or faults during data collection through experiments or automated sensors [1]. To address this issue, several relaxed clique models have also been extensively studied [46], including the k-plex [53], quasi-clique [33], r-clique [34], k-club [39], k-defective clique [64], and others.

In this paper, we primarily focus on the concept of the k-defective clique, which is formally defined as a subgraph $G(S)$ induced by the subset S of the graph G, such that it contains at least $\binom{|S|}{2} - k$ edges. This notion was originally introduced in [64] and has proven to be valuable in predicting implicit interactions among proteins in biological graphs. The rationale behind this concept is that the missing edges within the k-defective clique can be seen as indicative of implicit interactions between proteins. Due to the practical relevance to various real-world applications, including community detection in social networks [20, 22] and statistical analysis in financial networks [14], as well as its close relationship with other cohesive subgraph models, such as the clique [35] and k-plex [53], the maximum k-defective clique problem, which involves identifying a k-defective clique with the largest cardinality among all k-defective cliques in a given graph G, has recently garnered significant interest.

As shown in [58, 63], the problem of identifying the maximum k-defective clique of a given graph G is NP-complete, thereby establishing the infeasibility of a polynomial-time algorithm unless NP=P. To our knowledge, there are only a few solutions that address this challenging problem [13, 19, 21, 58]. Specifically, Trukhanov et al. [58] pioneer an exact algorithm for the maximum k-defective clique problem based on the Russian doll search technique [60]. Subsequently, Gschwinda et al. [21] further improve this algorithm by employing new preprocessing methods and an optimized implementation. Recently, several new enumeration algorithms [13, 19], based on a branch-and-bound technique [27], have also been developed to enhance the efficiency. Notably, Chen et al. [13] introduce a new branching rule and employ some reduction techniques to improve the search for the maximum k-defective clique. This novel branching rule prioritizes vertices with non-neighbors in the current k-defective clique for branching, ensuring a maximum of $k+1$ subbranches in each recursive call. Significantly, the authors establish that the worst-case time complexity of this technique for identifying the maximum k-defective clique is bounded by $O(P(n)\alpha_k^n)$, where n is the number of vertices in the graph G, $P(n)$ is a polynomial function dependent on n, and α_k is a real-number less than 2. To further mitigate unnecessary computations, an improved branch-and-bound enumeration algorithm is presented in [19] based on some newly branch pruning techniques. To our knowledge, this algorithm represents currently the most advanced solution to the problem of identifying the maximum k-defective cliques.

However, these existing solutions still exhibit several noteworthy issues. Firstly, the practical performance remains prohibitively expensive when processing real-world graphs. This issue primarily stems from the insufficient tightening of the upper bound-based pruning techniques and inefficient of the branching rules employed in these existing solutions. Specifically, the presence of overly loose upper bounds often hinders the timely termination of the branch-and-bound process. Moreover, the inefficient branching rules lead to a proliferation of duplicate results, resulting in numerous unnecessary computations within these existing algorithms. Secondly, the theoretical time complexity has not been sufficiently optimized. It is noteworthy that the majority of existing solutions [19, 21, 58] still have a worst-case time complexity of $O(P(n)2^n)$, with and only one approach [13] achieving a worst-case time complexity of $O(P(n)\alpha_k^n)$, where $\gamma_k < 2$. However, even for relatively small values of k, the corresponding of α_k approaches approximately 2. For instance, as reported in [13], when $k = 2$ and 3, the respective values of α_k are 1.984 and 1.996, which result is unacceptably high for the problem of finding the maximum k-defective clique in graph G. Consequently, there is an urgent demand for developing more efficient algorithms that can effectively identify the maximum k-defective clique of real-world graphs.

Contribution. In this paper, we extensively investigate the problem of finding maximum k-defective clique of a given graph G, and develop a novel algorithm that combines both theoretical advancements and practical efficiency to address aforementioned issues. The main contributions are summarized below.

Novel enumeration algorithms. To efficiently identify the maximum k-defective clique of G, we develop an elegant enumeration algorithm, which mainly combines two newly-developed branching rules. These rules ensure the algorithm's effectiveness in reducing search space. Firstly, if there exists a vertex with at most three non-neighbors within the search space, we employ the newly proposed branch reduction rules. Secondly, for cases where no such vertex exists, we further utilize a newly pivot-based branching rule to significantly reduce redundant branches. It is worth mentioning that we mathematically prove that the time complexity of this algorithm is bounded by $O(m\gamma_k^n)$, where γ_k takes the value of 1.414 if $k = 0$, or the maximum real-root of $x^{k+3} - 2x^{k+2} + x^2 - x + 1 = 0$ if $k \geq 1$. For example, when $k = 1$, 2, and 3, the corresponding values of γ_k are 1.466, 1.755, and 1.889, respectively. To our knowledge, our algorithm currently represents the most optimal solution in terms of worst-case time complexity.

New optimization techniques. To further improve the efficiency of our algorithm, we develop a set of optimization techniques. These include upper-bound based pruning and an ordering-based heuristic approach. Our research demonstrates that the size of the maximum k-defective clique in a graph G can be effectively bounded by considering several essential factors, such as the vertex degree, core number [52], and number of distinct colors present in G. Furthermore, we observe that the proposed color-based upper bound can be tightened by further considering the presence of non-neighbors among vertices. Leveraging these observations, we develop a highly efficient pruning algorithm with a time complexity of $O(kn + \overline{m})$, where n and $\overline{m}$ are the number of vertices and missing edges in G, respectively. In addition to the pruning algorithm, we also present a novel ordering-based heuristic algorithm. This algorithm functions as a preprocessing step, allowing us to identify a near-maximum k-defective clique and greatly reduce unnecessary vertices in G.

Extensive experiments. We construct extensive experiments to evaluate the efficiency of the proposed algorithms on 139 real-world graphs, 83 DIMACS10 graphs, and 114 Facebook graphs. The experimental results demonstrate that our algorithms substantially outperform the state-of-the-art algorithms in identifying the maximum k-defective clique by at least 3 orders of magnitude on the majority of real-world graphs. For example, On the flixster dataset (with 7.9 million edges), our algorithm takes less than one second to identify the maximum k-defective clique when $k = 1$. In contrast, all existing state-of-the-art algorithms failed to terminate within 3 hours under identical conditions.

2 PROBLEM DEFINITION

Consider an undirected and unweighted graph $G = (V, E)$, where V and E represent the sets of vertices and edges of the graph G, respectively. Let $n = |V|$ and $m = |E|$ denote the number of vertices and edges in G, respectively. For a vertex v of G, we define $N_v(G)$ as the set of neighbors of v in G, i.e., $N_v(G) = \{u \in V | (u, v) \in E\}$. The degree of v in G is denoted as $d_v(G) = |N_v(G)|$. Similarity, we refer to the set of non-neighbors of v in G as $\overline{N}_v(G) = V \setminus N_v(G)$, and the cardinality of $\overline{N}_v(G)$ as $\overline{d}_v(G) = |\overline{N}_v(G)|$. Given a vertex subset S of G, we let $G(S) = (S, E_S)$ be the subgraph of G induced by the subset S, where $E_S = \{(u, v) \in E | u \in S, v \in S\}$. To simplify notation, $N_v(G(S))$ ($\overline{N}_v(G(S))$) and $d_v(G(S))$ ($\overline{d}_v(G(S))$) are abbreviated as $N_v(S)$ ($\overline{N}_v(S)$) to $\overline{d}_v(S)$ ($\overline{d}_v(S)$), respectively. Below, we present the formal definition of the k-defective clique.

Definition 1 (k-defective clique [64]). Given a graph G and a non-negative integer k, the subgraph $G(S)$ induced by the vertex set $S \subseteq V$ is a k-defective clique if there exist at least $\binom{|S|}{2} - k$ edges in $G(S)$.

For simplicity, in the rest of this paper, we directly refer the set S as the k-defective clique of G. A k-defective clique S of G is considered maximal if there does not exist any other k-defective clique S' of G such that $S \subset S'$. Furthermore, a k-defective clique S of G is designated as maximum if its size is largest among all maximal k-defective clique of G, where the size of k-defective clique S is defined as the number of vertices it contains. Then, we introduce two useful properties of the k-defective clique, which are very helpful for designing our algorithms.

Property 1 (Hereditary [58]). Given a k-defective clique S of G, every subset of S is also a k-defective clique of G.

The hereditary property (Property 1) of a k-defective clique simplifies the maximality check process. Specifically, if a k-defective clique S of G is maximal, then we obtain that there is no vertex in $V \setminus S$ that can be used to expand S. Thus, this property forms the foundation for the design of our algorithms.

Property 2 (Small diameter [14]). Given a k-defective clique S of G, the diameter of $G(S)$ is no larger than 2 if $|S| \geq k + 2$.

Property 2 not only implies the internal density-connected nature (having a diameter of two with a size no less than $k + 2$) of the k-defective clique but also provides an acceleration for enumerating relatively-large maximal k-defective cliques [14]. However, the problem of enumerating maximal k-defective cliques often suffers from excessively long computational times, as there can be an exponential number of maximal k-defective cliques compared to the

number of vertices. To address this challenge, in this paper, we aim to the problem of finding a maximum k-defective clique of G and the formal problem definition is shown below.

Problem definition. Given a graph G and a non-negative integer k, the goal of this paper is to compute the maximum k-defective clique of G, i.e., finding a k-defective clique whose size is the largest among all maximal k-defective clique of G.

In Section 1, we have conducted extensive analysis that reveals the inefficiency of existing solutions [13, 19, 21, 58] in finding the maximum k-defective clique. To overcome these challenges, this paper will present a theoretically and practically efficient algorithm in the following sections.

3 THE EXACT ENUMERATION PARADIGM

In this section, we present a novel algorithm designed to efficiently identify the maximum k-defective clique within a given graph G. Our algorithm builds upon the widely recognized branch-and-bound technique [27], which centers around dividing the current problem into smaller sub-problems. Specifically, we define an instance $I = (G, S, C, k)$ that aims to compute the maximum k-defective clique containing the set S within the subgraph $G(S \cup C)$. Here, S represents the current partial k-defective clique, while C denotes the candidate set used to expand S. By selecting a vertex v from C, the instance I can be split into two sub-instances: $I_1 = (G, S \cup \{v\}, C \setminus \{v\}, k)$ and $I_2 = (G, S, C \setminus \{v\}, k)$, utilizing the branch-and-bound technique. Notably, the solution to instance I corresponds precisely to the larger result obtained from either I_1 or I_2. Consequently, in order to obtain the final solution for I, each sub-instance of I can be recursively divided until the candidate set C becomes empty. The overall outcome is determined by selecting the maximum solution among all sub-instances.

However, the total number of sub-instances for the instance $I = (G, S, C, k)$ can be exponentially large, specifically $O(2^n)$, when $S = \emptyset$ and $C = V$. Enumerating all possible sub-instances would be highly inefficient. In order to enhance the performance of such a procedure, it becomes crucial to identify and eliminate unnecessary sub-instances that cannot yield the maximum k-defective clique of G. Below, we first introduce some new branch reduction rules and then present our enumeration algorithm.

3.1 Branch Reduction Rules

Given the instance $I = (G, S, C, k)$ that focuses on computing the maximum k-defective clique containing set S in the subgraph $G(S \cup C)$, we observe that the sub-instances of I can be further reduced under specific conditions. Particularly, if there exists a vertex in C that has at most three non-neighbors within $S \cup C$, denoted as v with $\overline{d}_v(S \cup C) \leq 3$, the following three reduction rules apply.

(1) One non-neighbor reduction: $\overline{d}_v(S \cup C) = 1$**.** In this scenario, all other vertices within $S \cup C$ are the neighbors of v. Consequently, the maximum k-defective clique in $G(S \cup C)$ must necessarily include the vertex v, which leads us to obtain the following lemma.

Lemma 1. Given an instance $I = (G, S, C, k)$, if there exists a vertex v in C with $\overline{d}_v(S \cup C) = 1$, then the maximum k-defective clique for instance I must include in the sub-instance $I' = (G, S \cup \{v\}, C \setminus \{v\}, k)$.

(2) Two non-neighbors reduction: $\overline{d}_v(S \cup C) = 2$. Let u be the non-neighbor of v in $S \cup C$. It can be easily verified that the maximum k-defective clique in $G(S \cup C)$ must contain at least one vertex in $\{v, u\}$. Let S_1^* be the maximum k-defective clique that contains v. We observe that for any k-defective clique S_2^* where $u \in S_2^*$, it always holds that $|S_1^*| \geq |S_2^*|$. Therefore, in the case where $\overline{d}_v(S \cup C) = 2$, it is unnecessary to find the maximum k-defective clique that excludes v in instance I. This leads us to the following lemma.

Lemma 2. Given an instance $I = (G, S, C, k)$, if there exists a vertex v in C with $\overline{d}_v(S \cup C) = 2$, it follows that a maximum k-defective clique of instance I must exist in the sub-instance $I' = (G, S \cup \{v\}, C \setminus \{v\}, k)$.

Proof sketch. Assume that S^* is a maximum k-defective clique for instance I. It can be easily verified that $|S^* \cap \{v, u\}| \geq 1$, where u is the sole non-neighbor of v in $S \cup C$. When $v \notin S^*$, we can establish that $S^* \setminus \{u\} \cup \{v\}$ also forms a maximum k-defective clique if $u \in C$. Moreover, for the case where $u \in S$, we let w be a vertex in $S^* \setminus S$ with the minimum value of $d_w(S^*)$. It follows that S^* can be expanded by v, if $d_w(S^*) = |S^*| - 1$. Otherwise, $S^* \setminus \{w\} \cup \{v\}$ will form a maximum k-defective clique for instance I. Thus, there always exist a maximum k-defective clique for instance I that contains v.

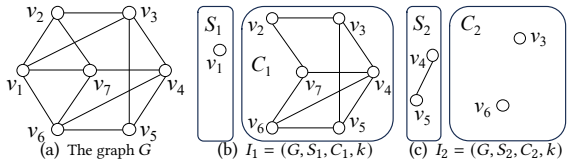
Based on Lemma 1 and Lemma 2, we can deduce that for a given instance $I = (G, S, C, k)$, if there exists a vertex v in C such that $\overline{d}_v(S \cup C) \leq 2$, then it is sufficient to consider the scenario where the maximum k-defective clique of I includes vertex v. Consequently, this reduces the need to explore sub-branches that aim to find the maximum k-defective clique excluding v.

(3) Three non-neighbors reduction: $\overline{d}_v(S \cup C) = 3$**.** Let u and w be the two non-neighbors of vertex v in $S \cup C$. In the instance $I = (G, S, C, k)$, the maximum k-defective clique must include at least one vertex from the set $\{v, u, w\}$. Moreover, based on Lemma 2, we obtain that if a maximum k-defective clique contains only u or only w among the vertices in $\{v, u, w\}$, there must also exist a maximum k-defective clique that includes vertex v. Hence, if the maximum k-defective clique excludes vertex v, it necessarily contains both vertices u and w. To further enhance such a result, we introduce the following lemma.

Lemma 3. Let S^* be a maximum k-defective clique for the instance $I = (G, S, C, k)$. If there exists a vertex v in C satisfying $\overline{d}_v(S \cup C) = 3$ and $\overline{d}_v(S) \leq 1$, with u and w denoting the two non-neighbors of v in $S \cup C$, the following results hold.

- *Case $\overline{d}_v(S) = 0$: If $(u, w) \notin E$ or $\overline{d}_u(S) + \overline{d}_w(S) \geq 1$, S^* is included in the sub-instance $I_1 = (G, S \cup \{v\}, C \setminus \{v\}, k)$; otherwise, S^* is either included in the sub-instance I_1 or the sub-instance $I_2 = (G, S \cup \{u, w\}, C \cap N_u(G) \cap N_w(G), k)$.*
- *Case $\overline{d}_v(S) = 1$: If $\overline{d}_u(S) \geq 1$ with $u \in C$, S^* is included in the sub-instance $I_1 = (G, S \cup \{v\}, C \setminus \{v\}, k)$; otherwise, S^* is either included in the sub-instance I_1 or the sub-instance $I_3 = (G, S \cup \{u\}, C \cap N_u(G), k)$.*

Proof sketch. For the case where $\overline{d}_v(S) = 0$, It can be easily verified that S^* contains either the vertex v, or both vertices u and w based on Lemma 2. We now consider the scenario where $\{u, w\} \subseteq S^*$. If $\overline{d}_u(S) \geq 1$ (or $\overline{d}_w(S) \geq 1$) or $(u, w) \notin E$, $S^* \setminus \{u\}$ (or $S^* \setminus \{w\}$) forms a $(k-1)$-defective clique in G, which can be expanded by v. However, if the conditions $\overline{d}_u(S) + \overline{d}_w(S) \geq 1$ and $(u, w) \notin E$ are not satisfied, the sub-instance $I' = (G, S \cup \{u, w\}, C \setminus \{u, w\}, k)$ is further invoked. We note that if there exists a vertex v' in $C \setminus N_u(G)$ (or $C \setminus N_w(G)$) included in S^*, then $S^* \setminus \{u\}$ (or $S^* \setminus \{w\}$) also forms a $(k-1)$-defective clique in G, expandable by v. Hence, the correctness has



(a) The graph G (b) $I_1 = (G, S_1, C_1, k)$ (c) $I_2 = (G, S_2, C_2, k)$

Figure 1: Three non-neighbor reduction rule, where the maximum k-defective clique S^* of G is either included in I_1 or in I_2 ($k \geq 2$).

been established for the case where $\overline{d}_v(S) = 0$. The case where $\overline{d}_v(S) = 1$ can be proven similarly.

The following example demonstrates the idea of Lemma 3.

Example 1. Consider a graph $G = (V, E)$ depicted in Fig. 1(a) where $k \geq 2$, we observe that $\overline{d}_{v_1}(G) = 3$. Utilizing the branch reduction rule (Lemma 3), we can identify the maximum k-defective clique S^* of G. Specifically, S^* is either included in $I_1 = (G, S_1 = \{v_1\}, C_1, k)$ or in $I_2 = (G, S_2 = \{v_4, v_5\}, C_2, k)$, as shown in Fig. 1(b) and Fig. 1(c), respectively. Furthermore, in the sub-instance I_2 for computing S^* containing $\{v_4, v_5\}$, the candidate set C_2 must be included in common neighbors of v_4 and v_5. Consequently, C_2 contains only the vertices v_3 and v_6. In addition, in the sub-instance I_1, we note that $\overline{d}_{v_4}(S_1 \cup C_1) = 3$. This observation allows us to further apply the three non-neighbor reduction rule to prune I_1. Thus, this example serves to illustrate the remarkable pruning capabilities of the proposed reduction rules.

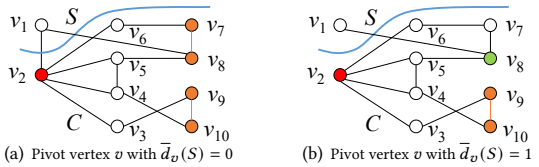
3.2 New Pivot-Based Techniques

Before unveiling our techniques, we first introduce a pivot-based solution initially developed for maximal k-defective clique enumerations [14]. The core concept behind this pivot-based technique is as follows: when given an instance $I = (G, S, C, k)$ aimed at enumerating all maximal k-defective cliques containing S in $G(S \cup C)$, if there exists a vertex $v \in C$ such that $S \subseteq N_v(G)$, then any maximal k-defective clique containing S in $G(S \cup C)$ either includes the vertex v or a non-neighbor vertex of v in C. This pivot-based technique is evidently applicable to solving the problem of finding the maximum k-defective clique.

However, we note that the restriction on the pivot vertex is overly stringent, resulting in numerous unnecessary computations when utilizing this pivot-based technique to identify the maximum k-defective clique of G. To illustrate, let us consider an instance $I = (G, S, C, k)$. If there exist two vertices $u \in S$ and $v \in S$ such that $N_v(G) \cap N_u(G) = \emptyset$, it becomes apparent that there is no vertex w in C that satisfies $S \subseteq N_w(G)$. Consequently, this instance I cannot be pruned using the pivot-based technique established in [14], leading to a substantial number of redundant computations. To address this concern, we introduce a novel pivot-based technique for finding the maximum k-defective clique of G, which is presented below.

Theorem 3.1 (New pivoting rule). *Given an instance $I = (G, S, C, k)$ aimed at finding the maximum k-defective clique that contains S in $G(S \cup C)$, let v, denoted by the pivot vertex, be a vertex in C with $\overline{d}_v(S) \leq 1$, then the maximum k-defective clique for instance I either contains v or a vertex in $C \setminus \{v\} \setminus N_v(G)$.*

Proof sketch. If $\overline{d}_v(S) = 0$, this theorem is clearly established [14]. For the case where $\overline{d}_v(S) = 1$, we obtain that S is a $(k-1)$-defective clique, as v can be used to expand S. Denote by $C_1 = C \cap N_v(G)$. This theorem disregards the maximum k-defective clique contained in



(a) Pivot vertex v with $\overline{d}_v(S) = 0$ (b) Pivot vertex v with $\overline{d}_v(S) = 1$

Figure 2: The pivot-based technique of Theorem 3.2, where the red vertices are the pivot vertices. Then, the maximum k-defective clique either contains a red or green vertex or an orange edge ($k \geq 1$).

$G(S \cup C_1)$. Let $S \cup D$ be the maximum k-defective clique in $G(S \cup C_1)$, where $D \subseteq C_1$. We now demonstrate that there exists a k-defective clique containing v with a size no less than $|S \cup D|$. Given a vertex $u \in D$ with the minimum $\overline{d}_u(S \cup D)$, we then observe that $S \cup D \cup \{v\}$ is a larger k-defective clique in $G(S \cup C)$ if $\overline{d}_u(S \cup D) = 1$. On the other hand, if $\overline{d}_u(S \cup D) \geq 2$, we obtain that $S \cup D \setminus \{u\} \cup \{v\}$ also constitutes a k-defective clique of $G(S \cup C)$. Thus, there exists a k-defective clique containing v with a size no less than $|S \cup D|$.

Although Theorem 3.1 effectively reduces redundant subbranches that cannot generate the maximum k-defective clique, we acknowledge that in instance $I = (G, S, C, k)$, there might still be unnecessary computations when expanding S with vertices in $C \setminus N_v(G)$, where v represents a selected pivot vertex from C. For instance, let us consider S^* as the maximum k-defective clique of instance I. If $|S^* \setminus \{v\} \setminus N_v(G)| \geq 2$, it becomes apparent that S^* can be identified by either $I' = (G, S \cup \{u\}, C \setminus \{u\}, k)$ or $I'' = (G, S \cup \{w\}, C \setminus \{w\}, k)$, where u and w are the two vertices in $S^* \setminus \{v\} \setminus N_v(G)$ that are used to expand S based on the pivot-based technique described in Theorem 3.1. Consequently, this leads to redundant computations. To address this concern, we propose an enhanced pivot-based technique, which is outlined below.

Theorem 3.2 (Improved pivoting rule). *Consider an instance $I = (G, S, C, k)$, where v is the pivot vertex in C with $\overline{d}_v(S) \leq 1$. Denote by $P = C \setminus \{v\} \setminus N_v(G)$. We then have the following results.*

- *Case $\overline{d}_v(S) = 0$: the maximum k-defective clique for instance I either contains v or an edge in $G(P)$.*
- *Case $\overline{d}_v(S) = 1$: the maximum k-defective clique for instance I either contains a vertex in $\{v\} \cup P_1$ or an edge in $G(P_2)$, where $P_1 = \{u \in P | \overline{d}_u(S) = 0\}$ and $P_2 = P \setminus P_1$.*

Proof sketch. Let S^* be the maximum k-defective clique containing S in $G(S \cup C)$. For the case where $\overline{d}_v(S) = 0$, suppose, on the contrary, that $D = S^* \cap P$ forms an independent set when $v \notin S^*$. Clearly, $D \neq \emptyset$, as $\overline{d}_v(S) = 0$. Given any vertex u in D, we obtain that $S^* \setminus \{u\}$ forms a $(k + 1 - |D|)$-defective clique. Moreover, since $\overline{d}_v(S^*) = |D|$, we conclude that $S^* \setminus \{u\} \cup \{v\}$ is also a k-defective clique in $G(S \cup C)$. Therefore, if $v \notin S^*$, there exists at least one edge in $G(D)$ for the case where $\overline{d}_v(S) = 0$. A similar analysis can be employed to prove the case where $\overline{d}_v(S) = 1$.

The example depicted in Fig. 2 serves as a practical illustration of the concept elucidated in Theorem 3.2.

Example 2. Consider the graph G shown in Fig. 2(a) with $k \geq 2$. Let $S = \{v_1\}$ and $C = \{v_2, v_3, ..., v_{10}\}$ be the current k-defective clique and the candidate set of C, respectively. By selecting v_2 as the pivot vertex, we can deduce that the maximum k-defective clique S^* of G either contains v_2 or an edge from $G(\{v_7, v_8, v_9, v_{10}\})$, as stated in

Theorem 3.2. However, if $(v_1, v_2) \notin E$ and we still choose v_2 as the pivot vertex, then S^* either contains a vertex from $\{v_2, v_8\}$ or an edge from $G(\{v_7, v_9, v_{10}\})$. Notably, since $G(\{v_7, v_9, v_{10}\})$ does not contain an edge involving v_7, it is unnecessary to consider the scenario where S^* includes v_7, as depicted in Fig. 2(b).

3.3 Algorithm Implementation

Based on the proposed branch reduction rules and pivoting rules, we introduce a novel branching rule for efficiently finding the maximum k-defective clique in graph G, which is outlined below.

Branching rule. Consider an instance $I = (G, S, C, k)$ aiming to identify the maximum k-defective clique containing S in $G(S \cup C)$. Let $N_S(C) = \{v \in C | S \subseteq N_v(G)\}$ be the set of common neighbors of S in C. Our branching rule is as follows:

- If there exists a vertex $v \in C$ satisfying $\overline{d}_v(S \cup C) \leq 3$ and $\overline{d}_v(S) \leq 1$, the branch reduction rules proposed in Sec. 3.1 are applied to determine the maximum solution for the instance I.
- Else if $|C \setminus N_S(C)| + \overline{d}(S) \geq k \geq 1$, a vertex $v \in C$ with the highest $\overline{d}_v(S)$ is selected to split the instance I into two sub-instances $I_1 = (G, S \cup \{v\}, C \setminus \{v\}, k)$ and $I_2 = (G, S, C \setminus \{v\}, k)$.
- Otherwise, the proposed pivoting rule described in Theorem 3.2 is employed to branch the instance I.

Implementations details. Armed with the proposed branching rule, we develop a new algorithm to identify the maximum k-defective clique of G, which is shown in Algorithm 1.

To begin, Algorithm 1 initializes the current maximum k-defective clique S^* as an empty set. Subsequently, it invokes the $Branch(S, C)$ procedure (line 2), which follows our proposed branching rules (lines 9-29). Here, the parameters S and C are denoted by the current k-defective clique and the candidate set used to expand S, respectively. Specifically, if there exists a vertex u in C that satisfies $\overline{d}_u(S \cup C) \leq 3$ and $\overline{d}_u(S) \leq 1$, the branch reduction rules (proposed in Sec. 3.1) are applied to find the maximum k-defective clique that contains S (lines 9-10). If branch reduction rules cannot be used, the procedure determines whether the size of $C \setminus N_S(C)$ is no larger than $|C| - k + \overline{d}(S)$ or each vertex in C has at least two non-neighbors in S (line 11). If this condition holds, the procedure directly identifies the maximum k-defective clique that includes or excludes vertex v (line 14), where v is a vertex in C with the maximum value of $\overline{d}_v(S)$ (line 12). If above conditions are not met, the maximum k-defective clique either contains a vertex in P_1 or an edge in $G(P_2)$, based on Theorem 3.2. Here, P_1 is defined as $\{v\}$ (or $\{v\} \cup \{u \in \overline{N}_v(C) | \overline{d}_v(S) = 0\}$ if $\overline{d}_v(S) = 1$), and P_2 as $\overline{N}_v(C) \setminus P_1$, where v is a pivot vertex selected from C to minimize the size of $P_1 \cup P_2$ (line 16). Subsequently, this procedure iteratively expands the current k-defective clique S by selecting the vertices in P_1 (lines 21-23) and the edges in $G(P_2)$ (lines 24-29). Finally, this recursion terminates when C becomes empty (lines 5-7). Note that if $C = \emptyset$ and the current k-defective clique S is larger than the current maximum result S^*, S^* is updated with the value of S (line 6).

In addition, to ensure that all remaining vertices in the candidate set can be utilized to expand $S \cup \{v\}$, it is necessary to update the candidate set when a vertex $v \in C$ is added to S. To address this requirement, we develop a procedure outlined in Algorithm 2. This algorithm involves the straightforward removal of each vertex u from $C \setminus \{v\}$ that possesses more than $k - s - \overline{d}_v(S)$ non-neighbors within $S \cup \{v\}$ (lines 2-6). Here, s represents the total number of missing edges in $G(S)$ (line 1). It can be easily verified that the time complexity of Algorithm 2 is bounded by $O(n)$.

Algorithm 1: The branch and bound algorithm

```
   Input: The graph G = (V, E) and a parameter k
   Output: The maximum k-defective clique S* of G
1  S* ← ∅;
2  Branch(∅, V);
3  return S*;
4  Function: Branch(S, C)
5      if C = ∅ then
6          if |S| > |S*| then S* ← S;
7          return;
8      C1 ← {u ∈ C | d̄_u(S) ≤ 1}; C2 ← C \ C1;
9      if ∃u ∈ C1 such that d̄_u(S ∪ C) ≤ 3 then
10         Apply the branch reduction rules in Lemma 1-3;
11     else if |C \ N_S(C)| + d̄(S) ≥ k ≥ 1 or C1 = ∅ then
12         v ← a vertex in C \ N_S(C) with largest d̄_v(S);
13         C' ← Update(S, C, v);
14         Branch(S ∪ {v}, C'); Branch(S, C \ {v});
15     else
16         v ← a vertex in C1 with the largest value of d_v(C);
17         P1 ← {v}; P2 ← N̄_v(C) \ P1;
18         if d̄_v(S) = 1 then
19             P1 ← {u ∈ N̄_v(C) | d̄_u(S) = 0} ∪ P1;
20             P2 ← N̄_v(C) \ P1;
21         foreach u ∈ P1 do
22             C' ← Update(S, C, u);
23             Branch(S ∪ {u}, C'); C ← C \ {u};
24         foreach u ∈ P2 do
25             C' ← Update(S, C, u); P2' ← C' ∩ P2;
26             foreach w ∈ P2' s.t. (u, w) ∈ E do
27                 C'' ← Update(S ∪ {u}, C', w);
28                 Branch(S ∪ {u, w}, C''); C' ← C' \ {w};
29             C ← C \ {u};
```

Algorithm 2: $Update(S, C, v)$

```
1  C' ← ∅; s ← the number of missing edges in G(S);
2  for u ∈ C, s.t. u ≠ v do
3      d̄ ← s + d̄_v(S) + d̄_u(S);
4      if d̄ ≤ k then
5          if u ∈ N_v(G) then C' ← C' ∪ {u};
6          else if d̄ < k then C' ← C' ∪ {u};
7  return C';
```

3.4 Complexity Analysis

We proceed to analyze the time and space complexity of the proposed algorithm, as outlined below.

Theorem 3.3. *The time complexity of Algorithm 1 is bounded by $O(my_k^n)$, where γ_k is the maximum real root of $x^{k+3} - 2x^{k+2} + x^2 -$*

$x+1=0$ *if* $k \geq 1$. *Specifically, when* $k = 1, 2$ *and* 3, *the corresponding values of* γ_k *are* 1.466, 1.755, *and* 1.889, *respectively.*

Proof sketch. Let $T(n)$ be the total number of leaves of $branch(S, C)$ outlined in Algorithm 1. Then, the time complexity of Algorithm 1 is bounded by $O(mT(n))$, as each recursive call of *branch* requires at most $O(m)$ time. We now analyze the size of $T(n)$.

(1) If $\exists v \in C$ with $\overline{d}_v(S \cup C) \leq 3$ and $\overline{d}_v(S) \leq 1$, the branch reduction rules outlined in Sec. 3.1 is used to identify the maximum k-defective clique. Let $D = \{u, w\}$ be the set of two non-neighbors of v in $S \cup C$. We then have the following recurrence relations:

$$\begin{cases} T(n) \leq T(n-1), & \text{if } \overline{d}_v(S \cup C) \leq 2; \\ T(n) \leq T(n-1) + T(|N_D(C)|), & \text{if } \overline{d}_v(C) = 3 \text{ and } \overline{d}_v(S) = 0; \\ T(n) \leq T(n-1) + T(|N_u(C)|), & \text{if } \overline{d}_v(C) = 2 \text{ and } \overline{d}_v(S) = 1. \end{cases} \quad (1)$$

It is easy to verify that $T(n) \leq T(n-1) + T(n-3)$ is the worst-case recurrence for the branch reduction rules.

(2) If $|C \setminus N_S(C)| + \overline{d}(S) \geq k$, a base recurrence of $T(n) \leq T(n-1) + T(n-1)$ is obtained. We note that this recurrence can be tightened, as in $branch(S \cup \{v\}, C \setminus \{v\})$, another vertex from $C \setminus N_S(C)$ will be selected to expand $S \cup \{v\}$. This means that at most $k - \overline{d}(S)$ vertices in $C \setminus N_S(C)$ are in preference to be added to S. If $\overline{d}_v(S) \geq 2$, it easy to obtain that:

$$T(n) \leq \sum_{i=1}^{k} T(n-i), \quad \text{if } k \geq 2. \quad (2)$$

If $\overline{d}_v(S) \leq 1$, we have $\overline{d}_v(S \cup C) \geq 4$. Consequently, we deduce that the size of $C \setminus N_{S \cup \{v\}}(C)$ is at least $k - \overline{d}(S) + 2$. Hence, the following recurrence relation can be obtained:

$$T(n) \leq \sum_{i=1}^{k} T(n-i) + T(n-k-2). \quad (3)$$

(3) If $C_1 = \emptyset$, we obtain that at most $k/2$ vertices in C are possible to be added to S. This leads to the following recurrence: $T(n) \leq \sum_{i=1}^{k/2} T(n-i)$, where $k \geq 2$.

(4) If $|C \setminus N_S(C)| + \overline{d}(S) < k$, The pivot-based branching rule gives rise to a recurrence of $T(n) \leq \sum_{i=1}^{|P_1|} T(n-i) + \sum_{i=1}^{|P_2|} \sum_{j=1}^{|P_2|-i} T(n-|P_1|-i-j)$. Building upon the based recurrence, we deduce that $T(n-i) \leq \sum_{j=1}^{n-i} T(n-i-j)$. Then, the recurrence of the pivot-based branching rule can be improved as:

$$T(n) \leq \sum_{i=1}^{|P_1|} T(n-i) + \sum_{i=1}^{|P_2|} T(n-|P_1|-i). \quad (4)$$

It is easy to verify that $T(n) \leq \sum_{i=1}^{k} T(n-i)$ if $\overline{d} = |P_1| + |P_2| \leq k$. For the case where $\overline{d} > k$, we observe that the first $\overline{d} - k$ sub-recursive calls of $Branch(S, C)$ will apply the branching rule of case (2). By combining Eq. (3) with Eq. (4), we obtain that $T(n) \leq \sum_{i=1}^{\overline{d}-k} \sum_{j=1}^{k} T(n-i-j) + \sum_{i=1}^{\overline{d}-k} T(n-\overline{d}-2) + \sum_{i=1}^{k} T(n-(\overline{d}-k)-i)$. Based on the conditions of $T(n) \leq 2T(n-1)$ and $\sum_{i=1}^{\overline{d}-k} T(n-\overline{d}-2) \leq T(n-k-2)$ if $\overline{d} > k$, we obtain the following recurrence:

$$T(n) \leq \sum_{i=1}^{k} T(n-i) + T(n-k-2). \quad (5)$$

To summary, we establish that the maximum size of $T(n)$ is bounded by Eq. (5). By utilizing the theoretical result in [17], we can deduce that the maximum size of $T(n)$ is bounded by $O(\gamma_k^n)$, where γ_k is the maximum real-root of function $x^{k+3} - 2x^{k+2} + x^2 - x + 1 = 0$ if $k \geq 1$. Thus, Theorem 3.3 establishes.

Theorem 3.4. *For the case where* $k = 0$, *the time complexity of Algorithm 1 is bounded by* $O(m1.414^n)$.

Proof sketch. When $k = 0$, Algorithm 1 employs either the branch reduction rules or the pivot-based branching rule. If the branch reduction rules are utilized, we obtain a recurrence of $T(n) \leq T(n-1) + T(n-4)$, as there is no vertex $v \in C$ satisfying $\overline{d}_v(S) \geq 1$. Moreover, if the pivot-based branching rule is employed, we can derive a recurrence of $T(n) \leq \overline{d}T(n-\overline{d})$. Since $\overline{d} \geq 4$, we establish that $T(n) \leq 4T(n-4) \leq \sqrt{2}^n$.

Theorem 3.5. *The space complexity of Algorithm 1 is* $O(\kappa n + m)$.

Proof. Based on the depth-first branching strategy, it is easy to verify that the $Branch(S, C)$ procedure consumes at most (κn) spaces. Since the algorithm also requires storing the entire graph in the main memory, then the overall space usage of Algorithm 1 is bounded by $O(\kappa n + m)$. □

4 FURTHER OPTIMIZATIONS

In this section, we introduce an improved algorithm based on several novel optimization techniques. Firstly, we develop a newly upper bound-based pruning algorithm that effectively reduces unnecessary branches in the branch-and-bound process. Secondly, we introduce an ordering-based heuristic approach as a preprocessing step to greatly reduce the size of the original graph. Below, we first introduce our proposed upper bounds

4.1 Upper Bounds

Let κ (or $\kappa(C)$) denote the sizes of the maximum k-defective clique in graph G (or subgraph $G(C)$). In this subsection, we explore both conventional and innovative upper bounds for κ and $\kappa(C)$, which play a crucial role in accelerating the computations of our algorithm.

Degree-based upper bound. The first upper bound is derived straightforwardly from the degree information of vertices in G, and we present the detailed result in the following lemma.

Lemma 4. For a given graph G, *the size of the maximum* k*-defective clique in* G *that contains a vertex* $v \in V$ *is at most* $d_v(G) + k + 1$. *As a consequence, we can conclude that* $\kappa \leq \max_{v \in V} d_v(G) + k + 1$.

Core-based upper bound. Now, we present a refined upper bound for both κ and $\kappa(C)$, drawing upon the well-established concept of k-core [52]. We provide the formal definition of k-core as follows.

Definition 2 ([52]). Given a graph G, *the subgraph* $G(C)$ *of* G *induced by the set* C *is a* k*-core of* G *if* $d_v(C) \geq k$ *for every* v *in* C.

Let C_k represent k-core subgraph of G. The core number of a vertex v in G, denoted by $core_v(G)$, is defined as the maximum value of k such that v belongs to the k-core subgraph C_k of G, i.e., $core_v(G) = \max\{k \mid v \in C_k\}$. Based on this concept, we can establish a tighter upper bound as follows.

Lemma 5. For a given graph G, *the size of the maximum* k*-defective clique in* G *containing a vertex* $v \in V$ *is bounded by* $core_v(G) + k + 1$. *Consequently, we can deduce that* $\kappa \leq \max_{v \in V} core_v(G) + k + 1$.

Lemma 5 clearly establishes as any k-defective clique S is also a $(|S|-k-1)$-core of G. Let δ be the maximum core number of G, representing the highest value of k for which a non-empty k-core exists in G. We also obtain that $\kappa \leq \delta + k + 1$. To determine the core number for each vertex in a given graph G, an algorithm with $O(m)$ time developed in [4] can be employed, indicating its remarkable efficiency in generating the core-based upper bound.

Color-based upper bound. We observe that the upper bound for κ and $\kappa(C)$ can be improved by a graph coloring technique. Below, we begin by providing the formal definition of graph coloring.

Definition 3. Given a graph G, the graph coloring is to assign a color number for each vertex v of G, denoted by $col_v(G)$, such that any two adjacent vertices have different colors. Formally, for every $(u,v) \in E$, it should hold that $col_v(G) \neq col_u(G)$.

Denote by ω and $\omega(C)$ the number of distinct colors in G and the subgraph $G(C)$ of G induced by C, respectively. Based on the concept of graph coloring, we can establish the following upper bound for κ and $\kappa(C)$.

Lemma 6. Given a coloring of the graph G and a subgraph $G(C)$ of G, the size of the maximum k-defective clique in G and $G(C)$ can be bounded by $\omega + k$ and $\omega(C) + k$, respectively.

Proof sketch. Given a k-defective clique S, we partition it into two disjoint subsets, S_1 and S_2, while ensuring the follows constraints: for each $v \in S_1$ (resp. $u \in S_2$), it holds that $\nexists w \in S_1 \setminus \{v\}$ with $col_v(G) = col_w(G)$ (resp. $\exists w \in S_1$ with $col_u(G) = col_w(G)$). It can be verified that $|S_1| \leq \omega$ and $|S_2| \leq k$. Thus, this lemma is obtained.

Lemma 6 emphasizes the importance of finding a smaller value for ω ($\omega(C)$) in order to achieve a better upper bound. However, it is worth noting that determining the smallest value of ω ($\omega(C)$) for graph coloring poses a computational challenge and is known to be NP-hard [24]. Thus, numerous heuristic approaches have been explored to address graph coloring problem [28, 56]. In this paper, we adopt a widely used degeneracy ordering for graph coloring. The definition of degeneracy ordering [32] is presented below.

Definition 4. Given a graph $G = (V, E)$, the degeneracy ordering is a permutation $\{v_1, v_2, ..., v_4\}$ of vertices in V such that for each vertex v_i, its degree is smallest in the subgraph $G(\{v_i, v_{i+1}, ..., v_n\})$.

The degeneracy ordering, akin to the technique employed for computing the k-core of a graph, can be obtained by the peeling technique [4]. Specifically, the vertex removal ordering aligns with the degeneracy ordering, which can be accomplished within a time complexity of at most $O(m)$. Subsequently, we can systematically assign colors to each vertex v of the graph G in a reverse order of the degeneracy ordering. As a result, the upper bound, derived from graph coloring, can be efficiently computed in $O(m)$ time.

Advanced color-based upper bound. Let S be a vertex subset of G, and $\kappa(S,C)$ represent the size of the maximum k-defective clique in $G(S \cup C)$ that includes all vertices in S. We define $\overline{d}_v(S)$ as the number of non-neighbors of vertex v in S, given by $\overline{d}_v(S) = |S \setminus N_v(S)|$. Moreover, we define $c_v(S)$ as the count of other vertices in S that share the same color as vertex v, denoted as $c_v(S) = |\{u \in S \setminus \{v\} | col_v(G) = col_u(G)\}|$. With these definitions established, we present the following lemma.

Lemma 7. Consider a graph G and a non-maximal k-defective clique S of G. If there exists a vertex set $D \subseteq V \setminus S$ that can form a larger k-defective clique with S, then for each vertex $v \in D$, there are at least $\overline{d}_v(S) + c_v(D)$ non-neighbors of v in $G(S \cup D)$.

Algorithm 3: Upperbound(S, C, k)

```
1 D ← ∅; s ← the missing edges in G(S);
2 while C ≠ ∅ do
3     v ← a vertex in C with minimum d̄_v(S) + c_v(D);
4     if s + d̄_v(S) + c_v(D) > k then break;
5     s ← s + d̄_v(S) + c_v(D);
6     D ← D ∪ {v}; C ← C \ {v};
7 return |S| + |D|;
```

Denote by $\overline{d}(S)$ the total number of missing edges in $G(S)$, i.e., $\overline{d}(S) = \frac{1}{2}\sum_{v \in S}(|S| - d_v(S) - 1)$. A lemma states the following.

Lemma 8. Given sets S and C, let D be the largest subset of C satisfying $\sum_{v \in D}(\overline{d}_v(S) + \frac{1}{2}c_v(D)) \leq k - \overline{d}(S)$. When finding the maximum k-defective clique containing S in the subgraph $G(S \cup C)$, we have $\kappa(S,C) \leq |S| + |D|$.

Proof sketch. Given the subset D of C, we observe that the number of missing edges in $G(D)$ is at least $\frac{1}{2}\sum_{v \in D} c_v(D)$. Moreover, since each vertex v in D has $\overline{d}_v(S)$ non-neighbors in S, we can deduce that the number of missing edges in $G(S \cup D)$ will increase by at least $\sum_{v \in D}(\overline{d}_v(S) + \frac{1}{2}c_v(D))$ if we add D to S. Thus, if D is largest subset of C satisfying $\sum_{v \in D}(\overline{d}_v(S) + \frac{1}{2}c_v(D)) \leq k - \overline{d}(S)$, we obtain that $\kappa(S,C) \leq |S| + |D|$.

Then, we present an algorithm, as shown in Algorithm 3, to compute the upper bound of $\kappa(S,C)$. This algorithm aims to determine the largest subset D of C. Initially, we initialize D as an empty set (line 1). Subsequently, the algorithm iteratively selects a vertex v from C that has the smallest value of $\overline{d}_v(S) + c_v(D)$ and adds it to the current subset D (lines 2-6). As v is selected to move from C to D, the missing edges in $G(S \cup D)$ increase by at least $\overline{d}_v(S) + c_v(D)$ (lines 5-6). The algorithm terminates and outputs $|S| + |D|$ as the upper bound of $\kappa(S,C)$ when either C becomes empty or the number of missing edges in $G(S \cup D)$ violates the definition of a k-defective clique (lines 2 and 4). The following theorem establishes the correctness of Algorithm 3.

Theorem 4.1. *Algorithm 3 correctly computes the upper bound of $\kappa(S,C)$.*

Proof sketch. On the contrary, assume that there exist a subset D' of C with $|D'| > |D|$ that satisfies $\sum_{v \in D'}(\overline{d}_v(S) + \frac{1}{2}c_v(D')\}) \leq k - \overline{d}(S)$. It can be seen that there exist two vertices $v \in D$ and $u \in D_1 \setminus D$ with $\overline{d}_v(S) + c_v(D \setminus \{v\}) > \overline{d}_u(S) + c_u(D \setminus \{v\})$. However, whether we consider the condition $col_v(G) = col_u(G)$ or $col_v(G) \neq col_u(G)$, we always conclude that the vertex u will be pushed into D in preference to v in our algorithm. Thus, this theorem is established.

Theorem 4.2. *The time complexity of Algorithm 3 is bounded by $O(kn + \overline{m})$, where $\overline{m}$ is the number of missing edges in $G(C)$.*

Proof. Algorithm 3 first involves sorting each vertex v in set C based on the size of $\overline{d}_v(S)$. This sorting process can be efficiently achieved in $O(kn)$ time using a bin sort. Furthermore, when a vertex v from C is added to set D, any vertex u in the set $C \setminus D$ that shares

Algorithm 4: The heuristic algorithm

Input: The graph $G = (V, E)$ and a parameter $k \geq 0$
Output: A near maximum k-defective clique S^* in G

1 Let $\{v_1, v_2, ..., v_n\}$ be the degeneracy ordering of vertices in G;
2 **for** $i = n$ *to* 1 *s.t.* $core(v_i) \geq |S^*| - k$ **do**
3 $S \leftarrow \{v_i\}$; $C \leftarrow N_{v_i}(G^+_{v_i})$;
4 **while** $\exists u \in C$ *with* $d_u(C) < |S^*| - k - 1$ **do**
5 $C \leftarrow C \setminus \{u\}$;
6 **while** $C \neq \emptyset$ **do**
7 $v \leftarrow$ a vertex in C with maximum degree (or maximum core number) in $G(S \cup C)$;
8 $S \leftarrow S \cup \{v\}$ and remove each vertex u from C if $\overline{d}_u(S)$ is larger than $k - \overline{d}(S)$;
9 **while** $\exists u \in C$ *s.t.* $d_u(N_S(C)) < |S^*| - |S| - k + \overline{d}(S)$ **do**
10 Remove u from C;
11 **if** $\exists u \in S$ *with* $d_u(N_S(C)) \leq |S^*| - |S| - k + \overline{d}(S)$ **then**
12 $S \leftarrow \emptyset$; $C \leftarrow \emptyset$;
13 **foreach** $v_j \in N^{=2}_{v_i}(G)$ *s.t.* $j > i$ **do**
14 **if** $d_{v_j}(S) \geq |S^*| - k + \overline{d}(S)$ **then** $C \leftarrow C \cup \{v_j\}$;
15 Further expand S with vertices in C as described in lines 6-12;
16 **if** $|S^*| < |S|$ **then** $S^* \leftarrow S$;
17 **return** S^*;

the same color as v will have its $c_u(D)$ value increased by 1. This particular operation takes at most $O(\overline{d}_v(C))$ time. Consequently, the overall time complexity of executing lines 2-6 in Algorithm 3 amounts to $O(\overline{m})$. Therefore, this theorem is proven. □

4.2 The Heuristic Algorithm

The basic idea of this heuristic approach is to incrementally enlarge the current k-defective clique S, by using a candidate set C. Initially, we initialize S as an empty set, while C is populated to V. During each iteration, we carefully select a vertex from C and attempt to enlarge S. Once no more vertices from C can be added to S (i.e., C becomes empty), we obtain a near-maximum maximal k-defective clique denoted as S^*. To maximize the size of S^*, we propose an ordering-based heuristic approach, which is outlined as follows.

Let $\boldsymbol{O} = \{v_1, v_2, ..., v_n\}$ be an ordering of vertices in G. We define $V^+_{v_i}$ as the set of vertices in G that rank higher than v_i in the ordering $\boldsymbol{O}$. Let $G^+_{v_i}$ be the subgraph of G induced by $V^+_{v_i}$. Our heuristic approach, based on this ordering, focuses on computing the near-maximum k-defective clique within the subgraph $G^+_{v_i}$ that includes vertex v_i for each v_i in the ordering $\boldsymbol{O}$. By executing this approach, we obtain several k-defective cliques, and the largest among them is selected as the near-maximum k-defective clique of G. Furthermore, we also employ some pruning techniques throughout this process.

Pruning techniques. When expanding the set S with vertices from C, we observe that many vertices in C can be pruned effectively. To achieve this, we employ three specific pruning techniques based on the current near-maximum k-defective clique denoted as S^*.

- *Distance-based pruning.* By Property 2, we determine that if $|S^*| \geq k + 2$, the diameter of $G(S^*)$ is at most 2. Consequently, during the expansion of $S = \{v_i\}$, only vertices in $G^+_{v_i}$ whose distance to v_i is not greater than 2 will be initialized to C.
- *Non-neighbor-based pruning.* We obtain that any vertex in C possessing more than $k - \overline{d}(S)$ non-neighbors in S can be safely excluded from C, as such vertices cannot contribute to the formation of a larger k-defective clique when combined with S.
- *Common neighbor-based pruning.* Let $N_S(C) = \{u \in C | S \subseteq N_u(G)\}$ be the set of common neighbors of S in C. Given a vertex $u \in C$, if $d_u(N_S(C)) < |S^*| - k - |S| + \overline{d}(S)$, it follows that u cannot be part of a maximum k-defective clique with a size equal to or greater than $|S^*|$. Consequently, such a vertex u can be safely removed from C.

Algorithm implementations. Equipped with the proposed techniques, we outline our heuristic approach in Algorithm 4.

Initially, Algorithm 4 computes the degeneracy ordering of vertices in G using a method described in [4]. Subsequently, the algorithm iteratively computes the near-maximum k-defective clique containing v_i in $G^+_{v_i}$ for each v_i in the degeneracy ordering (lines 2-16). The algorithm constructs the candidate set C with vertices in $N_{v_i}(G^+_{v_i})$ to expand the current k-defective clique $S = \{v_i\}$. Then, it progressively selects a vertex v from C with the largest degree (or maximum core number) to expand S until $C = \emptyset$. Notably, when a vertex v is added to S, all the remaining vertices in the candidate set C used to expand $S \cup \{v\}$ adhere to the non-neighbor-based pruning (line 8) and the common neighbor-based pruning (lines 4-5, lines 9-10). Furthermore, utilizing the diameter-based pruning, the algorithm further expands S by considering the vertices with a distance of 2 from v_i using a similar technique as before (lines 13-16), where $N^{=2}_{v_i}(G) = \{u \in V | u \notin N_{v_i}(G), N_u(G) \cap N_{v_i}(G) \neq \emptyset\}$. Finally, the heuristic algorithm terminates after each vertex in V has been processed and returns the largest k-defective clique detected as the final near-maximum k-defective clique of G (line 17). The time complexity of Algorithm 4 is provided below.

Theorem 4.3. *Let n' (m') be the maximum number of vertices (edges) in $G(S \cup C)$ obtained in Algorithm 4. Then, the time complexity of Algorithm 4 is bounded by $O(n(\kappa n' + m'))$.*

Proof. It is evident that the algorithm requires at most $O(m')$ time to perform the common neighbor-based pruning in $G(S \cup C)$ (lines 4-5 and lines 9-10). Additionally, when a vertex v is added into S, it necessitates at most $O(n')$ time to update the candidate set. Therefore, lines 7-8 of Algorithm 4 consume at most $O(\kappa n')$ time, as at most κ vertices in C can be added into S. Hence, the total time-consuming of Algorithm 4 is bounded by $O(n(\kappa n' + m'))$. □

Note that the practical performance of Algorithm 4 can be highly efficient (as highlighted in Sec. 5.2). This is mainly due to the fact that the size of C in lines 2-12 is bounded by δ, which is relatively small in real-world graphs. Moreover, for most of subgraphs $G(S \cup C)$, the number of vertices is much less than n'. Consequently, the practical performance of Algorithm 4 is considerably lower than its worst-case time complexity.

4.3 The Improved Algorithm

The pseudo-code of our improved algorithm is outlined in Algorithm 5. Specifically, it begins by employing the proposed heuristic algorithm (Algorithm 4) to acquire a near-maximum k-defective clique S^* in G (line 1). Subsequently, this algorithm identifies a $(|S^*| - k)$-core subgraph and focuses mainly on computing the maximum k-defective clique of G within this subgraph (line 2).

Algorithm 5: The heuristic-based improved algorithm

Input: The graph $G = (V, E)$ and a parameter k
Output: The maximum k-defective clique S^* of G

1 S^* returned by Algorithm 4;
2 $G \leftarrow (|S^*| - k)$-core of G;
3 Let $\{v_1, v_2, ..., v_n\}$ be the degeneracy ordering of vertices in G;
4 **for** $i = n$ *to* 1 *s.t.* $core(v_i) \geq |S^*| - k$ **do**
5 $S \leftarrow \{v_i\}$; $C_1 \leftarrow N_{v_i}(G^+_{v_i})$; $C_2 \leftarrow \emptyset$;
6 **while** $\exists u \in C_1$ *with* $d_u(C_1) < |S^*| - k - 1$ **do**
7 $C_1 \leftarrow C_1 \setminus \{u\}$;
8 **if** $|S \cup C_1| \leq |S^*| - k$ **then continue**;
9 **for** *each* $u \in N^{=2}_{v_i}(G^+_{v_i})$ **do**
10 **if** $d_u(C_1) \geq |S^*| - k$ **then** $C_2 \leftarrow C_2 \cup \{u\}$;
11 Coloring $G(S \cup C_1 \cup C_2)$ with degeneracy ordering;
12 $Branch(S, C_1 \cup C_2)$; `/* Algorithm 3 is also invoked */`

This is because other vertices cannot be part of a k-defective clique with a size surpassing $|S^*|$. The algorithm then iteratively computes the maximum k-defective clique containing v_i within G, following the reverse order of the degeneracy ordering (lines 3-12). Prior to the enumeration process, this algorithm also employs the pruning techniques outlined in Sec. 4.2 to reduce the size of the candidate set of $S = \{v_i\}$. Notably, each vertex in the candidate set $C_1 \cup C_2$ satisfies two conditions: it is at most 2 distances away from v_i, and it shares at least $|S^*| - k$ common neighbors with v_i (lines 5-10). Moreover, if the size of $S \cup C_1$ is not larger than $|S^*| - k$, the computation for v_i can be skipped by our observations (line 8). Following this, the algorithm employs the degeneracy ordering to color each vertex in $G(S \cup C_1 \cup C_2)$ (line 11), which serves as a prerequisite for Algorithm 3. Finally, the algorithm invokes the *Branch* procedure developed in Sec. 3.3 to compute the maximum k-defective clique containing v_i in G, and updates the current maximum result S^* if a larger k-defective clique is obtained (lines 12).

5 EXPERIMENTS

In this section, we conduct extensive experiments to evaluate the efficiency of the proposed algorithms. Below, we first introduce the experimental setup, and then report the experimental results.

5.1 Experimental Setup

Algorithms. We implement an algorithm called MDCE to identify the maximum k-defective clique of G, which contains all proposed techniques as detailed in Algorithm 5. To assess the performance of our proposed algorithms, we also use the state-of-the-art algorithms KDBB and MADEC as the baseline for performance evaluation, where KDBB and MADEC are developed in [19] and [13] respectively. It is worth noting that due to the absence of open-source code for KDBB, we utilize our own implementation for the experiments, which exhibits better performance compared to the reported results in the literature. All the tested algorithms are implemented in C++, and tested on a PC with one 2.2 GHz CPU and 64GB memory running CentOS operating system.

Datasets. We employ three distinct sets of datasets to evaluate the efficiency of the proposed algorithms. The first set of datasets, consisting of 139 massive real-world graphs, is originally obtained from the Network Data Repository [49]. These datasets have been widely used in various studies [18, 19, 65] and can be downloaded from http://lcs.ios.ac.cn/~caisw/graphs.html. The second set of datasets, which includes 114 Facebook graphs, is available at https://networkrepository.com/socfb.php. Lastly, The third set of datasets comprises 83 DIMACS10 graphs, which can be accessed at https://networkrepository.com/dimacs.php. These graphs have been utilized as benchmark graphs for evaluating the performance of the maximum k-defective clique enumeration algorithms [19].

Parameters. In our experimental evaluations, we follow a similar approach as [13, 19] by considering values of k as 1, 3, 5, and 10. However, we note that the size of the maximum k-defective clique in certain datasets is relatively small. Consequently, setting k to excessively large values may lack meaningful implications. Thus, we also impose an additional constraint of $k < \kappa - 1$, where κ is the size of the maximum k-defective clique in a given graph G.

5.2 Experimental Results

Exp-1: Performance evaluation on representative benchmark real-world graphs. In this experiment, we evaluate the performance of various algorithms in finding the maximum k-defective clique. Table 1 presents the results of each algorithm, including MDCE, KDBB and MADEC, on 38 benchmark real-world graphs with varying k, where "—" denotes that the algorithm failed to complete the computations within a time threshold of 10800 seconds (3 hours). As observed, the runtime of our algorithm MDCE consistently outperforms all existing algorithms (KDBB and MADEC) on all tested benchmark datasets across different values varying k. More specifically, our algorithm achieves at least 3 orders of magnitudes faster than KDBB and MADEC on most datasets. For instance, when $k = 1$ and considering the flixster dataset, MDCE only requires 0.59 seconds to identify the maximum k-defective clique, while KDBB and MADEC fail to complete the computation within a given 10800 seconds. Furthermore, we observe that the time-consuming of our algorithm is relatively insensitive to increase in k on most datasets, whereas the performance of existing algorithms decreases sharply with increasing k. For example, on the tech-as-skitter dataset, when $k = 1$, MDCE, KDBB and MADEC take 0.12 seconds, 0.824 seconds, and 705.63 seconds, respectively, to find the maximum k-defective clique. However, when k grows to 10, MDCE only requires 0.19 seconds, while KDBB and MADEC fail to complete the task in 10800 seconds. This notable performance improvement is due to the effectiveness of the proposed branching rules and upper-bound techniques in pruning unnecessary branches during the enumeration process. These experimental results clearly demonstrate the superior of our proposed algorithm in terms of runtime efficiency.

Exp-2: Solved instance of various algorithms on massive graphs. In this experiment, we aim to evaluate the performance of our proposed algorithm on massive datasets, comprising 139 real-world graphs, 83 DIMACS10 graphs, and 114 Facebook graphs. Fig. 3 showcases the number of solved instances with varying time thresholds for different values of k. From this figure, we observe that our algorithm, MDCE, consistently outperforms the state-of-the art algorithms, KDBB and MADEC, in terms of the number of solved instances. This result validates the efficiency of our propose algorithm in efficiently identifying the maximum k-defective clique of G. Furthermore, as the value of k increases, we observe

Table 1: Runtime of various algorithms on 38 real-world graphs (in seconds), where 1K=10^3, 1M=10^6.

Datasets	n	m	$k=1$			$k=3$			$k=5$			$k=10$		
			MDCE	KDBB	MADEC	MDCE	KDBB	MADEC	MDCE	KDBB	MADEC	MDCE	KDBB	MADEC
web-spam	4.8K	37.4K	**0.004**	0.652	8.13	**0.008**	5.720	1226.7	**0.02**	44.452	–	**0.35**	911.1	–
tech-WHOIS	7.5K	56.9K	**0.02**	7.08	3.50	**0.02**	287.4	321.3	**0.03**	5665.3	8794.9	**0.09**	–	–
scc_retweet	1.2K	65.9K	**0.001**	0.10	0.033	**0.08**	0.55	0.67	**0.013**	32.97	11.63	**0.026**	220.29	2606.7
scc_fb-forum	488	71K	**0.02**	0.22	0.05	**0.03**	13.19	1.38	**0.04**	1820.9	41.37	**0.18**	–	–
ia-enron-large	33.6K	180.8K	**0.021**	0.105	430.67	**0.033**	6.63	–	**0.057**	50.74	–	**0.52**	344.66	–
soc-douban	155K	327K	**0.01**	0.01	350.24	**0.01**	0.6	597.8	**0.01**	3.01	1063.2	**0.02**	1018.2	2472
soc-slashdot	70K	359K	**0.06**	197.9	1433.3	**0.14**	618.7	–	**0.28**	1499.9	–	**1.32**	5046.4	–
socfb-Duke14	9.9K	506K	**0.60**	7070	–	**1.52**	8529	–	**2.24**	–	–	**11.06**	–	–
socfb-UConn	17.2K	604.8K	**0.08**	2.67	4725.9	**0.085**	19.76	–	**0.095**	21.93	–	**0.132**	35.61	–
tech-RL-caida	191K	608K	**0.01**	0.06	98.02	**0.01**	1.13	737.27	**0.01**	3.38	–	**0.04**	51.10	–
socfb-wosn-friends	6.4K	817K	**0.13**	13.37	–	**0.14**	44.02	–	**0.18**	171.4	–	**0.23**	637.2	–
socfb-Wisconsin87	24K	836K	**0.32**	49.07	–	**0.34**	97.58	–	**0.30**	251.2	–	**0.39**	1787	–
socfb-Berkeley13	22.9K	852.4K	**0.23**	12.82	–	**0.23**	22.00	–	**0.24**	64.18	–	**0.29**	155.39	–
soc-gowalla	197K	950K	**0.001**	0.001	900.4	**0.001**	0.009	–	**0.041**	0.087	–	**0.059**	47.94	–
socfb-UGA50	24K	1.2M	**0.61**	684.53	–	**0.62**	1358.6	–	**0.68**	2175.4	–	**1.14**	6039.2	–
socfb-Texas80	31K	1.2M	**0.34**	257.0	7262	**0.32**	1529	–	**0.40**	7479	–	**0.42**	10258	–
socfb-Indiana	29K	1.3M	**0.56**	43.43	–	**0.57**	160.5	–	**0.64**	215.8	–	**0.67**	803.9	–
sc-nasasrb	55K	1.3M	**0.15**	153.9	1384.8	**0.23**	311.5	1400.2	**0.43**	1472.5	1400.1	**2.42**	7070.0	1428.8
soc-delicious	536K	1.4M	**0.011**	0.15	62.4	**0.014**	0.12	2242.5	**0.017**	3.38	–	**0.035**	56.93	–
socfb-UF	35K	1.5M	**0.62**	617.83	–	**0.64**	1207.0	–	**0.59**	1567.5	–	**0.68**	2459.9	–
socfb-Texas84	36K	1.6M	**0.58**	1148.5	–	**0.62**	1506.1	–	**0.70**	2452.3	–	**0.95**	9621.6	–
sc-shipsec1	140K	1.7M	**0.02**	0.12	2180.9	**0.03**	0.17	2555.6	**0.03**	0.22	3534.8	**0.26**	389.0	–
soc-youtube	496K	1.9M	**0.44**	104.8	–	**1.19**	620.2	–	**3.39**	2487.7	–	**26.73**	–	–
sc-shipsec5	179K	2.2M	**0.06**	3.55	–	**0.09**	50.58	–	**0.12**	107.2	–	**0.30**	424.7	–
sc-pkustk11	88K	2.56M	**0.29**	1.79	896.35	**0.28**	4.01	1843.2	**0.28**	4.40	2159.6	**0.38**	35.61	4572.7
sc-pkustk13	94.8K	3.26M	**0.636**	34.37	6685.4	**0.655**	469.54	6758.3	**0.709**	976.00	–	**1.148**	–	–
scc_reality	6.8K	4.7M	**0.001**	0.004	0.29	**0.001**	0.004	0.29	**0.14**	38.12	1.47	**1.08**	–	–
sc-pwtk	218K	5.6M	**0.92**	4406.3	–	**1.78**	–	–	**2.83**	–	–	**11.1**	–	–
soc-digg	771K	5.9M	**39.7**	–	–	**131**	–	–	**46.6**	–	–	**120.2**	–	–
web-it-2004	509K	7.2M	**0.001**	0.001	0.57	**0.13**	2.22	0.55	**0.14**	4.22	0.55	**0.34**	16.95	5.8
soc-flixster	2.5M	7.9M	**0.59**	–	–	**0.67**	–	–	**1.05**	–	–	**2.51**	–	–
tech-as-skitter	1.7M	11M	**0.12**	0.824	705.63	**0.12**	38.18	–	**0.14**	329.4	–	**0.19**	–	–
web-uk-2005	130K	12M	**0.18**	0.78	0.86	**0.29**	3.34	3.44	**0.32**	11.12	3.49	**0.53**	34.25	9.19
sc-ldoor	909K	21M	**7.17**	–	–	**17.4**	–	–	**34.7**	–	–	**983**	–	–
socfb-B-anon	2.9M	21M	**10.8**	194.1	–	**11.6**	504.3	–	**11.7**	1899	–	**14.2**	–	–
soc-pokec	1.6M	22M	**4.92**	4.225	–	**5.46**	8.51	–	**6.07**	11.61	–	**8.29**	121.0	–
socfb-A-anon	3.1M	23M	**11.3**	113.6	–	**12.4**	574.9	–	**12.9**	808.8	–	**15.7**	10623	–
soc-orkut	3M	106M	**78.5**	–	–	**132.5**	–	–	**192.6**	–	–	**350.4**	–	–

that the decrease in the number of solved instances for MDCE is much less significant compared to the state-of-the-art algorithms KDBB and MADEC. For instance, when $k = 1$, MDCE, KDBB, and MADEC solve 135, 113 and 87 instances within 100 seconds, respectively. However, when k grows to 10, MDCE solves 126 instances, while KDBB and MADEC can only handle 76 and 51 instances, respectively, under the same conditions. This further emphasizes the efficiency of our proposed techniques in reducing unnecessary computations, even when dealing with larger values of k.

Exp-3: Runtime of various algorithms with k growing. In this experiment, we further evaluate the performance of each algorithm on 4 representative datasets with varying k. Fig. 4 illustrates the detailed experimental results for three tested algorithms, with a time threshold of 3 hours. As can be seen, our algorithm, MDCE, successfully solves majority of tested graphs even when k is increased up to 30. However, the state-of-the-arts, KDBB and MADEC, are unable to complete the computations within a time threshold of 3 hours on most parameter settings. Furthermore, we observe that the runtime of our algorithm, MDCE, increases smoothly with the increase of k, whereas the existing algorithms, KDBB and MADEC, exhibit sharp increases. For instance, on the scc_retweet dataset, when k takes values of 1, 10, and 20, MDCE completes the computations in 0.001, 0.026, and 0.205 seconds, respectively. However, the existing algorithm KDBB (MADEC) requires 0.1 (0.33), 220.34 (2606.74), and >10800 (>10800) seconds, respectively. This experimental result demonstrates that our algorithm maintains excellent pruning performance even as k grows significantly large.

Exp-4: Results of the proposed heuristic algorithm. Denote by HMDC our proposed heuristic approach (Algorithm 4). In this experiment, we assess the efficiency and effectiveness of HMDC by examining the number of instances it solves under different time threshold and the difference in size between the results returned by HMDC and MDCE. Fig. 5 displays the experimental results on 139 real-world graphs. Here, σ represents $\kappa - |D^*|$, where κ is the size of the maximum k-defective clique and D^* is the result obtained by HMDC. Note that the results on other datasets are consistent. From this figure, we can note that the runtime of the proposed heuristic algorithm, HMDC, is highly efficient, taking less than 100 seconds for almost all tested datasets when $k \leq 10$. Moreover, we observe that the runtime of HMDC remains stable even with changes in k, indicating its ability to handle large real-world graphs effectively. Additionally, we observe that the size of D^* obtained by HMDC closely approximates κ. For instance, when $k = 1$ and $k = 3$, the gap σ between κ and $|D^*|$ consistently remains below or equal to 3 across all 139 real-world graphs, thus further affirming the efficacy of our proposed heuristic approach.

Exp-5: Efficiency of the proposed algorithm without the heuristic approach. We define our algorithm MDCE without

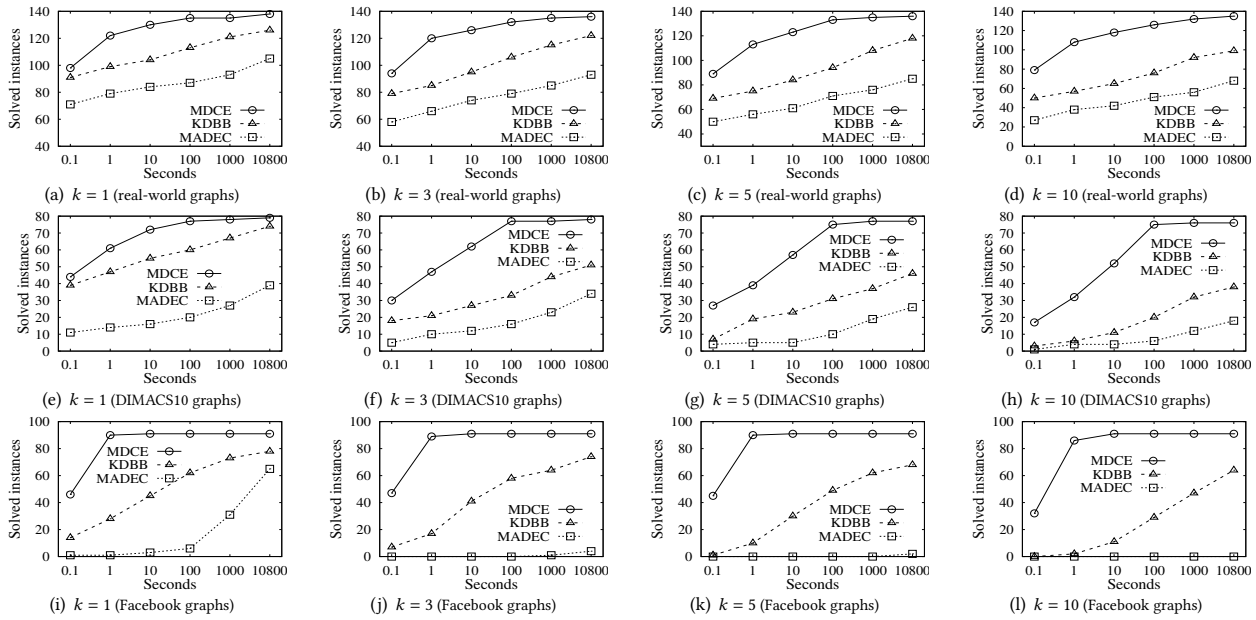


Figure 3: Number of solved instances of various algorithms on massive graphs with different time thresholds.

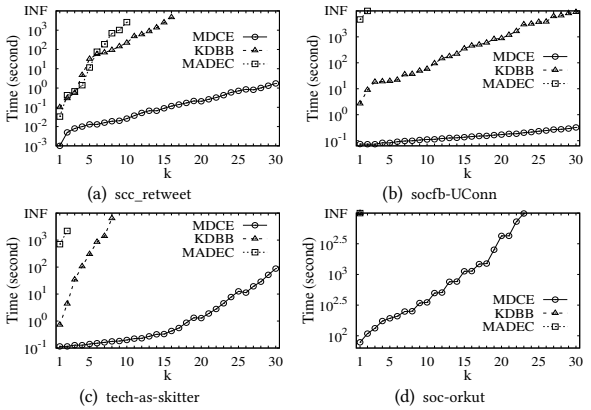


Figure 4: Runtime of various algorithms with k growing.

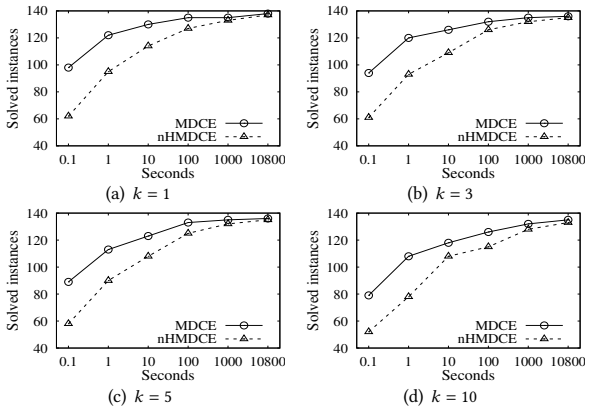


Figure 6: Efficiency of MDCE without the heuristic approach.

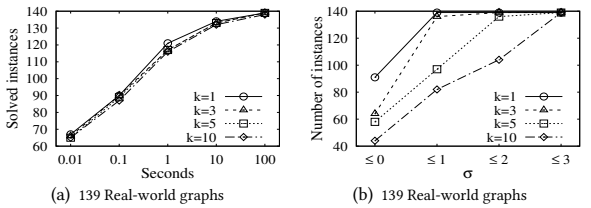


Figure 5: Results of the heuristic approach.

the heuristic approach as nHMDCE, which refers to Algorithm 5 without lines 1-2. In this experiment, we test the effectiveness of algorithm nHMDCE in finding the maximum k-defective clique of G. Fig. 6 illustrates the number of solved instanced of nHMDCE and MDCE on 139 real-world graphs with different time thresholds when varying k. From the results, we note that MDCE consistently solves more instances than nHMDCE. This disparity arises because the proposed heuristic algorithm can efficiently identify a near-maximum k-defective clique, enabling significant pruning of vertices based on the obtained result. Consequently, the efficiency of the enumeration algorithm is substantially improved. Nevertheless, it is worth noting that nHMDCE still outperforms the existing solutions KDBB and MADEC in most parameter settings, reinforcing the effectiveness of the proposed branching rules in identifying the maximum k-defective clique in graph G.

Exp-6: Efficiency of proposed upper bound techniques. In this experiment, we test the effectiveness of the proposed upper bounds. We designate MDCE-N as Algorithm 5 without any upper bounds, and let MDCE-C and MDCE-L be Algorithm 5 augmented with core-based (Lemma 5) and color-based (Lemma 6) upper bounds, respectively. We conduct experiments on a set of 139 real-world graphs, as described in Fig. 7. As can be seen, we note that MDCE consistently demonstrates superior performance compared to all other tested algorithms. This can be attributed to the tightness of the proposed advanced color-based upper bound and the algorithm's efficiency in computing our proposed upper bound. Additionally, we observe that within a given runtime threshold, the gap in number of solved instances between the algorithm MDCE and the other algorithms (MDCE-N, MDCE-C, and MDCE-L) increases

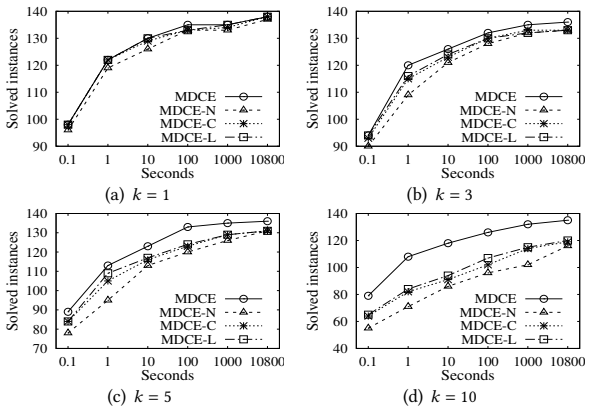


Figure 7: Efficiency of MDCE with various upper bounds.

as k grows. For instance, with a time threshold of 100 seconds, when $k = 1$, MDCE solves 135 instances, while both MDCE-N, MDCE-C, and MDCE-L solve 133 instances each. However, when k grows to 10, MDCE solves 126 instances, whereas MDCE-N, MDCE-C, and MDCE-L only manage to solve 96, 102, and 107 instances, respectively. This experiment further highlights the efficiency of the proposed upper bound pruning technique.

Exp-7: Efficiency of proposed branch reduction rules. This experiment aims to evaluate the performance of the proposed branch reduction rules. Let us denote MDCE-R the algorithm MDCE without the graph reduction rules developed in Sec. 3.1. Table 2 presents the experimental results obtained by executing MDCE and MDCE-R on 7 representative real-world graphs with varying k. The results clearly demonstrate that the runtime of MDCE consistently outperforms that of MDCE-R across all tested datasets. Moreover, even as k increases, MDCE maintains its superior performance compared to MDCE-R. These findings provide important evidence supporting the efficiency of the proposed branch reduction rules in effectively reducing unnecessary branches of our proposed algorithm.

6 RELATED WORKS

Maximum clique enumerations. The problem of determining the maximum clique in a graph G has been proven to be NP-hard [8], with approximating a satisfactory solution being a challenging task [66]. Over the past few decades, numerous exact algorithms have been developed to tackle this problem [10, 11, 29–31, 43, 50, 51, 54–56]. Most of these algorithms are built upon a branch-and-bound framework, and employing various enumeration strategies to find the maximum clique. Among the existing approaches, those proposed by Tomita et al. [54–56] and Li et al. [29–31] have gained significant popularity. Specifically, Tomita et al. [54] introduced an algorithm based on degeneracy ordering and further improved it using the graph-recoloring technique [56] and the adjunct coloring-based ordering [55]. On the other hand, Li et al. proposed a branch-and-bound algorithm based on MaxSAT reasoning[31], and further improving it with incremental upper bounds [30] and dynamic and static vertex ordering strategies [29]. Additionally, several parallel approaches utilizing multi-cores have also been developed to enhance practical efficiency [50, 51]. However, the aforementioned upper bound techniques based on coloring and MaxSAT reasoning face challenges when extended to solve the problem of finding the maximum k-defective clique, wherein the subgraph allows at most k missing edges. To address this issue, this paper introduces a novel upper bound approach based on graph coloring, which significantly differs from existing color-based upper bounds.

Table 2: Runtime of MDCE without branch reduction rules.

	$k = 1$		$k = 5$		$k = 10$	
Datasets	MDCE	MDCE-R	MDCE	MDCE-R	MDCE	MDCE-R
scc_fb-messages	**0.29**	1.38	**0.32**	1.39	**0.54**	1.61
scc_reality	**2.29**	7.27	**2.64**	7.48	**3.80**	8.59
sc-ldoor	**7.17**	10.23	**34.75**	45.36	**983.3**	1373.1
socfb-Duke14	**0.60**	0.70	**2.24**	2.84	**11.06**	14.66
socfb-Texas84	**0.58**	0.65	**0.70**	0.88	**0.95**	1.41
soc-pokec	**4.92**	5.25	**6.07**	7.35	**8.29**	10.22
tech-WHOIS	**0.022**	0.023	**0.032**	0.042	**0.092**	0.27

Maximum relaxed-clique enumerations. Since the clique model is often too restrictive for many real-world applications, several relaxed-clique models have also been developed to address this limitation [46]. These include the k-plex [53], s-clique [46], and γ-quasi-clique [33], and others. Among these models, significant attention has been given to the problems of finding the maximum k-plex [3, 12, 18, 23, 37, 40, 62, 65] and maximum γ-quasi-clique [36, 38, 42, 44, 45, 48, 59] in recent years. Regarding the maximum k-plex problem, Balasundaram et al. [3] proposed an integer programming formulation and a branch-and-cut algorithm. McClosky et al. [37] introduced a combinatorial algorithm based on co-k-plex coloring as an upper bound technique. Xiao et al. [62] developed an exact algorithm with a time complexity of $O(P(n)\alpha^n)$, employing a symmetric branching rule, where $\alpha < 2$. More recently, several novel techniques have also been developed to further improve the efficiency, including dynamic vertex selection strategies [18], second-order reduction and coloring-based upper bounds [65], partition-based upper bounds [23], and exploiting small dense subgraphs [12]. Concerning the maximum γ-quasi-clique problem, Pattillo et al. [45] and Veremyev et al. [59] formulated the problem using integer programming. Pajouh et al. [42], Pastukhov et al. [44], and Ribeiro et al. [48] respectively developed branch-and-bound algorithms incorporating various pruning techniques. Additionally, upper bounds on the maximum γ-quasi-clique number have been further explored in [36, 38]. Unfortunately, all these existing algorithms still face challenges when efficiently extended to solve the problem of finding the maximum k-defective clique. In this paper, we propose a theoretically and practically efficient solution to find the maximum k-defective clique.

7 CONCLUSION

In this paper, we focus on the problem of identifying the maximum k-defective clique of a given graph G. To address this problem, we introduce an efficient enumeration algorithm accompanied by a series of novel optimization techniques. Specifically, our enumeration algorithm leverages newly-developed graph reduction rules and a pivot-based branching rule. Our analysis demonstrates that the proposed algorithm achieves a time complexity of $O(m\gamma_k^n)$, where γ_k is a real value strictly less than 2. To further enhance efficiency, we also present an efficient pruning algorithm based on novel upper bounds that we developed. Moreover, we make additional improvements to our algorithm by incorporating an ordering-based heuristic-based algorithm as the preprocessing step. Finally, we conduct comprehensive experiments to validate the effectiveness and efficiency of our proposed approaches.

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