

Finding conserved low-diameter subgraphs in social and biological networks

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Abstract

The analysis of social and biological networks often involves modeling clusters of interest as *cliques* or their graph-theoretic generalizations. The *k*-club model, which relaxes the requirement of pairwise adjacency in a clique to length-bounded paths inside the cluster, has been used to model cohesive substructures in social networks and functional modules or complexes in biological networks. However, if the graphs are time-varying, or if they change under different conditions, we may be interested in clusters that preserve their property over time or under changes in conditions. To model such clusters that are conserved in a collection of graphs, we consider a *cross-graph k-club* model, a subset of nodes that forms a *k*-club in every graph in the collection. In this article, we consider the canonical optimization problem of finding a cross-graph *k*-club of maximum cardinality in a graph collection. We develop integer programming approaches to solve this problem. Specifically, we introduce strengthened formulations, valid inequalities, and branch-and-cut algorithms based on delayed constraint generation. The results of our computational study indicate the significant benefits of using the approaches we introduce.

KEYWORDS

k-clubs, cross-graph mining, integer programming, temporal networks

1 | INTRODUCTION

In graph-based data mining (or graph mining), a node models a data item with different attributes, and two nodes are joined by an edge if they are “close” in each other based on similarity measures. Graph mining in social and biological networks involves modeling clusters of interest using nodes and their graph-theoretic generalizations. In these graphs, a cohesive/tight-knit subgraph is a subset of nodes whose members are believed or verified to interact cooperatively with each other toward some specific goal. Cohesive subgraphs in social networks could be identified for use in recommendation systems, marketing campaigns, community detection, influence maximization, and so forth [3]. In biological networks like protein interaction networks, gene co-expression networks, and metabolic networks, clusters and network motifs are commonly used to identify functional modules that could represent protein complexes, or signaling pathways [19]. The clique and its graph-theoretic generalizations have been extensively studied and used as models of cohesive subgroups or clusters in diverse fields including social and biological network analysis [36]. Many categories include the distance based clusters *k*-clique and *k*-club [8], and the edge count, degree, and edge density based relaxations *k*-defective clique [43], *k*-plex [7], and *k*-quasi clique [28], respectively.

A significant body of literature on optimization methods for cluster detection seeks to find a subset of nodes satisfying a graph property while optimizing a measure of fitness like cluster size or weight. One common characteristic shared by optimization approaches to graph mining is that they identify cohesive subgraphs, critical nodes, most central actors, or other graph structures of interest in a single graph. However, in many settings the graphs are time-varying as the underlying dynamic systems they

model evolve over time. In this case, the single graph under consideration is typically a snapshot that reflects node relationships at the point in time it is recorded, or it aggregates information over a period of time in some manner.

Alternatively, relationships between pairs of nodes (and hence the graph model) may be different under different conditions. Jointly mining the graphs corresponding to different conditions might uncover novel clusters that cannot be found by individually analyzing the network corresponding to each condition. An example in cross-market consumer segmentation is finding customers who have similar behaviors across different markets as a more robust cohesive subgraph than those found in a single market [38]. Similarly, systems biologists are interested in finding groups of co-expressing genes or interacting proteins that are conserved under different biological conditions or between different species [37]. These approaches are based on the belief that conserved modules are more likely to govern core biological functions [29, 43].

Broadly, we call the process of simultaneously mining a collection of two or more graphs for conserved structures and patterns as *cross-graph mining*. Despite its potential applications previous work on this topic is limited in the literature. Algorithms for enumerating cross-graph quasi-cliques to extract hidden patterns crossing multiple pieces of data were developed in [37]. This work was extended in [18] for finding frequent cross-graph quasi-cliques, wherein the detected clusters are required to form a quasi-clique in at least a fixed number of graphs in the collection. An approach to clustering nodes that exhibit homogeneous financial status values by mining the complete sets of cross-graph quasi-cliques in a bipartite graph was introduced in [44]. This bipartite graph has stocks on nodes in one partition and different features of the stocks data in the other partition. The cross-graph quasi-clique model was used to handle the issue of missing values in stock data. Models and methods for mining conserved clusters in a collection of graphs without strictly imposing the cross-graph requirement can also be found in [9, 16, 17, 41, 48].

In this article, we consider a *cross-graph k-club* model to represent low-diameter clusters that are conserved in a collection of graphs. Note that the graph collection may represent temporal graphs with an implicit ordering, or may be obtained under different experimental conditions without any natural ordering. Although our focus is on clusters of conserved low-diameter subgraphs, one may investigate any graph relation or another graph property in the same setting. Our main contributions in this article are integer programming (IP) approaches to find a cross-graph *k*-club of the largest cardinality in a given collection of graphs. Specifically, we introduce strengthened formulations, valid inequalities, and branch-and-cut algorithms based on delayed cut generation that are evaluated on a test bed of instances in our computational study (see also [33]).

The remainder of this article is organized as follows. We formally define the problem of interest and briefly review IP formulations for the maximum *k*-club problem in Section 2. In Section 3, we introduce a straightforward conjunctive formulation for the maximum cross-graph *k*-club problem and propose techniques to strengthen the constraints. Then in Section 4, we discuss valid inequalities for the problem, including extensions of those known in the literature for the single-graph problem. In Section 5, we introduce branch-and-cut algorithms together with preprocessing techniques to solve the problem. We compare the computational results from using the algorithms based on different IP formulations, and verify the computational effectiveness of approaches we developed for the cross-graph *k*-club problem in solving another related problem in temporal graph mining called the *k*-club separation problem [6]. We conclude this article with a summary of our contributions and identify future extensions in Section 7.

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2 | BACKGROUND

For a single graph G , we use $V(G)$ and $E(G)$ to denote its node and edge sets respectively. For simplicity we use u to denote an edge $(u, v) \in E(G)$. For a node set $S \subseteq V(G)$, we use $G[S]$ to denote the graph obtained from G by deleting the nodes in A along with its incident edges and we let $G[S]$ denote the subgraph induced by S (obtained by deleting nodes outside S with the edges incident to these nodes). We use $N_G(u)$ and $N_G(v)$ to denote the complement of graph G and the neighborhood of u in G , respectively. We use $N_G(u, v)$ to denote the common neighborhood of u and v in graph G . We denote by $\text{dist}_G(u, v)$ the minimum number of edges on a path connecting nodes u and v in graph G , and its diameter is given by $\text{diam}(G) := \max\{\text{dist}_G(u, v) : u, v \in V(G)\}$.

Definition 1 ([25]). Given a graph G and a positive integer k , a subset of nodes $S \subseteq V(G)$ is called a *k-club* if $\text{dist}_G(u, v) \leq k$ for every pair of nodes $u, v \in S$.

Definition 2 ([12, 30] (see also [30])). Given a graph G and a positive integer k , a subset of nodes $S \subseteq V(G)$ is called a *k-club* if $\text{diam}(G[S]) \leq k$.

A *k-club* S allows two nodes u and v to be included even if every path between u and v of length at most k in G includes nodes outside (see Figure 1). By contrast, in the *k*-club model at least one of those paths should be contained in $G[S]$. Together, *k*-cliques and *k*-clubs are well-known distance-based clique relaxations [42]. The structural guarantees they provide typically determine their suitability for any particular graph mining application. The *k*-cliques, for instance, are hereditary; that is, the

Definition 1 implies that every path of length at most k in G between nodes u and v , uses nodes from S . Let $S_G(u, v)$ denote the collection of all length- k u, v -separators that are minimal by exclusion. For the case $k = 2$, the unique minimal length-2 u, v -separator is the common neighborhood $N_G(u, v)$.

Formulation 1 that follows is the conjunctive cut-like formulation (CCF) of the maximum cross-graph *k*-club problem over a collection \mathcal{G} . For a subset of nodes $S \subseteq V(\mathcal{G})$, we use the shorthand $s(S) := \sum_{u,v \in S} s(u, v)$ is readily verified that s is an incidence vector of a cross-graph *k*-club if and only if it is feasible to the CCF:

$$\max s(V(\mathcal{G})), \quad \forall S \subseteq V(\mathcal{G}), s(S) \leq 1, \quad \forall S \subseteq S_G(u, v), u, v \in E(\mathcal{G}), \quad (1a)$$

$$s(u, v) + s(v, u) \leq 1, \quad \forall u, v \in V(\mathcal{G}), \quad (1b)$$

$$s(u, v) \leq 1, \quad \forall u, v \in V(\mathcal{G}). \quad (1c)$$

Formulation 1 can be strengthened by noting that if a node w that belongs to some minimal length- k u, v -separator of graph $G \in \mathcal{G}$ [i.e., $u, v \in S$ and $w \notin S$] is also at a distance strictly greater than k from either u or v in some other graph $H \in \mathcal{G}$ in the collection, then w cannot be included in a cross-graph *k*-club that contains both u and v . Consequently, constraints (1b) can be replaced by

$$s_u + s_v - s(S \cap D_{u,v}) \leq 1, \quad (2)$$

where $D_{u,v}$ is the set of nodes that are at distance at most k from u and v in all the graphs in \mathcal{G} , defined as:

$$D_{u,v} := \{w \in V(\mathcal{G}) \setminus \{u, v\} : \text{dist}_G(u, w) \leq k \text{ and } \text{dist}_H(v, w) \leq k \text{ for all } G, H \in \mathcal{G}\}.$$

The validity of constraints (2) follows from the validity of (1b) and from the observation that if $s_u + s_v = 1$, then $s(S \cap D_{u,v}) = 0$, because no nodes from the set $S \cap D_{u,v}$ can be included in a cross-graph *k*-club containing u and v . Alternatively, we can think of $S \cap D_{u,v}$ as further reducing the size the separator S by removing nodes that are not in any path of length at most k between u and v in some graph in the collection. Observe that the resulting formulation is at least as tight as the CCF. Moreover, there are instances where $S \cap D_{u,v} \subset S$, for at least one separator $S \in S_G(u, v)$, as illustrated in the following example, which means that there are instances where the resulting formulation is strictly tighter than (1).

Consider the maximum 2-graph 2-club problem on the graph collection in Figure 2. Formulation 1 includes the constraint $s_1 + s_2 \leq 1$ due to node pair 1 and 2 in G and constraint $s_1 + s_2 - s_6 \leq 1$ due to the same node pair in H . Note that $\text{dist}_G(1, 3) = 3$. We can therefore tighten the first constraint by intersecting the minimal separator (3) with $D_{1,2} = \{5, 6, 7\}$ to obtain the constraint $s_1 + s_2 - s_6 \leq 1$ that dominates both previous constraints.

Based on the foregoing observations, we can now envision an approach in which we further tighten the constraints with respect to each u, v pair, by *recursively* deleting nodes which are too far from either u or v in any graph in the collection. This is a recursive operation because the deletion of nodes can have a domino effect on pairwise distances in graphs, leading to more nodes meeting the condition for deletion. The resulting inequalities will be at least as strong as their counterpart in constraints (2). However, it is important to recognize that this operation is node pair specific, that is, the graph collection obtained by deleting nodes based on a particular u, v pair is only valid for generating constraints with respect to that pair. This is because nodes deleted based on u and v might be within distance k of a different node pair.

To illustrate this idea, consider the maximum 2-graph 3-club problem on the graph collection in Figure 3. Constraints (2) are listed below for the node pair 1 and 6, for graphs G and H , by noting that $D_{1,6} = \{3, 4, 5\}$, $S_{G,1,6} = \{1, 2, 3, 4, 5\}$, and $S_{H,1,6} = \{1, 2, 3, 4, 5, 6\}$.

FIGURE 2 Inequality $s_1 + s_2 \leq 1$ is valid for the problem on $\mathcal{G} = \{G, H\}$ when $k = 2$

Peritently, given a graph G , a positive integer k , and a (possibly fractional) point $x^* \in [0, 1]^{|V(G)|}$, finding a length- k u, v -separator for some node pair u, v such that $x^*_u + x^*_v - x^*_{S \cap D_{u,v}} > 1$ is known to be NP-hard for $k \geq 5$ and is solvable in polynomial time for $k \in \{2, 3, 4\}$ (see [5, 39]). The case $k = 2$ is straightforward, as the common neighborhood $N_G(u, v)$ is the unique minimal separator. The cases $k \in \{3, 4\}$ require solving the maximum flow problem on an auxiliary network and applying the maximum flow-minimum cut theorem to identify a “violated separator,” or conclude that none exists.

Proposition 2. The pairwise peeling algorithm will delete the some set of nodes independent of the order in which the graphs in \mathcal{G} are processed by the algorithm.

Proof. Suppose for a specific $u \in \mathcal{G}$, (w_1, w_2, \dots, w_k) is the order in which nodes were deleted using an ordering x^* of the graphs in \mathcal{G} . Then, w_1 is too far from either u or v in some graph in the original collection, and hence, must be deleted by Algorithm 1 using any other ordering of graphs in \mathcal{G} . If w_2 was deleted following w_1 , when using x^* , then in any other ordering, after w_1 is deleted, we know that w_2 must be too far from either u or v in \mathcal{G} , and therefore, must also be deleted. By repeating this argument, $\{w_1, w_2, \dots, w_k\}$ must be deleted under any ordering that is different from x^* . As x^* is arbitrary, we can conclude that the final outcome of Algorithm 1 is independent of the order in which graphs in \mathcal{G} are processed. ■

Hereafter, we refer to this new formulation as the *pairwise peeling cut-like formulation* (PPCF). For each $u, v \in \mathcal{G}$, constraint (3) is at least as strong as constraint (2) (which in turn dominates constraint (1b)). In our computational experiments reported in Section 6, we assess the gains made by using Algorithm 1 to generate potentially stronger constraints.

4 | VALID INEQUALITIES

In this section, we introduce a family of valid inequalities for arbitrary k obtained by lifting selected zero coefficient variables in inequality (3) and another for the special case $k = 2$ that extends a result from literature for the 2-club polytope [27].

4.1 | Lifted cut-like constraints

We can strengthen constraint (3) by lifting the coefficients of some of the variables under certain conditions, similar to the approach taken in [39]. Consider a pair of nodes u, v for which we have produced a peeled collection $\mathcal{G}_{u,v}$. For graphs $G, H \in \mathcal{G}$ (not necessarily distinct), consider a node w with $\text{dist}_G(u, w) > k$ and $\text{dist}_H(v, w) > k$. We know that w cannot belong to any minimal length- k u, v -separator in G or H before the collection is peeled for the pair u, v . After peeling, w will no longer exist in any of the graphs, and therefore cannot belong to $S \in S_G(u, v)$ for any $G \in \mathcal{G}_{u,v}$. We are interested in finding an s_u such that inequality $s_u + s_v - s(S \cap D_{u,v}) \leq 1$ remains valid. Let $XCLUB(\mathcal{G}_{u,v})$ denote the cross-graph *k*-club polytope of $\mathcal{G}_{u,v}$ that is, the convex hull of feasible solutions to the formulation (1). We need:

$$s_u \leq 1 - \max\{s_u + s_v - s(S \cap D_{u,v}) : S \in XCLUB(\mathcal{G}_{u,v}), s(S \cap D_{u,v}) = 1\} = 1,$$

because $s_u = s_v = 0$ for every feasible S with $s_u = 1$ by our choice of w . We can repeat this argument by lifting another node at distance greater than k from each of the nodes u, v , and w in some graph in the collection, also with coefficient one. We can now generalize this observation to based on the following definition to yield valid inequality (4). Define a subset of nodes $S \subseteq V(\mathcal{G})$ in a cross-graph distance- k independent set if every pair of distinct nodes in S are at distance greater than k in every graph in \mathcal{G} .

Proposition 3. Given a collection \mathcal{G} , a positive integer k , let $\mathcal{G}_{u,v}$ denote the collection peeled for the node pair u, v . Consider a length- k u, v -separator $S \in S_G(u, v)$ for some $G \in \mathcal{G}_{u,v}$. Suppose $1 \in V(\mathcal{G}_{u,v}) \setminus \{u, v\}$ is a maximal subset (by inclusion) of nodes such that $\{u, v\}$ and $1 \cup \{v\}$ are cross-graph distance- k independent sets in \mathcal{G} . The following inequality is valid for $XCLUB(\mathcal{G}_{u,v})$:

$$s_u + s_v + s(1) - s(S) \leq 1. \quad (4)$$

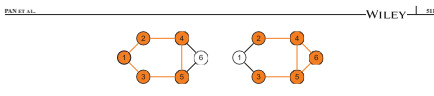
If $\text{dist}_G(u, v) > k$ for some graph $G \in \mathcal{G}_{u,v}$, the empty set is the unique minimal length- k u, v -separator in G and inequality (4) includes the special case $s_u + s_v + s(1) \leq 1$, where $1 \cup \{u, v\}$ forms a maximal cross-graph distance- k independent set.

4.2 | Independent set inequality for cross-graph 2-clubs

Mahdavi Pajouh et al. [27] introduced the following independent set cut-like inequality for the (single graph) 2-club polytope of graph G :

$$s(C) = \sum_{u,v \in C} (|N_G(u) \cap C| - 1) \cdot s_u \leq 1, \quad (5)$$

FIGURE 1 The set $\{1, 2, 3, 4, 5\}$ on the left forms a 2-club, the set $\{2, 3, 4, 5, 6\}$ on the right forms a 2-club, but does not induce a 2-club [3].



property is preserved under vertex deletion. In contrast, the *k*-club property is not preserved under vertex deletion. Nonetheless, the lack of heredity may be acceptable when it is more important to ensure that nodes on at least one of the length-bounded paths is completely contained within the subgraph induced by the club [2]. Since their introduction in social network analysis [49], these distance-based clique relaxations have been used in social and biological network analysis [8, 21, 35], as well as other areas. For low values of parameter k , typically no more than four, the *k*-club can be an appropriate choice for modeling tightly-knit clusters.

We define the cross-graph counterpart of the *k*-club, based on the cross-graph quasi-clique model introduced by Pei et al. [38], which also appears to be the earliest formal study of a cross-graph model. Let $\mathcal{G} = (G_1, G_2, \dots, G_p)$ denote a collection of p simple, undirected graphs, all defined on a common node set denoted by $V(\mathcal{G})$.

Definition 3. A subset of nodes $S \subseteq V(\mathcal{G})$ is called a *cross-graph k-club* if S is a *k*-club in each graph in collection \mathcal{G} .

This article focuses on the maximum cross-graph *k*-club problem, which seeks to find a cross-graph *k*-club of maximum cardinality in \mathcal{G} . We use the alternate term “*p*-graph” *k*-clubs if we wish to specify that there are p graphs in the collection. Otherwise, in line with past usage, we simply refer to it as a cross-graph *k*-club [39]. The 1-graph maximum *k*-club problem is NP-hard for every fixed k [11], and remains so on graphs of diameter $k + 1$ [8]. Consequently, the maximum cross-graph *k*-club problem is NP-hard for every fixed positive integer k as it includes the maximum *k*-club problem as special case when p is a singleton. In our previous study on this topic we show that this problem is NP-hard even if it contains exactly two distinct graphs [32]. Moreover, verifying if a given cross-graph *k*-club can be strictly enlarged (the complementary problem to verifying maximality by inclusion) is also shown to be NP-complete for a collection containing two distinct graphs [32]. This result extends the analogous result known for 1-graph 2-clubs to the cross-graph setting [26].

The first IP formulation in the literature for the maximum *k*-club problem was introduced in [11]. This so-called chain formulation introduces a binary variable for each path of length at most k connecting a nonadjacent pair of nodes. For the special case of $k = 2$, this reduces to the so-called common neighbor formulation for the maximum 2-club problem. As path enumeration gets increasingly challenging as k takes values larger than 2, it can take up to $O(n^k)$ binary variables and constraints to fully describe the chain formulation. To the best of our knowledge, no systematic computational studies have been reported on the chain formulation when $k \geq 3$.

Two polynomial-sized IP formulations, one using binary variables and the other using integer variables were introduced in [46]. Fully described by $O(n^2)$ variables and constraints, these are the first compact formulations for the maximum *k*-club problem for general k . A decomposition and branch-and-cut algorithm to find a maximum *k*-club that employs canonical hypercube cuts as delayed constraints is introduced in [31] (see also [73]). A cut-like formulation and a path-like formulation that use respectively, length-bounded separation and length-bounded connectors are introduced in [39]. The cut-like formulation could use exponentially many constraints, but only a binary variables. The computational superiority of this formulation is demonstrated by the numerical results reported in [39], which makes this the state-of-the-art mathematical programming approach to solve the maximum *k*-club problem for general k .

3 | INTEGER PROGRAMMING FORMULATIONS

An IP formulation for the maximum cross-graph *k*-club problem can be obtained by simply taking the conjunction of any IP formulation for the maximum *k*-club problem over all graphs in the collection. We refer to this straightforward approach as the *conjunctive formulation*. In this section, we first extend the cut-like formulation of the maximum *k*-club problem [39] to the cross-graph setting through conjunction. We present ideas which strengthen this formulation, and eventually arrive at a new formulation based on a preprocessing procedure that we call *pairwise peeling*. We also identify new valid inequalities for the problem and cross-graph extensions of existing valid inequalities from the literature.

Definition 4. Given a graph G and a pair of nonadjacent nodes u and v , a subset of nodes $S \subseteq V(G) \setminus \{u, v\}$ is called a length- k u, v -separator if $\text{dist}_{G \setminus S}(u, v) > k$.

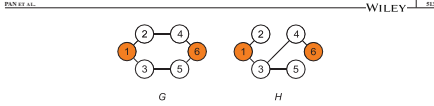


FIGURE 3 Inequality $s_1 + s_6 \leq 1$ is valid for the problem on $\mathcal{G} = \{G, H\}$ when $k = 3$.
(2, 3), (2, 5), (3, 4), (4, 5), and $S_{H,1,6} = \{1, 3\}$, (4),
 $s_1 + s_6 - s_3 \leq 1$,
 $s_1 + s_6 - s_5 \leq 1$,
 $s_1 + s_6 - s_4 \leq 1$,
 $s_1 + s_6 - s_2 \leq 1$,
 $s_1 + s_6 - s_3 \leq 1$,
 $s_1 + s_6 - s_5 \leq 1$.

However, the inequality $s_1 + s_6 \leq 1$ that can replace all of the foregoing constraints for the node pair 1 and 6 can be derived as follows: observe that $\text{dist}_G(1, 6) = 4 > 3$, thus if we want to simultaneously include nodes 1 and 6 in a 2-graph 3-club, then we cannot include node 2 and 3 and 4 can be deleted from G and H . Then, $\text{dist}_{G \setminus \{2, 3\}}(1, 6) = 4 > 3$, and consequently we cannot include node 4 either. Upon deleting nodes 2 and 4 from G and H , we find that nodes 1 and 6 are disconnected in H ; so, $s_1 + s_6 \leq 1$ is valid.

Algorithm 1 formalizes the idea illustrated by the foregoing example to generate tighter constraints, and we refer to it as the *pairwise peeling algorithm*. Let us denote the node pairs that are nonadjacent in some graph in the collection \mathcal{G} by $\mathcal{J} := \{(u, v) \in V(\mathcal{G}) : u, v \in E(\mathcal{G})\}$ for some $G \in \mathcal{G}$. The algorithm takes a graph collection \mathcal{G} , a positive integer k , and a node pair $u, v \in \mathcal{J}$ as input, and creates an auxiliary graph collection $\mathcal{G}_{u,v}$ by recursively deleting from every graph in the collection, nodes that are more than distance k from either u or v in some graph in the collection. The constraints for the node pair u and v can then be generated based on the minimal separators for graphs in this auxiliary collection $\mathcal{G}_{u,v}$. Thus, we can replace constraints (1b) by the following based on the pairwise peeled collection:

$$s_u + s_v - s(S \cap D_{u,v}) \leq 1 \quad \forall S \in S_G(u, v) \text{ and } G \in \mathcal{G}_{u,v}. \quad (3)$$

Proposition 1. Replacing constraints (1b) in formulation (1) by constraints (3) produces a correct formulation for the maximum cross-graph *k*-club problem.

The claim follows from the observation that the incidence vector of a cross-graph *k*-club satisfies constraints (3) and every binary vector satisfying these constraints also satisfies constraints (1b). Furthermore, constraints (2) and (3) coincide when $k = 2$, because the unique minimal length-2 u, v -separator in G

where C is an independent set in graph G and the notation $(\cup)^+$ denotes the $\max(\cdot, 0)$ given some real number r . Inequality (5) is valid for $\text{XCLUB}_k(G)$ if C is an independent set in some graph G by distance at every 2-club in G is based on the result in [27], and every cross-graph 2-club of G is a 2-club in G . The following theorem shows that we can further strengthen this inequality for our setting. We use $N_G^2(u)$ to denote the subset of nodes at distance at most two from vertex u in every graph in the collection, that is, $N_G^2(u) := \{v \in V(G) : \text{dist}_G(u, v) \leq 2 \forall G \in \mathcal{G}\}$.

Theorem 1. Given a graph collection \mathcal{G} and a set $C \subseteq V(G)$ that is independent in some graph $G \in \mathcal{G}$, inequality (6) is valid for $\text{XCLUB}_k(G)$:

$$|C|C| - \sum_{u \in V(G)} (|N_G(u) \cap C \cap N_G^2(u)| - 1)^+ \leq 1. \quad (6)$$

Proof. Let S be an arbitrary cross-graph 2-club of G and s^* be its incidence vector. It suffices to show that the following inequality holds in order to show that s^* satisfies inequality (6):

$$|C|C| - \sum_{u \in V(G)} (|N_G(u) \cap C \cap N_G^2(u)| - 1)^+ \leq 1.$$

As $s \in S$ and S is a cross-graph 2-club, we know that $S \subseteq N_G^2(u)$. Therefore,

$$|C|C| - \sum_{u \in V(G)} (|N_G(u) \cap C \cap N_G^2(u)| - 1)^+ \leq |C|C| - \sum_{u \in V(G)} (|N_G(u) \cap C \cap S| - 1)^+.$$

Next, we use induction on the cardinality of $C \cap S$ to prove that:

$$|C|C| - \sum_{u \in V(G)} (|N_G(u) \cap C \cap S| - 1)^+ \leq 1.$$

If $|C \cap S| = 1$, the inequality is trivially true. For some integer $q \geq 2$, we prove the claim for $|C \cap S| = q$, by assuming the claim to hold for all C' and S' such that $|C' \cap S'| \leq q - 1$.

Arbitrarily pick a node $a \in C \cap S$ and let $C_a = C \cap S \setminus \{a\}$. Note that $C_a \cap S$ is a nonempty independent set in G . By induction hypothesis,

$$|C_a|C_a| - \sum_{u \in V(G)} (|N_G(u) \cap C_a \cap S| - 1)^+ \leq 1.$$

We can now rewrite the inequality above as:

$$\begin{aligned} |C|C| - 1 - (|N_G(a) \cap C_a \cap S| - 1)^+ &= \sum_{u \in V(G)} (|N_G(u) \cap C_a \cap S| - 1)^+ \leq 1, \text{ or} \\ |C|C| - 1 - \sum_{u \in V(G)} (|N_G(u) \cap C_a \cap S| - 1)^+ &\leq 1. \end{aligned} \quad (7)$$

because node a belongs to the independent set C implying that $N_G(a) \cap C_a = \emptyset$.

Now, consider a node $b \in C_a$. As nodes a and b are contained in the independent set C and the cross-graph 2-club S , $\text{dist}_G(a, b) = 2$ and a and b have common neighbors u of nodes a and b must exist in S and that node u cannot be inside the independent set C . Hence, we know that $u \in S \setminus C$ and that $|N_G(u) \cap C \cap S| = |N_G(u) \cap C_a \cap S| + 1 \geq 2$.

From inequality (7) we obtain,

$$1 \geq |C \cap S| - 1 - \sum_{u \in V(G)} (|N_G(u) \cap C_a \cap S| - 1)^+.$$

$$|C|C| - 1 - (|N_G(a) \cap C_a \cap S| - 1)^+ - \sum_{u \in V(G)} (|N_G(u) \cap C_a \cap S| - 1)^+.$$

$$|C|C| - 1 - (|N_G(a) \cap C \cap S| - 1) - \sum_{u \in V(G)} (|N_G(u) \cap C_a \cap S| - 1)^+.$$

$$\geq |C|C| - \sum_{u \in V(G)} (|N_G(u) \cap C \cap S| - 1)^+, \text{ establishing our claim.} \quad \blacksquare$$

Theorem 1 includes as a special case, the independent set valid inequality (5) for the single-graph 2-club polytope established in [27] by observing that if \mathcal{G} is a singleton, then $N_G(u) \subseteq N_G^2(u)$. The induction approach used offers an alternate proof of that result. Another consequence is that the separation of these more general inequalities is also NP-hard, as inequality (5) is known to be NP-hard to separate [27].

with degree less than $|S|$ in $J(G^S)$, and also from every graph in \mathcal{G} . After core peeling, $J(G^S)$ will be an $|S|$ -core as long as it is not null. Next, a pair of nodes u and v that are adjacent in $J(G^S)$ can belong to a cross-graph k -club larger than $|S|$ only if they have at least $|S| - 1$ common neighbors in $J(G^S)$. If not, during community peeling step, the edge uv can be deleted from $J(G^S)$ and from every graph in the collection in which u and v are adjacent.

The power intersection graph $J(G^S)$ may contain more connected components after core and community peeling than before. As a result, there may exist an edge $uv \in E(G)$ for some $G \in \mathcal{G}$ whose end points u and v belong to different connected components of $J(G^S)$. The edge uv can be removed from every $G \in \mathcal{G}$ containing the edge. Doing so may disconnect a graph $G \in \mathcal{G}$ so that not only u and v belong to different components, but so do some other nodes a and b that are adjacent in $J(G^S)$; then, we can delete edge ab from $J(G^S)$. In other words, during the "cross-edge" peeling step, we recursively delete an edge uv from every graph in the expanded collection $\mathcal{G}(u, v)$ in which it is present, if u and v are in different connected components of some graph in \mathcal{G} or $J(G^S)$. When this recursive procedure finishes, every graph in the expanded collection $\mathcal{G}(u, v)$ will have connected components with identical node subsets inducing the components (see also [22] for a similar approach) used in a different context. As this may result in changes to the graphs in \mathcal{G} , we iterate over these peeling steps until no longer changes. Although, we chose not to do so, one might also look for a new feasible solution in $J(G)$ before repeating the peeling steps. Next, we describe our decomposition BC algorithms as applied to the collection of graphs \mathcal{G} output by Algorithm 2.

5.2 Initial root node relaxation

Denote by E the edge set of the complement graph of the power intersection graph of $J(G^S)$, that is, $E := \{u, v \in V(G) : \text{dist}_G(u, v) > 1 \text{ in some graph } G \in \mathcal{G}\}$. Like the single-graph counterparts, a cross-graph k -club is a graph-theoretic relaxation of a cross-graph k -club. The maximum cross-graph k -club problem is equivalent to the classical maximum clique problem on $J(G^S)$ formulated as:

$$\max |x(V(G))|, \quad x: x_u + x_v \leq 1 \quad \forall uv \in E, x_u \in \{0, 1\} \quad \forall u \in V(G), \quad (8a)$$

where x is the incidence vector of cross-graph k -cliques in \mathcal{G} . This formulation based on *conflict constraints* serves as the *initial root relaxation* that we start solving in both variants of our decomposition BC algorithms. To avoid having conflict constraints in the initial root relaxation for pairs of nodes that reside in different components of $J(G^S)$, we extend the initial relaxation by using a binary variable for each connected component of $J(G^S)$ and enforce that nodes selected must belong to the same component. Let C denote the set of components of $J(G^S)$. The initial root relaxation problem we use is given in formulation (8),

$$\max |x(V(G))|, \quad (8a)$$

$$\text{s.t. } x_u + x_v \leq 1, \quad \forall uv \in E(H) \text{ and } H \in C, \quad (8b)$$

$$x_u \leq y_H, \quad \forall u \in V(H) \text{ and } H \in C, \quad (8c)$$

$$y_H \in \{0, 1\}, \quad \forall H \in C, \quad (8d)$$

$$y_H \in \{0, 1\}, \quad \forall H \in C. \quad (8e)$$

Recall that every $G \in \mathcal{G}$ and the graph $J(G^S)$ have a set of connected components that are induced by the identical node subsets of $V(G)$. Therefore, we could alternatively solve the maximum cross-graph k -club problem on the collection of connected components corresponding to one such identical node subset at a time. We chose to use the extended formulation (8) in order to eliminate from experimental consideration, variations that consider greedy or reverse greedy orderings based on component sizes, and those that iteratively fix a node to be included in the solution permitting us to solve the problem in the k -neighborhood of the fixed node. Although, our purpose here is to demonstrate the effectiveness of using one formulation over another in a decomposition BC algorithm, we do recognize that incorporating more ideas from the literature on k -clubs and its variants [15, 20, 24, 31, 39, 40] could potentially improve the effectiveness of our methods.

The two decomposition BC algorithms, henceforth referred to by the underlying formulations CCF and PPCF, would detect a violated constraint (10) and (1), respectively, whenever an *integral solution* is encountered in the BC tree that corresponds to a cross-graph k -club that is not a cross-graph k -club. We chose not to separate fractional solutions based on our preliminary experiments that did not indicate noticeable performance gains for our test bed. For the special case $k = 2$, we also separate the independent set valid inequality (6). We discuss our separation procedures next.

5.3 Separation procedures

Given a graph $G \in \mathcal{G}$, a positive integer k , and a (possibly fractional) point $x^* \in [0, 1]^{V(G)}$, finding a length- k , x^* -separator S in G , for some node pair u, v such that $x_u^* + x_v^* > 1$ is known to be NP-hard for $k \geq 5$ and is solvable in polynomial-time for

Algorithm 5. Independent set inequality separation heuristic

Input: $G, x^*, \epsilon \in [0, 1]^{V(G)}$, minimum cut violation ϵ , time limit t

- 1 **for** $G \in \mathcal{G}$ **do**
- 2 Find a "good" feasible solution by solving formulation (10) for input (x^*, G) with time limit t and minimum objective target of $1 + \epsilon$ to obtain (x'', G) \triangleright Feasibility of (10) is guaranteed
- 3 **if** objective value at x'' is at least $1 + \epsilon$ **then**
- 4 **return** Cutting plane (6) for independent set $C := \{u \in V(G) : x_u'' = 1\}$

$$w_i \geq \sum_{u \in V(G)} x_u - 1 - |N_G(u) \cap N_G^2(u)|, \quad \forall i \in V(G), \quad (10c)$$

$$w_i \geq 0, \quad \forall i \in V(G), \quad (10d)$$

$$z_i + z_j \leq 1, \quad \forall ij \in E(G), \quad (10e)$$

$$z_i \in \{0, 1\}, \quad \forall i \in V(G). \quad (10f)$$

Rather than attempting to solve the separation MILP (10) to optimality, we utilize it as a heuristic. Our approach, summarized in Algorithm 5, is to solve formulation (10) on each graph $G \in \mathcal{G}$ whenever the LP relaxation optimizes at x^* at BC node is binary, with the aim of finding a good feasible solution or fail to find one after $J(G)$ attempts. Hence, we terminate the Gurobi solver early once a feasible solution of objective at least $1 + \epsilon$ is detected or the time limit t is reached.

6 COMPUTATIONAL STUDY

We report results from our computational experiments conducted on 64-bit Linux[®] compute nodes with Intel[®] "Skylake" X30 CPUs with 96 GB RAM. The algorithms are implemented in C++ and the optimization models are solved using Gurobi[®] Optimizer v9.0.1 (1) with a solve time limit of 7200 s. The global cut aggressiveness parameter in Gurobi is configured to cut off all general purpose cutting planes in order to ensure that our comparisons are a better representation of the effectiveness of the user-defined cutting planes added. All unspecified Gurobi settings, including rounding heuristics and number of threads are left at their default settings.

In general, we consider the following parameter values in our experiments: $k \in \{2, 3, 4\}$, and the number of graphs in the collection $p \in \{2, 3, 4, 5\}$. Our test bed is generated from the following three groups of graphs: the Tenth DIMACS Implementation Challenge benchmarks (1) (DIMACS-10 graphs), graphs used in computational studies in [40] (VB graphs), and graphs used in computational studies in [23, 27, 31] (BG graphs). These graphs are commonly used benchmarks for the maximum k -club problem. It is also known that the edge densities of these graphs have a discernible impact on either or not the instances are challenging for particular values of parameter k [26]. We incorporate this observation by appropriately matching the BG graphs to the value of parameter k for which we solve the maximum cross-graph k -club problem. For DIMACS-10 and VB graphs, we first conduct a set of preliminary experiments to recognize challenging graph k and combinations. Graph collections for our computational experiments are generated from these graphs, and the generation procedure varies by group. In Sections 6.1 and 6.2, we discuss our experimental results by groups of graphs in our test bed, explain the generation procedures, and the selection of challenging instances in greater detail. In Section 6.3, we consider the impact of the independent set inequality on PPCF for the special case of $k = 2$. In Section 6.4, we conduct a computational case study on the effectiveness of PPCF on a related problem of finding maximum k -club signature, which can be reduced to solving a series of maximum cross-graph k -club problems. Codes and instances used in our computational experiments are publicly available on GitHub [34].

For most of our experiments, we report results averaged over $11 - p$ runs, that is, on graph collections $\{G_1, \dots, G_{p-1}\}, \dots, \{G_{11-p}, \dots, G_{11}\}$. The only exception being the results reported from solving the maximum k -club signature problem in Section 6.4, where we report the largest solution from solving a series of maximum cross-graph k -club problems, following the definition of a signature. We use consistent column headings in all tables reported in this section, with any differences in the club signature results identified in corresponding table notes. We report under column headings "N" and "P" the corresponding parameter values and the graph collection is indicated under the column heading "Collection." Under the column heading "Nodes" and "Edges" we report the number of nodes and edges, respectively, that were removed from the graph collection in the preprocessing step using the pairwise peeling Algorithm 2. Columns labeled "obj" and "time (s)", respectively report the average optimal objective value and average running time in seconds of the corresponding approach,

It is also worth noting that our valid inequality (6) dominates inequality (5), which is also valid for $\text{XCLUB}_k(G)$. Consider the two-graph collection $\mathcal{G} = \{G, H\}$ in Figure 2. For the set $C = \{1, 5, 6\}$, which is independent in G , inequality (5) yields $|C|C| - \sum_{u \in V(G)} (|N_G(u) \cap C \cap N_G^2(u)| - 1)^+ \leq 1$, whereas inequality (6) yields $|C|C| - \sum_{u \in V(G)} (|N_G(u) \cap C \cap N_G^2(u)| - 1)^+ \leq 1$.

Both valid inequalities (4) and (6) we have considered in this section relate to inequalities established in the literature for single-graph k -clubs [27, 39]. These inequalities, under suitable conditions, are also known to induce facets of the 2-club polytope. However, we have not identified nontrivial sufficient conditions that do the same in the cross-graph setting. The primary challenge with identifying the required number of affinely independent incidence vectors of cross-graph k -clubs that lie on the face of the convex hull induced by our valid inequalities, in order to demonstrate the dimension of that face. In contrast to the single-graph counterpart, the shortest path that connect the same pair of nodes in a cross-graph k -club can be different in each graph in the collection, making the task of identifying affinely independent feasible solutions very challenging. Identifying faces of $\text{XCLUB}_k(G)$, especially when $k = 2$, is an interesting problem for future study.

5.1 DELAYED CONSTRAINT GENERATION

The main goal of our computational study in Section 6 is to compare the performance of a general purpose IP solver when using WCF and PPCF to solve the maximum cross-graph k -club problem. As both formulations use exponentially many constraints in the worst case, we implement them in a delayed fashion in the two decomposition branch-and-cut (BC) algorithms that use the same initial root node relaxation based on cross-graph k -cliques. These delayed constraint generation approaches and preprocessing ideas are described in this section.

5.1.1 Preprocessing

Before applying the decomposition BC algorithms, we apply extensions of some preprocessing techniques that are known to be effective for the single-graph counterpart to our cross-graph setting [23, 31, 39]. Algorithm 2 describes this preprocessing scheme based on a feasible solution S obtained using the "DROP heuristic" [10] for k -clubs, applied to the intersection graph $J(G)$ with node set $V(G)$ and edge set $\bigcap_{G \in \mathcal{G}} E(G)$. Every k -club in $J(G)$ is a cross-graph k -club in \mathcal{G} , although the converse is not true.

Peeling based on this cross-graph k -club S is designed to remove nodes and edges from graphs in the collection without affecting any feasible solution of $\text{XCLUB}_k(G)$ more than $|S|$. To this end, we first construct the power intersection graph $J(G^S)$ by $J(G^S)$. The node set of $J(G^S)$ is $V(G)$ and a pair of nodes are made adjacent in $J(G^S)$ if the distance between them is at most k in every graph in the collection. Finally, we use the observation that every cross-graph k -club and every cross-graph k -club defined next forms a clique of the same size in $J(G^S)$, allowing us to apply peeling ideas from the maximum clique literature.

Definition 5. Given a graph collection \mathcal{G} , a subset of nodes $S \subseteq V(G)$ is called a cross-graph k -clique if S is a k -club in each graph in \mathcal{G} .

Once a feasible solution S is available, we implement core peeling [1] followed by community peeling [47] procedures on $J(G^S)$; the peeling actions are mirrored on \mathcal{G} . If node u has fewer than $|S|$ neighbors in $J(G^S)$, it cannot belong to a cross-graph k -club larger than $|S|$ (because if it did, node u would have degree at least $|S|$ in $J(G^S)$). Core peeling recursively deletes nodes

Algorithm 2. Preprocessing

Input: A graph collection \mathcal{G} , a positive integer $k \geq 2$

Output: A preprocessed graph collection \mathcal{G}

- 1 obtain the intersection graph $J(G)$
- 2 compute a k -club S of $J(G)$ using the DROP heuristic
- 3 **do**
- 4 obtain the power intersection graph $J(G^S)$
- 5 CorePeel($J(G^S)$, $|S|$)
- 6 CommunityPeel($J(G^S)$, $|S|$)
- 7 CrossEdgePeel($J(G^S)$)
- 8 **while** \mathcal{G} is modified;
- 9 **return** \mathcal{G}

$k \in \{2, 3, 4\}$ (see [5, 39]). The case $k = 2$ is trivial as a unique minimal separator exists in the form of the common neighborhood $N_G(u, v)$. The cases $k \in \{3, 4\}$ require a transformation to an auxiliary network on which we need to solve the maximum flow problem. However, we solved the separation problems using a heuristic procedure following the approach taken in [39]. Moreover, we separate constraint (1b) in CCF and constraint (1a) in PPCF using Algorithm 1 and Algorithm 4, respectively, only if the BC node linear programming (LP) relaxation optimizes at x^* is binary. The BC node initial relaxation (1) ensures that such an x^* corresponds to a cross-graph k -club. All optimized constraints that are detected at x^* is not a cross-graph k -club are added to the lazy cut pool. The BC node relaxation is re-solved by applying at least some of these cuts, as determined by the solver.

The separation problem for valid inequality (5) for the maximum (single-graph) k -club problem was shown to be NP-hard, and its exact and heuristic separation was computationally investigated in [27]. The separation problem for valid inequality (6) for the special case $k = 2$ can be formulated as a mixed-integer nonlinear program (MINLP) similar to the single-graph counterpart defined in [27]. The following MINLP formulation (10) is the starting point for our approach to using them as cutting planes. However, our subsequent linearization uses fewer variables to handle the nonlinear objective compared to the approach used in [27]. Furthermore, based on the computational experience reported in [27], in our experiments, we favor the use of general-purpose mixed-integer linear programming (MILP) rounding heuristics available in the solver rather than attempting exact solution, or using simple greedy combinatorial heuristics for this separation problem.

Iterating over each graph $G \in \mathcal{G}$, we seek an independent set in G that underlies inequality (6), in order to separate the point $x^* \in [0, 1]^{V(G)}$. Let the binary variable z_i indicate if node i is selected in the independent set in graph $G \in \mathcal{G}$:

$$z_i(x^*, G) := \max_{x^* \in [0, 1]^{V(G)}} \sum_{i \in V(G)} x_i^* (1 - z_i) - \sum_{i \in V(G)} x_i^* (1 - z_i) \quad (9)$$

A violated independent set inequality exists for graph G if and only if $z_i(x^*, G) > 1$. We can introduce variables y_H to linearize the objective function and obtain the following separation MILP:

$$z_i(x^*, G) := \max_{x^* \in [0, 1]^{V(G)}} \sum_{i \in V(G)} x_i^* (1 - z_i) - \sum_{i \in V(G)} x_i^* (1 - z_i) \quad (10a)$$

$$\text{s.t. } y_H \leq |N_G(u) \cap N_G^2(u)| (1 - z_u), \quad \forall u \in V(G). \quad (10b)$$

Algorithm 3. CCF separation heuristic

Input: $G, x^*, \epsilon \in [0, 1]^{V(G)}$

$k \in \{2, 3, 4\}$ and $|C| = 1$ $\triangleright K$ is a cross-graph k -clique

- 1 **for** each $u \in K$ and $G \in \mathcal{G}$ **do**
- 2 **if** $\text{dist}_G(u, v) > 1$ **then**
- 3 Apply MINIMALIZE from 39 to the trivial length- k , u , v -separator $V(G) \setminus K$ to obtain a minimal separator S in G
- 4 **add** constraint $x_u + x_v - x_S \leq 1$ violated by x^* to lazy-cut pool
- 5 **return** x^* corresponds to a cross-graph k -club

Algorithm 4. PPCF separation heuristic

Input: $G, x^*, \epsilon \in [0, 1]^{V(G)}$

$k \in \{2, 3, 4\}$ and $|C| = 1$ $\triangleright K$ is a cross-graph k -clique

- 1 **for** each $u \in K$ and $G \in \mathcal{G}$ **do**
- 2 **if** $\text{dist}_G(u, v) > 1$ **then**
- 3 Apply Pairwise Peeling Algorithm 1 on a copy of G, k, u, v to obtain \mathcal{G}_{uv}
- 4 Let $G' \in \mathcal{G}_{uv}$ correspond to $G \in \mathcal{G}$
- 5 Apply MINIMALIZE from 39 to the trivial length- k , u , v -separator $V(G') \setminus K$ to obtain a minimal separator S in G'
- 6 **add** constraint $x_u + x_v - x_S \leq 1$ violated by x^* to lazy-cut pool
- 7 **return** x^* corresponds to a cross-graph k -club

unless indicated otherwise in the table notes. Columns labeled "RLC" under CCF and PPCF report the average number of lazy constraints added, namely CCF constraint (1b) and PPCF constraint (1a), respectively. The average number of branch-and-cut nodes encountered is reported under the column heading "BNCN". The column heading "BNCN" report the average number of terms with coefficient -1 on the left hand side of the added lazy constraints $x_u + x_v - x_S \leq 1$, that is, $|S|$. This is an indirect indicator of the strength of the constraints. Generally, the smaller this number, the stronger the constraint. The extra column labeled "RLC" (only under PPCF) reports the average number of strengthened PPCF constraints of type (1) added. In order to count the constraints of type (1) that are not of type (1b), we check if the length- k , u -separator S in G' obtained in step 6 of Algorithm 4 is not a length- k , u -separator in any $G \in \mathcal{G}$. That is, we only count under RLC k -clubs for every $G \in \mathcal{G}$, $\text{dist}_G(u, v) \leq k$. This implies that such a PPCF constraint could not have been obtained as a CCF constraint from any graph.

6.1 BG graphs

The BG graphs we use are part of the test bed used in [31], which was generated based on the procedure outlined in [11] (see also [13]). There are four classes of 200-node BG graphs, with 10 samples each from a random generation procedure, designated by their (average) edge density: BG-1.5 and BG-10 have densities 15% and 10% respectively and are challenging when $k = 2$; BG-2.5 have densities of 5% and are challenging for $k = 3$; BG-2.5 with densities around 2.5% are challenging for $k = 4$. We report results for the challenging instances in Table 1.

PPCF based branch-and-cut takes, on average, 47.2% less time than CCF for instances solved to optimality. Note that the wall-clock time for PPCF also includes the time spent in computing the statistics reported under columns RSLC, PPCF and CCF did not reach optimality for five and six BG-15 instances, respectively, for the case $k = 2$ and $k = 3$, and the statistics for these cases are very similar between the two approaches. For PPCF, over 72% of the lazy constraints added are of the stronger type (1), which could explain the noticeably better running time performance of this approach. For most of the instances, we observe a smaller value under PPCF than CCF. Note that the value of PPCF is zero for six groups of instances under PPCF. The lazy constraints of this type are actually conflict constraints with no negative terms on the left hand side. Across all instances solved to optimality, CCF enumerated over 21% more BC nodes on average than PPCF. The foregoing observations strongly suggest that PPCF approach based on pairwise peeling constraints significantly improves our ability to find maximum cross-graph k -clubs on this group of instances.

TABLE 1 Comparison of CCF and PPCF on BG instances

k	p	Collection	References by type				CCF				PPCF				
			Nodes	Edges	obj.	time (s)	RLC	BNCN	BNCN	BNCN	RLC	BNCN	BNCN	BNCN	
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
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2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
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2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
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2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	WL10	0	0	0	0	0	0	0	0	0	0	0	0	0
2															

TABLE 2 DIMACS-10 test graphs used in generating graph collections.

G_i	#(V)	#(E)	Edge density (%)
karate	34	1,150	0.9
karate	77	254	8.68
polbooks	105	441	8.08
adjoint	112	636	8.66
football	115	613	9.35
crkmap	453	2025	1.58
email	1113	5451	0.85
polblogs	1400	16,715	1.91
netcience	1589	2742	0.22
power	4046	4046	0.01
hsp-h	8361	17,751	0.05
PCPmapcar	10,680	24,316	0.04

6.2 DIMACS-10 and VB graphs

We used 12 graphs from the DIMACS-10 benchmarks, listed in Table 2, each serving as a “seed graph” to generate a corresponding total of 10 graphs. The edge set of each graph in the collection is constructed at random, we start with an empty graph and add edges from the seed graph with a probability of 0.8. These are the same graph collections used in the computational studies reported in [6]. VB graphs are from the test bed used in [46], and all their subcollections in this graph contain 10 graphs randomly generated with the same target (average) edge density using the same generation procedure as [11, 13]. Each of these graphs has 300 nodes and the three classes are designated as VB_0.5, VB_1.0, and VB_1.5, respectively for their edge densities 0.5%, 1.0%, and 1.5%.

The results from our preliminary experiments to identify challenging collections based on DIMACS-10 and VB graphs for the cross-graph problem are reported in tab. 10–21. We solve the collection $\{G_1, \dots, G_n\}$ (recall that we have 10 graphs corresponding to each subcollection inside each group for each value of parameter k and of interest using both algorithms. We observe that when solving most of these instances there are very few (sometimes zero) lary constraints added by both CCF and PCCF. If the initial relaxation is practically sufficient to solve the problem using both approaches, we consider these instances not to be sufficiently challenging for the problem, and therefore no meaningful distinction can be made between the performance of the two approaches. Based on our preliminary experiments, we only include those instances that required over 100 lary constraints using either CCF or PCCF. We rerun the two BC algorithms and report results averaged over 11 r -runs (as described before in Table 3). As a larger number of lary constraints is needed to solve the instances, the benefits of using PCCF over CCF is also observed in the results in Table 1. Across this test bed, on average, PCCF is 12.8% faster and over 33% of the lary constraints added by PCCF are the stronger type (3) constraints.

6.3 PCCF with independent set inequality for cross-graph 2-clubs

In this section, we report on our experiment adding the independent set inequality (6) to our PCCF method for the special case of cross-graph 2-clubs and assess its performance on the BG instances, which are among the more challenging instances in our test bed. In our experiments, we set the minimum constraint violation parameter $\epsilon = 0.5$ with a time limit of $T = 30$ seconds for each G_i . As we only separate binary points, constraint violation will always be a positive integer (within numerical tolerance). We also apply the PCCF separation Algorithm 4 to generate violated PCCF constraints following the attempt at finding a violated independent set inequality using Algorithm 5. The overall correctness of our algorithm, MLP formulation (10) is also incrementally updated before it is solved at the integral point x^* being separated only influences the objective function of this MLP. The results are reported in Table 4.

Although, we expected these cuts to improve overall performance for $k = 2$ for the challenging BG instances in our test bed, we observed a deterioration in performance in terms of average running time/optimality gap and true size. We observed similar performance losses for other values of k and termination time. It also appears based on the numbers reported under the column labeled HS/Cut that a relatively small number of violated independent set cuts were found. The average ratio of HS/Cut is just 3.7%. Adding only the PCCF constraints and letting the tree enumeration appear to be the better choice in our experimental set up. However, it is possible that a entirely different approach to adding these cutting planes could lead to better performance. For instance, we could attempt aggressive fractional separation at the root, adding a round of cutting planes simultaneously by generating one cut for each graph, and/or adding these cutting planes only at the top levels of the tree. These are directions worth

TABLE 3 Comparison of CCF and PCCF on DIMACS and VB instances.

k	r	Collection	Reduction by PCCF				PCCF				Avg. ratio of HS/Cut	Avg. number of branch-and-cut tree nodes			
			Nodes	Edges	Time (s)	RLC*	Nodes	Edges	Time (s)	RLC*					
3	2	email	209	825	1272	664.3	4830	31	48,617	1272	666.1	5213	308	30	49.94
3	2	football	0	0	367	0.5	1428	2.2	438	367	0.5	1468	0.5	2.1	452
3	3	email	207	1152	1112	701.8	7098	34	7018	1112	1412	7029	829	3.3	86.56
3	3	football	0	0	261	0.6	1512	2.4	365	261	0.6	1622	264	2.1	417
3	4	email	248	1485	1041	905.5	8870	36	51957	1041	7502	9552	1411	3.3	32.434
3	4	football	0	0	251	0.5	251	0.5	299	251	0.5	1298	285	2.2	183
3	5	email	249	1824	973	1003.9	13726	38	49,415	973	1232	1222	2239	3.4	34.256
3	5	football	0	0	247	0.5	1605	2.6	220	247	0.5	1612	396	2.1	184
4	2	VB_1.0	0	100	2.1	6.9	3399	1.2	4252	2.1	7.8	3328	3239	0.0	1155
4	2	VB_1.5	0	30	4	336.8	27301	1.9	22386	4	155.1	27421	27447	0.0	21598
4	2	email	183	462	462.9	13.6	1310	3.7	530	462.9	16.8	1380	29	3.6	346
4	3	VB_1.5	0	100	1.6	238.3	39386	1.8	17336	1.6	72.2	38490	36999	0.0	19497
4	3	email	167	876	432.5	23.4	2211	6.3	912	432.5	25.0	239	62	6.4	798
4	4	hsp-h	7384	29380	1759	2068	2315	34	8007	1759	2363	3308	240	3.2	534
4	4	VB_1.5	0	100	1.8	108.7	29420	1.7	4315	1.8	47.9	49430	29430	0.0	11840
4	4	email	150	805	411.3	27.0	2615	6.0	1284	411.3	29.1	2086	105	5.0	1186
4	4	hsp-h	7248	38182	1546	1392	4073	3.2	2311	1546	1363	3660	490	3.1	1600
4	5	VB_1.5	0	100	1.8	101.4	29184	1.7	3928	1.8	35.8	29187	29187	0.0	4489
4	5	email	152	729	396.2	26.6	2642	5.2	1454	396.2	29.0	2349	213	4.0	1392
4	5	hsp-h	7036	44855	1383	607.8	5489	3.8	2206	1383	555.9	4040	717	3.7	1021

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