Exact Algorithms with New Upper Bounds for the Maximum k-plex Problem

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Abstract

The Maximum k-plex Problem (MKP) is a degree relaxation of the widely known Maximum Clique Problem. As a practical NP-hard problem, MKP has many important real-world applications, such as the analysis of various complex networks. Branch-and-bound (BnB) algorithms are a type of well-studied and effective exact algorithms for MKP, and the key for BnB algorithms is the bound design. Recent BnB MKP algorithms involve two kinds of upper bounds based on graph coloring and partition, respectively, that work in different perspectives and thus are complementary with each other. We first propose a new coloring-based upper bound, termed Relaxed Graph Color Bound (RelaxGCB), that significantly outperforms the previous coloring-based upper bound. Then we further propose another new upper bound, termed RelaxPUB, that incorporates RelaxGCB and a partition-based upper bound in a novel way, making use of their complementarity. We apply RelaxGCB and RelaxPUB to state-of-the-art BnB MKP algorithms and produce eight new BnB algorithms. Extensive experiments using diverse k values based on dense or massive sparse graphs demonstrate the excellent performance and robustness of our methods.

1 Introduction

Given an undirected graph $G = (V, E)$, a clique is a set of vertices that are pairwise adjacent, and a k-plex [Seidman and Foster, 1978] is a set of vertices $S \subseteq V$ where each vertex $v \in S$ is non-adjacent to at most k vertices (including v itself) in S. Thus, a clique is a 1-plex, and k-plex is a relaxation structure of clique. The Maximum Clique Problem (MCP) is to find the largest clique in G, while the Maximum k-plex Problem (MKP) is to find the largest k-plex in G.

MCP is a famous and fundamental NP-hard problem, and the clique model has been widely investigated in the past decades. However, in many real-world applications, such as social network mining [Seidman and Foster, 1978; Pattillo *et al.*, 2013; Conte *et al.*, 2018; Zhu *et al.*, 2020; Wang *et al.*, 2023a] and biological network analysis [Grbic *et al.*, 2020], dense subgraphs need not to be restrictive cliques but allow missing a few connections. Therefore, investigating relaxation clique structures like k-plex is significant, and studies related to k-plex have sustainably grown in recent decades [Balasundaram *et al.*, 2011; McClosky and Hicks, 2012; Berlowitz *et al.*, 2015; Conte *et al.*, 2017; Wang *et al.*, 2022; Matsugu *et al.*, 2023].

Many efficient exact methods for the NP-hard MKP have been proposed [Xiao *et al.*, 2017; Gao *et al.*, 2018; Zhou *et al.*, 2021; Jiang *et al.*, 2021; Chang *et al.*, 2022; Wang *et al.*, 2023b; Jiang *et al.*, 2023; Chang and Yao, 2024], resulting in various effective techniques, such as reduction rules, upper bounds, inprocessing methods, etc. Most of these studies follow the branch-and-bound (BnB) framework [Lawler and Wood, 1966], whose performance heavily depends on the quality of the upper bounds.

A BnB MKP algorithm usually maintains the current growing partial k-plex $S \subseteq V$ and the corresponding candidate vertex set $C \subseteq V \backslash S$. Existing methods for calculating the upper bound on the number of vertices that C can provide for S can be divided into two categories. The first considers the connectivity between vertices in C only, such as the graph color bound (GCB) proposed in the Maplex algorithm [Zhou *et al.*, 2021]. The second considers the connectivity between vertices in C and vertices in S, including the partition-based upper bounds (PUB) proposed in the KpLeX [Jiang *et al.*, 2021] algorithm and also used in the kPlexS [Chang *et al.*, 2022] and KPLEX [Wang *et al.*, 2023b] algorithms.

In this work, we observe that the existing upper bounds are still not very tight. For a graph G, an independent set I is a subset of V where any two vertices are non-adjacent. Graph coloring assigns a color to each vertex such that adjacent vertices are in different colors, which is widely used for finding independent sets in graphs. GCB [Zhou *et al.*, 2021] claims that an independent set $I \subseteq C$ can provide at most $\min\{|I|, k\}$ vertices for S, ignoring the connectivity between vertices in I and vertices in S. While PUB [Jiang *et al.*, 2021] simply regards C as a clique. Also, due to different motivations of the two kinds of upper bounds, they show complementary performance in various instances, as indicated in our follow-up examples and experiments.

Based on our observation, We propose a new upper bound based on graph coloring called Relaxed Graph Color Bound

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(RelaxGCB) with two new techniques, bringing new ideas for coloring-based upper bounds in relaxation clique problems. RelaxGCB first calculates an upper bound for each independent set $I \subseteq C$ that is strictly no worse than GCB by considering the connectivity between not only vertices in I themselves but also vertices in I and vertices in S. Furthermore, RelaxGCB relaxes the restrictive structure of independent sets, allowing to add some extra vertices to a maximal independent set (*i.e.*, not contained by any other independent set) $I \subseteq C$ without increasing the upper bound.

Based on our another observation that the coloring-based and partition-based upper bounds are complementary, we propose another new upper bound called RelaxPUB. RelaxPUB combines our RelaxGCB with a refined PUB called DisePUB [Jiang *et al.*, 2023]. Different from common methods for combining various upper bounds that sequentially calculate them until the branch can be pruned or cannot be pruned by any upper bound, RelaxPUB combines RelaxGCB and DisePUB in a novel and compact way. When calculating the upper bound of the number of vertices that C can provide for S, both of them iteratively extracts a subset $I \subseteq C$ from C, calculating the upper bound of the number of vertices that I can provide for S and accumulating the upper bounds. In each iteration, RelaxPUB uses RelaxGCB and DisePUB to respectively extract a subset from C and selects the better one, and repeats this process until C is empty.

We evaluate our proposed two upper bounds by applying them to state-of-the-art (SOTA) BnB MKP algorithms, including Maplex, kPlexS, DiseMKP, and KPLEX. Among them, Maplex only applies coloring-based upper bound, *i.e.*, GCB, and the others only apply PUB. We replace their original upper bounds with our RelaxGCB and RelaxPUB and gain new BnB algorithms. Extensive experiments show that in both dense and massive sparse graphs using various k values, RelaxGCB significantly outperforms GCB, and RelaxPUB can significantly improve the baselines and lead to SOTA BnB algorithms, indicating the excellent and generic performance of our methods.

2 Preliminaries

2.1 Definitions

Given an undirected graph $G = (V, E)$, where V is the vertex set and E the edge set, the density of G is $2|E|/(|V|(|V|-1))$, we denote $N(v)$ as the set of vertices adjacent to v, which are also called the neighbors of v. Given a vertex set $S \subseteq V$, we denote $G[S]$ as the subgraph induced by S. Given an integer k, $S \subseteq V$ is a k-plex if each vertex $v \in S$ satisfies that $|S \backslash N(v)| \leq k$.

For a growing partial k-plex S, we define $\omega_k(G, S)$ as the size of the maximum k-plex that includes all vertices in S, and $\delta(S, v) = |S \backslash N(v)|$ as the number of non-neighbors of vertex v in S. Given an integer k, we further define $\delta_k^-(S, v) = k - \delta(S, v)$ to facilitate our algorithm description. If $v \in S$, $\delta_k^-(S, v)$ indicates the maximum number of non-adjacent vertices of v that can be added to S. Otherwise, it indicates that, including v itself, the maximum number of its non-adjacent vertices that can be added to S.

2.2 Framework of BnB MKP Algorithms

During the course of a general BnB MKP algorithm, a lower bound lb on the size of the maximum k-plex is maintained, which is usually initialized by some heuristic algorithms [Zhou *et al.*, 2021; Jiang *et al.*, 2021; Chang *et al.*, 2022], and is updated once a larger k-plex is found.

A general BnB MKP algorithm usually contains a preprocessing stage and a BnB search stage. During the preprocessing, the algorithm uses some reduction rules [Gao *et al.*, 2018; Zhou *et al.*, 2021; Chang *et al.*, 2022] to remove vertices that are impossible to belong to a k-plex of size larger than lb. In the BnB search stage, the algorithm traverses the search tree to find the optimal solution. During the search, the algorithm always maintains two vertex sets, the current growing partial k-plex S, and its corresponding candidate set C containing vertices that might be added to S. Once the algorithm selects a branching vertex v to be added to S from C, it calculates an upper bound ub on the size of the maximum k-plex that can be extended from $S \cup \{v\}$, and the branch of adding v to S will be pruned if $ub \leq lb$.

3 The RelaxGCB Bound

The proposed RelaxGCB brings two new ideas of using the coloring technique for calculating the upper bound. Specifically, it first calculates a tighter bound for each independent set $I \subseteq C$, and then allows add extra vertices to a maximal independent set without changing the upper bound.

In the following, we first introduce our two improvements and provide an example for illustration, then present our RelaxColoring algorithm for calculating the RelaxGCB bound.

3.1 A Tighter Upper Bound for Independent Sets

Since vertices in the candidate set C might be non-adjacent to some vertices in the growing partial k-plex S, an independent set $I \subseteq C$ actually cannot provide k vertices for S sometimes even when $|I| > k$. We introduce a Tighter Independent Set Upper Bound (TISUB) on the number of vertices that an independent set $I \subseteq C$ can provide for S.

Lemma 1 (TISUB). *Suppose $I = \{v_1, v_2, \cdots, v_{|I|}\} \subseteq C$ is an independent set and $\delta_k^-(S, v_1) \geq \delta_k^-(S, v_2) \geq \cdots \geq \delta_k^-(S, v_{|I|})$, $\max\{i|\delta_k^-(S, v_i) \geq i\}$ is an upper bound of the number of vertices that I can provide for S.*

Proof. Firstly, ignoring the constraint of at most k non-neighbors of vertices in S, $v_1, v_2, \cdots, v_{|I|}$ is one of the best orders for adding vertices in I to S to obtain the largest k-plex in $G[S \cup I]$, because the more non-neighbors in S (as indicated by $\delta(S, v)$), the easier it is for vertices to violate the constraint. Secondly, suppose vertices $v_1, \cdots, v_i$ are going to be added to S, further adding v_{i+1} to S leads to $\delta(S, v_{i+1}) + i + 1$ non-neighbors of v_{i+1} in S (including v_{i+1} itself). Therefore, only vertices $v_i \in I$ with $\delta(S, v_i) + i \leq k$, *i.e.*, $\delta_k^-(S, v_i) \geq i$, can be added to S, and I can provide at most $\max\{i|\delta_k^-(S, v_i) \geq i\}$ vertices for S. □

To better understand the TISUB, we suggest borrowing from the h-index defined in Wikipedia. If you regard each vertex $v \in I$ as a paper of an author and $\delta_k^-(S, v)$ as the citation times of this paper. Then, *TISUB*(I, S) equals the h-index of this author.

For convenience, in the rest of this paper, we regard the vertices in any independent set $I \subseteq C$, *i.e.*, $\{v_1, v_2, \cdots, v_{|I|}\}$, as sorted in non-ascending order of their $\delta_k^-(S, v)$ values. We further define *TISUB*$(I, S) = \max\{i|\delta_k^-(S, v_i) \geq i\}$ as the upper bound calculated by TISUB on the number of vertices that I can provide for S. Note that the value of *TISUB*(I, S) is bounded by $|I|$ since $i \leq |I|$, which eliminates the need for term $|I|$ in TISUB. Moreover, since $\delta(S, v) \geq 0$, $\delta_k^-(S, v) \leq k$ holds, and *TISUB*(I, S) is also bounded by k. Therefore, we have *TISUB*$(I, S) \leq \min\{|I|, k\}$, and TISUB is strictly never worse than GCB, which claims that I can provide at most $\min\{|I|, k\}$ vertices for S.

3.2 Relax the Independent Sets

Since the relaxation property of k-plex over clique, an independent set $I \in C$ can usually provide more than one vertices for the growing partial k-plex S, and the restriction of independent sets can be relaxed to contain more vertices.

In the following, we define two kinds of vertices and then introduce two different rules for relaxing the restriction of independent sets and making maximal independent sets contain extra vertices without increasing their TISUB.

Definition 1 (Conflict Vertex)**.** *Given a vertex set I, we denote vertices $v \in I$ that are adjacent to at least one vertex in I as conflict vertices.*

Definition 2 (Loose Vertex)**.** *Given a k-plex S and a vertex set $I \subseteq C$, suppose UB is an upper bound of the number of vertices that I can provide for S, we denote each vertex $v \in I$ with $\delta_k^-(S, v) > UB$ as a loose vertex.*

Rule 1. Suppose UB is an upper bound of the number of vertices that a vertex set $I \subseteq C$ can provide for S. It is allowed to add vertex v to I if the number of vertices that are loose or conflict in $I \cup \{v\}$ is no more than UB.

Lemma 2. *After adding any vertex v to $I \subseteq C$ according to Rule 1, UB is still an upper bound of the number of vertices that $I' = I \cup \{v\}$ can provide for S.*

Proof. On one hand, if adding a vertex $v \in I'$ that is neither *conflict* nor *loose* to S, then at most $\delta_k^-(S, v) - 1 < UB$ other vertices in I' can be added to S. On the other hand, by Rule 1, we require the number of *conflict* or *loose* vertices in I' to be no more than UB. Therefore, at most UB vertices in I' can be added to S. □

Rule 2. Suppose UB is an upper bound of the number of vertices that a vertex set $I \subseteq C$ can provide for S. It is allowed to add vertex v to I if v is adjacent to at most $UB - \delta_k^-(S, v)$ vertices in I.

Lemma 3. *After adding any vertex v to $I \subseteq C$ according to Rule 2, UB is still an upper bound of the number of vertices that $I' = I \cup \{v\}$ can provide for S.*

Proof. On one hand, if adding v to S, at most $\delta_k^-(S, v) - 1$ other vertices that are non-adjacent to v in I' can be added to S. Since v is adjacent to at most $UB - \delta_k^-(S, v)$ vertices in I', thus after adding v to S, I' can still provide at most $UB - 1$ vertices for S. On the other hand, if not adding v to S, I' itself can only provide at most UB vertices for S. □

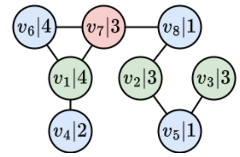


Figure 1: An example for comparing the upper bounds.

Given a maximal independent set $I \subseteq C$, both Rule 1 and Rule 2 can add extra vertices to I without increasing its TISUB. Actually, Rule 1 allows us to add finite (at most *TISUB*(I, S) - 1) *conflict* vertices to I, and Rule 2 can be repeatedly used to add any vertex satisfying the rule to I.

3.3 An Example for Illustration

We provide an example in Figure 1 to show how the upper bounds are calculated and rules are used. Figure 1 shows a subgraph of G induced by the candidate set $C = \{v_1, v_2, \cdots, v_8\}$, *i.e.*, $G[C]$, of a 4-plex S, where $v_i|t$ identifies vertex $v_i \in C$ with $\delta_k^-(S, v_i) = t$. For simplification, we hide the 4-plex S and only depict the candidate vertices.

Suppose we sequentially color vertices $v_1, v_2, \cdots, v_8$ under the constraint that adjacent vertices cannot be in the same color, C can be partitioned into 3 independent sets, $I_1 = \{v_1, v_2, v_3\}$, $I_2 = \{v_4, v_5, v_6, v_8\}$ and $I_3 = \{v_7\}$, as indicated by the colors of the vertices. The GCB of $\omega_4(G, S)$ is $|S| + \sum_{i=1}^{3} \min\{|I_i|, 4\} = |S| + 3 + 4 + 1 = |S| + 8$. The TISUB of $\omega_4(G, S)$ is $|S| + \sum_{i=1}^{3}$ *TISUB*$(I_i, S) = |S| + 3 + 2 + 1 = |S| + 6$.

Then, let us use Rule 1 to make independent set I_1 contain more vertices. For I_1, since *TISUB*$(I_1, S) = 3$, there is only one *loose* vertex v_1 in I_1. By applying Rule 1, we can add vertices v_6 and v_7 to I_1 without increasing the upper bound of $\omega_4(G[S \cup I_1], S)$, since there are only 3 *loose* or *conflict* vertices, *i.e.*, v_1, v_6, v_7, in $I_1 \cup \{v_6, v_7\}$. After the operation, C is partitioned into two sets, $I_5 = I_1 \cup \{v_6, v_7\}$ and $I_6 = \{v_4, v_5, v_8\}$. The new upper bound of $\omega_4(G, S)$ is $|S| +$ *TISUB*$(I_5, S) +$ *TISUB*$(I_6, S) = |S| + 3 + 1 = |S| + 4$.

Finally, let us use Rule 2 to further make set I_5 contain more vertices. According to Rule 2, all vertices in I_6 can be added to I_5 without increasing the upper bound of $\omega_4(G[S \cup I_5], S)$. After the operation, the final RelaxGCB of $\omega_4(G, S)$ is $|S| +$ *TISUB*$(I_5, S) = |S| + 3$.

3.4 The RelaxColoring Algorithm

The RelaxColoring algorithm for calculating the RelaxGCB is summarized in Algorithm 1. The algorithm first uses $|S|$ to initialize the upper bound UB (line 1), and then repeatedly uses the TryColor() function to extract a subset $I \subseteq C$ and calculate the upper bound on the number of vertices that I can provide for S, *i.e.*, ub (line 3) until $C = \emptyset$ (line 2). After each execution of function TryColor(), the candidate set C and upper bound UB are both updated (line 4).

Function TryColor() is summarized in Algorithm 2, which first finds a maximal independent set $I \subseteq C$ (lines 1-3) and calculates its TISUB (line 4). Then, the algorithm initializes

Algorithm 1: RelaxColoring(G, k, S, C)

Input: A graph $G = (V, E)$, an integer k, the current partial k-plex S, the candidate set C
Output: RelaxGCB of $\omega_k(G, S)$
initialize the upper bound $UB \leftarrow |S|$;
while $C \neq \emptyset$ **do**
  $\{I, ub\} \leftarrow$ TryColor(G, k, S, C);
  $C \leftarrow C \backslash I$, $UB \leftarrow UB + ub$;
return UB;

Algorithm 2: TryColor(G, k, S, C)

Input: A graph $G = (V, E)$, an integer k, the current partial k-plex S, the candidate set C
Output: A vertex set I, an upper bound ub of the number of vertices that I can provide for S
1 initialize $I \leftarrow \emptyset$;
2 **for each** vertex $v \in C$ **do**
3   **if** $N(v) \cap I = \emptyset$ **then** $I \leftarrow I \cup \{v\}$;
4 $ub \leftarrow$ *TISUB*(I, S);
5 initialize the set of *loose* or *conflict* vertices $LC \leftarrow \{v \in I | \delta_k^-(S, v) > ub\}$;
6 **if** $|LC| < ub$ **then**
7   **for each** vertex $v \in C \backslash I$ **do**
8     $CV \leftarrow \{v\} \cup \{N(v) \cap I \backslash LC\}$;
9   **if** $|LC| + |CV| \leq ub$ **then**
10       $I \leftarrow I \cup \{v\}$;
11       $LC \leftarrow LC \cup CV$;
12   **if** $|LC| = ub$ **then break**;
13 **for each** vertex $v \in C \backslash I \wedge \delta_k^-(S, v) < ub$ **do**
14   **if** $|N(v) \cap I| \leq ub - \delta_k^-(S, v)$ **then**
15     $I \leftarrow I \cup \{v\}$;
16 **return** $\{I, ub\}$;

the set of *loose* or *conflict* vertices LC (line 5) and tries to add as many vertices as possible to I according to Rule 1 (lines 6-12). Once trying to add each vertex v, the algorithm uses CV to denote the extra *conflict* vertices caused by adding v to I (line 8). Since I is a maximal independent set in C, adding any vertex v to I increases at least one *conflict* vertices, *i.e.*, v itself (line 8). Thus, the utilization of Rule 1 can be terminated when $|LC| \geq ub$ (lines 6 and 12). Finally, the algorithm applies Rule 2 to further add vertices to I (lines 13-15). Since for each vertex $v \in C \backslash I$, $|N(v) \cap I| > 0$ holds, only vertex $v \in C \backslash I$ with $\delta_k^-(S, v) < ub$ can be added to I according to Rule 2 (line 13).

The time complexities of RelaxColoring algorithm and TryColor function are $O(|C|^2 \times T)$ and $O(|C| \times T)$, respectively, where $O(T)$ is the time complexity of the intersection operation between $N(v)$ and I (or $I \backslash LC$) used in lines 3, 8, and 14 in Algorithm 2. Actually, $O(T)$ is bounded by $O(|V|)$ and much smaller than $O(|V|)$ with the bitset encoding [Segundo *et al.*, 2011].

Algorithm 3: SelectPartition(G, k, S, C)

Input: A graph $G = (V, E)$, an integer k, the current partial k-plex S, the candidate set C
Output: A vertex set I, an upper bound ub of the number of vertices that I can provide for S
initialize $dise^* \leftarrow 0, ub^* \leftarrow 0, I^* \leftarrow \emptyset$;
for each vertex $v \in S \wedge \delta_k^-(S, v) > 0$ **do**
  $I \leftarrow C \backslash N(v)$;
  $ub \leftarrow \min\{|I|, \delta_k^-(S, v)\}$;
  if $|I|/ub > dise^* \vee (|I|/ub = dise^* \wedge |I| > |I^*|)$ **then** $dise^* \leftarrow |I|/ub, ub^* \leftarrow ub, I^* \leftarrow I$;
return $\{I^*, ub^*\}$;

4 The RelaxPUB Bound

Motivated by the complementarity of the coloring-based and partition-based upper bounds, we propose to combine RelaxGCB with the newest PUB, DisePUB [Jiang *et al.*, 2023], and propose a better and generic upper bound for MKP. In this section, we first introduce DisePUB, then provide two examples to illustrate the complementarity of the coloring-based and partition-based upper bounds, and finally present our new upper bound, RelaxPUB.

4.1 Revisiting DisePUB

Given a growing partial k-plex S and the corresponding candidate set C, for each vertex $v \in S$, DisePUB claims that a subset $I \subseteq C$ can provide at most $\min\{|I|, \delta_k^-(S, v)\}$ vertices for S if $N(v) \cap I = \emptyset$. Given a vertex $v \in S$, let $I = C \backslash N(v)$ and $ub = \min\{|I|, \delta_k^-(S, v)\}$, DisePUB defines a metric for I, *i.e.*, $dise(I) = |I|/ub$, to evaluate the extraction of vertex set I. The larger the value of $dise(I)$, the more vertices that can be extracted from C and the fewer increments on the upper bound of $\omega_k(G, S)$.

In each step, DisePUB traverses each vertex $v \in S$ with $\delta_k^-(S, v) > 0$ and selects the corresponding set $I = C \backslash N(v)$ with the largest value of $dise(I)$. Ties are broken by preferring larger extractions. We use function SelectPartition() to describe the selection, which is shown in Algorithm 3. Then, DisePUB extracts $C \backslash N(v)$ from C and increases the upper bound of $\omega_k(G, S)$ by $\min\{|C \backslash N(v)|, \delta_k^-(S, v)\}$.

DisePUB repeats the above process until vertices remaining in C are adjacent to all vertices in S. DisePUB denotes the set of remaining vertices in C as π_0 and finally increases the upper bound of $\omega_k(G, S)$ by $|\pi_0|$.

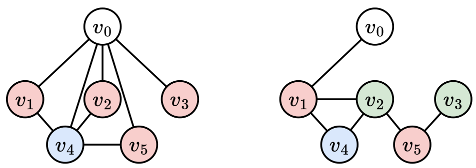
4.2 Complementarity of GCB and PUB

To better illustrate the complementarity of the coloring-based and partition-based upper bounds (*i.e.*, GCB and PUB), we provide two examples in Figure 2, where the growing 2-plex S contains only one vertex v_0 and its corresponding candidate set $C = \{v_1, v_2, v_3, v_4, v_5\}$.

In Figure 2(a), the GCB is tighter than the PUB. The vertices in C are all adjacent to v_0, which means the vertices in C are all in π_0. Thus, the PUB is $|S| + |\pi_0| = 6$. While by coloring the vertices in C, it can be partitioned into 2 independent sets $I_1 = \{v_1, v_2, v_3, v_5\}$ and $I_2 = \{v_4\}$, and the GCB is

Algorithm 4: SelectUB(G, k, S, C)

Input: A graph $G = (V, E)$, an integer k, the current partial k-plex S, the candidate set C
Output: RelaxPUB of $\omega_k(G, S)$
initialize the upper bound $UB \leftarrow |S|$;
while $C \neq \emptyset$ **do**
  $\{I_C, ub_C\} \leftarrow$ TryColor(G, k, S, C);
  $\{I_P, ub_P\} \leftarrow$ SelectPartition(G, k, S, C);
  if $|I_C|/ub_C > |I_P|/ub_P \vee (|I_C|/ub_C = |I_P|/ub_P \wedge |I_C| > |I_P|)$ **then**
    $C \leftarrow C \backslash I_C$, $UB \leftarrow UB + ub_C$;
  else
    $C \leftarrow C \backslash I_P$, $UB \leftarrow UB + ub_P$;
return UB;



(a) GCB prevails (b) PUB prevails

Figure 2: Examples for demonstrating the complementarity.

$|S| + \sum_{i=1}^{2} \min\{|I_i|, 2\} = 4$. In contrast, the PUB is tighter than the GCB in Figure 2(b), where C can be partitioned into 3 independent sets $I_1 = \{v_1, v_5\}$, $I_2 = \{v_2, v_3\}$, and $I_3 = \{v_4\}$. Thus, the GCB is $|S| + \sum_{i=1}^{3} \min\{|I_i|, 2\} = 6$. While vertices in C except v_1 are non-adjacent to v_0, $\pi_0 = \{v_1\}$, thus the PUB is $|S| + |\pi_0| + \delta_2^-(S, v_0) = 3$.

4.3 Combining RelaxGCB and DisePUB

Both RelaxGCB and DisePUB extract a subset from C and accumulate the upper bound of $\omega_k(G, S)$. The $dise$ metric in DisePUB can also be used for the vertex set returned by TryColor(). RelaxPUB combines RelaxGCB and DisePUB by using them to select a promising extraction in each step.

We propose an algorithm called SelectUB for calculating the RelaxPUB of $\omega_k(G, S)$, which is presented in Algorithm 4. The algorithm calls TryColor() and SelectPartition() in each step and figures out whose returned vertex set is better according to the $dise$ metric. Ties are broken by preferring larger extraction. Once a better extraction is selected, The algorithm updates the candidate set C and accumulates the upper bound of $\omega_k(G, S)$.

The time complexities of functions TryColor() and SelectPartition() are $O(|C| \times T)$ and $O(|C| \times |S|)$ [Jiang *et al.*, 2023], respectively, where $O(T)$ is much smaller than $O(|V|)$ as referred to Section 3.4. The time complexity of the SelectUB algorithm is $O(|C|^2 \times (|S| + T))$.

5 Experimental Results

This section presents experiments to evaluate the performance of RelaxGCB and RelaxPUB. Baselines contain SOTA BnB algorithms with GCB and PUB, *i.e.*, Maplex [Zhou *et al.*, 2021], kPlexS [Chang *et al.*, 2022], DiseMKP [Jiang *et al.*, 2023], an improvement version of KpLeX [Jiang *et al.*, 2021], and KPLEX [Wang *et al.*, 2023b]. We replace the original bounds in these baselines with RelaxGCB and RelaxPUB, conducting eight new BnB algorithms. Moreover, the recent kplexT algorithm [Chang and Yao, 2024] is also considered as a baseline, which does not contain GCB or PUB, and we compare it with our RelaxPUB-based algorithms.

5.1 Experimental Setup

All the algorithms[1] were implemented in C++ and run on a server using an AMD EPYC 7H12 CPU, running Ubuntu 18.04 Linux operation system. We test the algorithms on two public benchmarks that are widely used in the literature of the baselines, the 2nd DIMACS benchmark[2] that contains 80 (almost dense) graphs with up to 4,000 vertices and densities ranging from 0.03 to 0.99, and the Real-world benchmark[3] that contains 139 real-world sparse graphs from the Network Data Repository [Rossi and Ahmed, 2015].

We choose the two datasets because the 2nd DIMACS benchmark is also widely used to evaluate MCP, one of the most closely related problems to MKP, and the Real-world benchmark is widely used for analyzing various complex networks, one of the most important application areas of MKP. Moreover, the structures of the two benchmarks are distinct, helping evaluate the robustness of the algorithms.

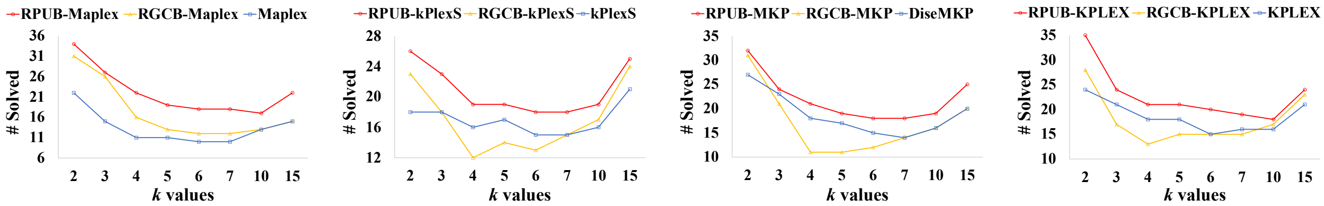
For each graph, we generate 8 MKP instances with $k \in \{2, 3, 4, 5, 6, 7, 10, 15\}$, and set the cut-off time to 1,800 seconds per instance, following the settings of the baselines.

5.2 Performance Evaluation

The comparison results between the algorithms with RelaxGCB and RelaxPUB (RGCB and RPUB in short) and the baselines in dense 2nd DIMACS and sparse Real-world benchmarks are summarized in Figures 3 and 4, respectively. The results are expressed by the number of MKP instances solved by each algorithm within the cut-off time for different k values. Note that Maplex only contains the GCB, and the other three baselines only contain the PUB. 1) From (a) of the two figures, one can observe that our RelaxGCB significantly outperforms GCB. 2) From (b) to (d) of the two figures, one can observe that RelaxGCB is complementary to PUB. 3) From all the figures, one can observe that our RelaxPUB makes full use of the complementarity of RelaxGCB and PUB, and significantly improves all the baselines in solving both dense and massive sparse graphs over diverse k values, indicating its dominant performance over the SOTA baselines, excellent generalization over different graphs, and strong robustness over diverse k values.

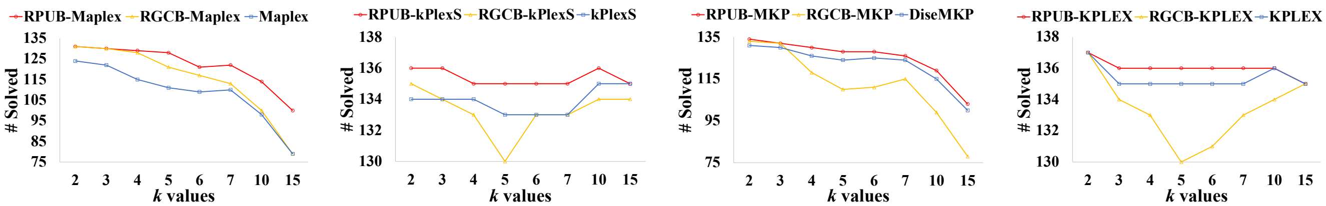
Following the convention of the baselines, we also present detailed results of the baselines and their improvements with RelaxPUB in solving 30 representative 2nd DIMACS and Real-world instances with $k = 2, 3, 6, 10, 15$ in Table 1. We report their running times in seconds (column *Time*), the sizes

[1] Source code: https://github.com/JHL-HUST/RelaxPUB
[2] http://archive.dimacs.rutgers.edu/pub/challenge/graph/benchmarks/clique/
[3] http://lcs.ios.ac.cn/%7Ecaisw/Resource/realworld%20graphs.tar.gz



(a) Comparison with Maplex (b) Comparison with kPlexS (c) Comparisons with DiseMKP (d) Comparison with KPLEX

Figure 3: Comparisons on the 2nd DIMACS benchmark. Note that Maplex is based on GCB while the other baselines on PUB.

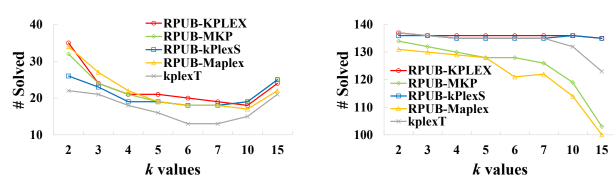


(a) Comparison with Maplex (b) Comparison with kPlexS (c) Comparison with DiseMKP (d) Comparison with KPLEX

Figure 4: Comparisons on the Real-world benchmark. Note that Maplex is based on GCB while the other baselines on PUB.

k	Instance	RelaxPUB-Maplex			Maplex		RelaxPUB-kPlexS			kPlexS		RelaxPUB-MKP			DiseMKP		RelaxPUB-KPLEX			KPLEX	
		Tree	*Time*	*Percent*	*Tree*	*Time*	*Tree*	*Time*	*Percent*	*Tree*	*Time*	*Tree*	*Time*	*Percent*	*Tree*	*Time*	*Tree*	*Time*	*Percent*	*Tree*	*Time*
2	brock200-3	**9.432**	**10.06**	49.7%	790.8	107.8	**8.343**	**292.0**	49.9%	52.35	1,615	**7.393**	**21.93**	46.2%	85.88	26.06	**27.43**	**34.63**	79.8%	225.2	80.52
	brock200-4	**24.99**	**30.07**	50.2%	4015	576.9	**23.84**	**695.8**	49.7%	-	-	**12.60**	**47.20**	49.8%	279.6	103.1	**68.81**	**84.81**	78.8%	780.2	250.0
	C125.9	**88.36**	**186.3**	66.3%	-	-	**24.56**	**162.8**	71.8%	-	-	**15.32**	**69.65**	70.5%	-	-	**29.61**	**37.93**	88.0%	-	-
	keller4	**3.715**	**4.015**	46.1%	1273	182.3	**3.961**	**87.18**	44.3%	92.45	1,238	**2.666**	**8.016**	42.0%	69.11	21.15	**19.29**	**17.38**	79.6%	562.6	105.3
	san200-0-9-1	**0.004**	**0.051**	93.0%	-	-	**0.024**	**0.660**	94.8%	-	-	**0.003**	**0.105**	95.2%	-	-	**0.057**	**0.619**	98.4%	64.21	27.33
	sanr200-0-7	**96.72**	**135.8**	49.5%	-	-	**66.05**	**1,656**	51.5%	-	-	**40.59**	**153.0**	49.9%	1130	475.4	**171.7**	**206.6**	79.5%	2681	752.0
	socfb-Duke14	**0.579**	**2.313**	78.7%	195.6	45.05	**0.110**	**4.397**	85.8%	1.046	36.58	**0.213**	**2.121**	83.4%	243.6	154.5	**0.281**	**2.403**	94.3%	1.598	2.957
	socfb-UF	**0.253**	**3.217**	88.3%	-	-	**0.094**	**2.012**	93.2%	0.190	3.310	**0.069**	**2.800**	91.5%	413.1	299.3	**0.107**	**1.741**	91.9%	0.234	1.850
	socfb-Uillinois	**0.229**	**7.991**	89.3%	-	-	**0.022**	**2.224**	92.8%	0.023	2.628	**0.168**	**4.138**	81.0%	18.33	13.05	**0.024**	**1.774**	85.8%	0.027	1.845
3	hamming6-2	**393.2**	**399.6**	57.6%	-	-	**204.4**	**349.2**	49.8%	-	-	**137.4**	**234.1**	49.1%	826.6	304.6	**197.0**	**136.2**	60.2%	1157	203.3
	MANN-a81	**0.001**	**0.001**	100%	-	-	**0.001**	**534.9**	96.3%	0.001	556.1	**0.001**	**62.67**	98.3%	0.003	63.61	**0.004**	**568.4**	98.9%	0.406	605.2
	p-hat300-2	**174.7**	**340.9**	57.0%	-	-	**123.6**	**1,565**	57.2%	-	-	**36.99**	**200.0**	59.2%	-	-	**401.9**	**470.9**	75.3%	1293	529.0
	socfb-UF	**82.41**	**254.3**	87.3%	-	-	**0.094**	**1.975**	82.1%	0.324	4.172	**6.950**	**40.60**	86.7%	440.6	413.4	**0.067**	**1.877**	89.4%	0.079	2.104
	socfb-Indiana	**2.437**	**8.069**	89.1%	1002	308.6	**0.007**	**1.722**	82.8%	0.008	1.879	**1.110**	**7.302**	84.9%	587.8	391.5	**0.006**	**1.436**	89.9%	0.006	1.708
	soc-flixster	**8.732**	**20.00**	74.6%	-	-	**0.725**	**8.152**	73.5%	7.394	110.5	**2.084**	**13.15**	76.2%	118.0	85.04	**0.280**	**3.982**	84.7%	0.470	5.674
	soc-lastfm	**1.384**	**6.018**	54.8%	78.33	29.91	**0.327**	**17.86**	60.2%	0.785	43.87	**0.729**	**9.750**	52.4%	7.163	10.26	**1.549**	**53.88**	77.5%	2.819	95.76
	soc-slashdot	**1.607**	**1.922**	74.2%	2461	289.2	**0.095**	**0.715**	72.3%	0.299	2.825	**0.245**	**0.910**	76.9%	7.847	4.577	**0.096**	**0.829**	82.4%	0.131	0.766
	tech-WHOIS	**24.96**	**72.23**	85.3%	-	-	**0.049**	**0.451**	84.4%	0.134	1.647	**0.384**	**2.514**	89.8%	6.996	6.043	**0.028**	**0.279**	90.9%	0.034	0.483
6	c-fat200-1	**0.001**	**0.001**	92.8%	0.003	0.001	**0.001**	**0.001**	80.6%	0.001	0.002	**0.002**	**0.014**	82.9%	0.002	0.018	**0.001**	**0.001**	66.0%	0.001	0.001
	san200-0-7-1	**0.001**	**0.017**	95.9%	-	-	**0.001**	**0.040**	93.3%	3.163	4.928	**0.001**	**0.037**	93.7%	0.329	0.177	**0.001**	**0.043**	87.1%	-	-
	san200-0-7-2	**0.001**	**0.012**	80.1%	11.99	6.417	**0.004**	**0.156**	70.4%	-	-	**0.005**	**0.066**	68.8%	-	-	**0.002**	**0.122**	81.8%	-	-
	socfb-Berkeley13	**0.078**	**1.514**	94.4%	1780	249.5	**0.001**	**0.890**	50.0%	0.001	0.905	**0.244**	**1.890**	90.4%	4.509	4.586	**0.001**	**0.828**	28.2%	0.001	0.867
	socfb-MIT	**0.189**	**0.591**	78.4%	15876	1684	**0.002**	**0.317**	70.7%	0.002	0.319	**0.041**	**0.523**	91.4%	2.220	1.764	**0.002**	**0.271**	57.0%	0.002	0.340
	soc-gowalla	**12.45**	**11.61**	54.2%	779.5	120.1	**0.003**	**0.430**	63.4%	0.005	0.572	**6.042**	**16.65**	53.1%	59.68	43.12	**0.004**	**0.199**	69.3%	0.004	0.242
10	bio-dmela	**1.245**	**14.64**	39.1%	-	-	**0.004**	**0.067**	48.7%	0.007	0.076	**0.085**	**0.113**	30.9%	4.615	0.221	**0.019**	**0.037**	57.1%	0.030	0.038
	ia-enron-large	**5.779**	**4.850**	55.4%	156.3	24.10	**0.001**	**0.103**	76.3%	0.001	0.115	**14.80**	**24.89**	39.6%	266.7	178.1	**0.002**	**0.064**	72.1%	0.002	0.065
	tech-RL-caida	**0.662**	**0.803**	46.9%	18.52	4.693	**0.001**	**0.251**	65.9%	0.001	0.258	**0.017**	**0.363**	73.2%	1.160	0.500	**0.001**	**0.067**	83.3%	0.001	0.068
15	C125-9	**152.7**	**507.5**	79.6%	-	-	**5.460**	**30.22**	70.4%	12.21	96.15	**2.712**	**16.10**	82.6%	7.771	22.62	**1.194**	**5.414**	83.5%	17.47	40.32
	bio-diseasome	**0.234**	**0.145**	80.1%	1011	169.0	**0.001**	**0.001**	81.3%	0.001	0.001	**0.055**	**0.024**	57.7%	80.71	2.321	**0.000**	**0.000**	100%	0.000	0.001
	socfb-uci-uni	**22.61**	**107.5**	47.9%	-	-	**0.019**	**49.43**	58.1%	0.517	53.96	**26.93**	**295.4**	35.6%	-	-	**0.185**	**6.775**	62.7%	1.096	9.322

Table 1: Comparisons on 30 representative instances with five k values. The search tree size is in 10^5, and the time is in seconds. The percent indicates the percentage of times RelaxGCB is used in RelaxPUB. Better results appear in bold.



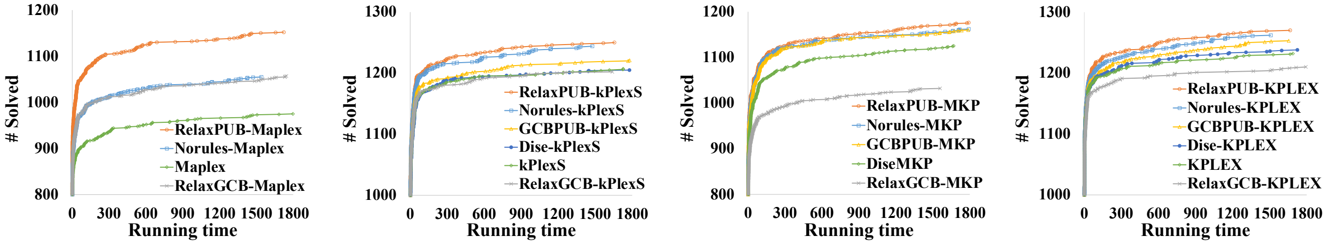
(a) On DIMACS2 benchmark (b) On Real-world benchmark

Figure 5: Comparisons of our RelaxPUB algorithms and kplexT.

of their entire search trees in 10^5 (column *Tree*) to solve the instances, and the percentage of the number of times RelaxGCB is selected and outperforms the DisePUB in RelaxPUB (column *Percent*). Better results are highlighted in bold, and symbol '-' means the algorithm cannot solve the instance within the cut-off time.

The results show that for each pair of tested algorithms, our new upper bounds can help the baseline algorithm prune significantly more branches, reducing its search tree sizes by several orders of magnitude for instances that both can solve within the cut-off time. There are also many instances that the baseline algorithms cannot solve within the cut-off time, while the algorithms with our upper bounds can solve with few branches and much less calculation time. Moreover, we can observe that RelaxGCB contributes a lot in solving these instances, indicating again the complementarity of RelaxGCB and DisePUB.

Moreover, we compare our RelaxPUB algorithms with



(a) On Maplex (b) On kPlexS (c) On DiseMKP (d) On KPLEX

Figure 6: Ablation studies on each baseline over all the tested instances.

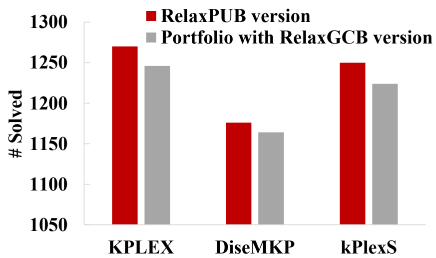


Figure 7: Comparison of the RelaxPUB algorithms with the portfolios of the baselines and their RelaxGCB algorithms.

the kplexT algorithm. The results are shown in Figure 5. We can observe that in Real-world benchmark, RelaxPUB-kPlexS and RelaxPUB-KPLEX show better performance than kplexT, and in DIMACS2 benchmark, kplexT shows the worst performance, indicating that our method indeed leads to SOTA BnB algorithms for MKP. By the way, kplexT mentioned that the PUB may be used to improve it in its future work [Chang and Yao, 2024], indicating that our method indeed improves a general and popular technique.

5.3 Ablation Study

The ablation studies contain two parts. The first part is to evaluate the effectiveness of the proposed TISUB and the two rules (see Lemmas 1, 2, and 3) in our proposed upper bounds. For the kPlexS, DiseMKP, and KPLEX baselines having the PUB, we generate a "Norules" variant, which uses our RelaxPUB without Rules 1 and 2, and a "GCBPUB" variant, which uses our RelaxPUB and replaces its RelaxGCB with the GCB in Maplex. Moreover, since the kPlexS and KPLEX algorithms use the previous PUB proposed in [Jiang *et al.*, 2021], we apply the newest DisePUB to them and obtain two variants: Dise-kPlexS and Dise-KPLEX. For the Maplex baseline that is only based on GCB, its "Norules" variant uses our RelaxGCB without Rules 1 and 2.

We perform four groups of ablation studies based on each baseline over all the 1,752 instances, as summarized in Figure 6. The results are expressed by the variation in the number of solved instances for each algorithm over the running time (in seconds). The results show that the "GCBPUB" variants are better than the baselines, indicating that combining coloring-based and partition-based upper bounds by the mechanism in RelaxPUB can make use of their complementarity. The "Norules" variants are better than the "GCBPUB" variants, indicating that TISUB is a significant improvement over GCB. The new algorithms with RelaxPUB are better than the "Norules" variants, indicating that our proposed two rules can further improve TISUB. Moreover, DisePUB can hardly improve kPlexS and KPLEX, indicating that the improvements of the RelaxPUB series over the baselines originate from RelaxGCB rather than using the newest DisePUB.

The second part is to evaluate the effectiveness of the combination scheme designed in RelaxPUB. In this part, we compare each of the RelaxPUB algorithms with the portfolio consist of the corresponding baseline and its RelaxGCB algorithm. For example for the KPLEX algorithm, the portfolio version outputs the better result found by KPLEX and RelaxGCB-KPLEX, *i.e.*, if any of KPLEX and RelaxGCB-KPLEX solve the solution, the portfolio solves the solution. The comparison results on all the 1,752 tested instances are shown in Figure 7. Note that we only perform on the baselines with PUB, *i.e.*, KPLEX, DiseMKP, and kPlexS. The results show that the RelaxPUB algorithms can solve more instances than the portfolio ones, indicating the advantages of the combination scheme in RelaxPUB, which can make fully use of the complementarity of RelaxGCB and PUB.

6 Conclusion

We proposed two new upper bounds for the Maximum k-plex Problem (MKP), termed RelaxGCB and RelaxPUB. RelaxGCB considers the connectivity between vertices more thoroughly and relaxes the restrictive independent set structure to contain more vertices without increasing the upper bound. Provided theoretical proof indicates that RelaxGCB is strictly better than the previous graph color bound (GCB). RelaxPUB further combines RelaxGCB and an advanced partition-based upper bound in a novel way, making fully use of their complementarity. We replaced the GCB in Maplex and the partition-based upper bounds in kPlexS, DiseMKP, and KPLEX with RelaxGCB and RelaxPUB, respectively, producing eight new BnB MKP algorithms. Experiments on both dense and sparse graph datasets show that RelaxGCB significantly outperforms GCB, and RelaxPUB exhibits clearly priority over the baselines and exhibits excellent robustness over various k values and high generalization capability over different graphs and algorithms.

RelaxGCB contains ideas of enhancing coloring-based upper bounds in relaxation clique problems, and RelaxPUB contains ideas of combining complementary upper bounds. We believe our methods can be applied for improving BnB algorithms of other relaxation clique problems.

Contribution Statement

The first two authors, Jiongzhi Zheng and Mingming Jin, contributed equally.

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