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Independence Systems and Stable Set Relaxations

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Abstract

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Many fundamental combinatorial optimization problems involve the search for subsets of graph elements which satisfy some notion of independence. This thesis develops techniques for optimizing over a class of independence systems and focuses on systems having the vertex set of a finite graph as a ground set. The search for maximum stable sets in a graph offers a well-studied example of such a problem. More generally, for any integer $k \geq 1$, the maximum co- k -plex problem fits into this framework as well. Co- k -plexes are defined as a relaxation of stable sets.

This thesis studies co- k -plexes from polyhedral, algorithmic, and enumerative perspectives. The polyhedral analysis explores the relationship between the stable set polytope and co- k -plex polyhedra. Results include generalizations of odd holes, webs, wheels, and the claw. Sufficient conditions for the integrality of some related linear systems and results on the composition of stable set polyhedra are also given. The algorithmic analysis involves the development of heuristic and exact algorithms for finding maximum k -plexes. This problem is closely related to the search for co- k -plexes. The final chapter includes results on the enumerative structure of co- k -plexes in certain graphs.

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Chapter 1

Introduction

Graphs are often used to model relationships among elements of a system. For example, suppose a retail company desires to open a large number of outlets in a developing area. If research indicates that the market can sustain at most one outlet per five-mile radius, how should the company choose from a set of potential locations in order to maximize the total number of new outlets? This problem can be solved by analyzing a related graph.

To see the connection, let $V = \{v_1, \dots, v_n\}$ denote the (finite) set of potential outlet locations. Let E be the set of unordered pairs $v_i v_j$ such that location v_i is within five miles of location v_j . Notice that $S \subseteq V$ represents a feasible set of locations whenever

$$v_i v_j \notin E \quad \text{for all } v_i, v_j \in S.$$

In other words, the elements of S are pairwise nonadjacent in the graph $G = (V, E)$. The set S defines a *stable set* in G , and the company's problem is solved by finding a maximum cardinality stable set in G .

A natural extension of this location problem would be to allow at most k outlets

per five-mile radius for some integer $k \geq 1$. Note that the stable sets of G remain feasible. In general, though, the company will have the option of opening more outlets. Define the neighbor set of v_i as $N_G(v_i) := \{v_j \mid v_i v_j \in E\}$. $N_G(v_i)$ denotes the set of locations within five miles of v_i . The problem now requires a feasible solution $S \subseteq V$ to satisfy the following:

$$|N_G(v_i) \cap S| \leq k - 1 \quad \text{for all } v_i \in S.$$

In other words, each element of S has at most $k - 1$ neighbors in S . The set S defines a *co- k -plex* in G , and the company's problem is solved by finding a maximum cardinality *co- k -plex* in G .

The abstract notions of finding maximum stable sets and *co- k -plexes* in a graph are thus seen to have a useful application. Unfortunately, the ability to phrase a problem in graph-theoretic terms does not imply that an efficient solution method exists. Indeed, the decision versions of the Maximum Stable Set Problem (MSSP) and the Maximum *Co- k -plex* Problem (MCP- k) belong to the class of NP-hard problems. This suggests that any exact solution method for MSSP or MCP- k probably requires exponential, with respect to the size of the input parameters, time to identify an optimal solution in a general graph. Garey and Johnson (31) and Papadimitriou and Steiglitz (57) offer precise treatments of these complexity issues.

The complexity results on MSSP and MCP- k may seem discouraging, but they do not indicate that all problem instances of practical size are intractable. In fact,

an extensive body of research has led to the solution of challenging MSSP instances on graphs with hundreds of vertices (68; 73; 18; 4; 54). Much of this research was conducted in response to an implementation challenge coordinated by the center for *Discrete Mathematics and Theoretical Computer Science* (DIMACS) in 1992.

Since 1992, algorithms for solving MSSP are primarily tested on the well-known DIMACS (26) benchmark graphs, many of which have industrial applications. A survey of methods as of 1999 is given by Bomze et al.(10). More recent research (65; 60) has improved the running time for solutions on the DIMACS graphs and found solutions for random graphs on the order of 15,000 vertices. MCPP- k is far less studied (6; 49), but one purpose of this thesis is to analyze MCPP- k on graphs of comparable size.

This thesis shows that many results first discovered in the context of stable sets have analogues in the context of co- k -plexes. The new co- k -plex analogues reveal that certain properties of stable sets do not strictly depend on the definition of a stable set. Instead, it turns out that an arbitrary, but fixed, level of degree-boundedness suffices to obtain much of the structure associated with stable sets. The analysis focuses on finding co- k -plex analogues for polyhedral, algorithmic, and enumerative properties of stable sets.

The polyhedral analysis deals with linear systems of inequalities. In principle, polyhedral results facilitate the use of linear programming techniques to solve co- k -plex optimization problems. Chapter 4 introduces four new classes of facets for the

co- k -plex polytope. Chapter 4 also shows that the exclusion of certain subgraphs causes the co-2-plex polytope to have a relatively simple facial structure. This result characterizes a class of graphs for which co-2-plex optimization is tractable. In addition, the polyhedral analysis includes a generalized notion of graph perfection and results on composition of co-1-plex polyhedra.

Combinatorial algorithms provide another solution method for co- k -plex optimization problems. Rather than mapping the problem into a polyhedron, combinatorial algorithms operate directly on the graph elements. Chapter 5 describes various new combinatorial algorithms related to co- k -plex optimization. The heuristics generalize well-known algorithms by Brèlaz (11) and Balas and Xue (5). The exact algorithms generalize well-known algorithms by Applegate and Johnson (1), Carraghan and Pardalos (18), and Östergård (54).

The co- k -plex polynomials in Chapter 6 carry information on the combinatorial structure of co- k -plexes in a graph. Although tractable co- k -plex optimization and nice combinatorial structure often coincide, the study of co- k -plex polynomials has other benefits including visualization. For example, the problem of counting and characterizing binary strings with no consecutive triplet of ones is equivalent to computing the co-2-plex polynomial of the path P^n . Chapter 6 introduces co- k -plex polynomials and obtains recursive formulas for structured graphs such as paths and cycles.

This thesis is organized as follows. Chapter 2 introduces notation and definitions used throughout the thesis. Chapter 3 discusses composition of stable set polyhe-

dra. Chapter 4 studies the co- k -plex polytope. Chapter 5 contains heuristic and exact algorithms for detecting cohesive subgraphs, a problem intimately related to the search for co- k -plexes. All algorithms were implemented and run on a 2.2 GHz Dual-Core AMD Opteron processor with 3 GB of memory. Chapter 6 introduces co- k -plex polynomials. Chapter 7 offers some concluding remarks and discusses future research.

Chapter 2

Notation and Definitions

This section discusses notation and definitions relating to graphs, polyhedra, independence systems, and generating functions. An in-depth treatment of graph theory is given by Diestel (25). Polyhedral theory is discussed in Cook et al. (23). Stanley's book (64) develops the theory of generating functions. Most of what follows can be found in these references. The remainder of this thesis will make extensive use of the material in this chapter.

2.1 Graph Preliminaries

Let $G = (V, E)$ be a graph with vertices $V(G) := V$ and edges $E(G) := E$. All graphs considered will be finite, simple, and undirected. The vertices $v, u \in V$ are said to be *adjacent* if $uv \in E$. A *stable set* consists of pairwise nonadjacent vertices. The cardinality of a largest stable set in G is denoted $\alpha(G)$. A *complete* graph consists of pairwise adjacent vertices. Maximal complete subgraphs are called cliques. The cardinality of a largest clique in G is denoted by $\omega(G)$. Let $\bar{G} = (V, \bar{E})$ denote the *complement graph* of G , where $e \in \bar{E} \Leftrightarrow e \notin E$. Notice that the complement of a

stable set is a complete graph.

A *path* P^k in G is a subgraph with vertex set $\{v_1, \dots, v_k\} \subseteq V$ and edge set $\{v_1v_2, \dots, v_{k-1}v_k\} \subseteq E$ where the v_i are all distinct. A *cycle* C^k in G is a subgraph with vertex set $\{v_1, \dots, v_k\} \subseteq V$ and edge set $\{v_1v_2, \dots, v_{k-1}v_k, v_kv_1\} \subseteq E$ where the v_i are all distinct. The length of a path (cycle) is defined to be $|E(P^k)|$ ($|E(C^k)|$). An edge $e \in E \setminus E(C^k)$ which joins two vertices in C^k is a *chord*. Chordless cycles of length at least four are called induced cycles or *holes*.

For all $v \in V$, let $N_G(v) := \{u \in V \mid uv \in E\}$ be the neighbor set of v , and let $deg_G(v) = |N_G(v)|$ be the degree of v in G . Define the closed neighbor set as $N_G[v] := N_G(v) \cup \{v\}$. Define $\Delta(G) := \max_{v \in V} \{deg_G(v)\}$ and $\delta(G) := \min_{v \in V} \{deg_G(v)\}$. Let $V' \subseteq V$ and $E(V') := \{uv \in E \mid u, v \in V'\}$. The subgraph *induced* by V' is $G[V'] := (V', E(V'))$.

Fix an integer $k \geq 1$. A subset $S \subseteq V$ induces a *co- k -plex* if $\Delta(G[S]) \leq k - 1$. The term *co- k -plex* refers to both the graph $G[S]$ and the set S . Notice that *co-1-plexes* are stable sets. A subset $K \subseteq V$ induces a *k -plex* whenever $\delta(G[K]) \geq |K| - k$. The term *k -plex* refers to both the graph $G[K]$ and the set K . Notice that *1-plexes* are complete graphs. The set S is a *co- k -plex* in G if and only if S is a *k -plex* in \bar{G} . Consequently, the Maximum *co- k -plex* and Maximum *k -plex* problems are intimately related. This is analogous to the relationship between stable sets in G and complete graphs in \bar{G} .

2.2 Polyhedral Preliminaries

Given vectors $x_1, \dots, x_k \in \mathbf{R}^n$ and nonnegative scalars $\lambda_1, \dots, \lambda_k \in \mathbf{R}_+$, the vector $\sum_{i=1}^k \lambda_i x_i$ is a *convex combination* of the x_i 's if $\sum_{i=1}^k \lambda_i = 1$. The *convex hull* of a finite set $S \subset \mathbf{R}^n$ is the set of all convex combinations of S . The convex hull of S is the smallest convex set containing S .

The vectors $x_1, \dots, x_k \in \mathbf{R}^n$ are said to be *affinely independent* if $\sum_{i=1}^k \lambda_i x_i = 0$ and $\sum_{i=1}^k \lambda_i = 0$ imply that $\lambda_i = 0$ for all i . The more familiar concept of linear independence implies affine independence. The *dimension* of $K \subseteq \mathbf{R}^n$, i.e. $\dim K$, is one less than the maximum cardinality of an affinely independent set contained in K .

A *polyhedron* is the solution set to a finite system of linear inequalities. In other words, for any polyhedron P , there exists some (A, b) such that $P = \{x \mid Ax \leq b\}$. A polyhedron $P \subseteq \mathbf{R}^n$ is *full-dimensional* if $\dim P = n$. A vector $v \in P$ is a *vertex* if and only if v is not the convex combination of vectors in $P \setminus \{v\}$. Bounded polyhedra are called *polytopes*. A polytope can be characterized as the convex hull of its vertices.

An inequality $c^T x \leq d$ is *valid* for P if $P \subseteq \{x \mid c^T x \leq d\}$. The inequality is *supporting* if $P \cap \{x \mid c^T x = d\} \neq \emptyset$. The set $F = P \cap \{x \mid c^T x = d\}$ is called a *face* of P . More generally, any subsystem $A'x \leq b'$ of $Ax \leq b$ *induces* the face $F = P \cap \{x \mid A'x = b'\}$, and every face of P is defined by some subsystem of valid inequalities. If $F \neq \emptyset$ and $F \neq P$, then F is a *proper* face of P .

A polyhedron is *integral* if every nonempty face contains an integral vector. The

set of faces, \mathcal{F} , of the polyhedron P and the set inclusion relation define a partially ordered set (\mathcal{F}, \subseteq) . The maximal elements of (\mathcal{F}, \subseteq) are called *facets*. If P is a polytope, then the minimal elements of (\mathcal{F}, \subseteq) are exactly the vertices of P . Thus, a polytope is integral if its vertices are integral vectors.

For the remainder of this section, let P be a full-dimensional polytope. All facets F of P satisfy $\dim F = n - 1$. Consequently, F is a facet whenever it contains n affinely independent points. Any facet F of P also satisfies the following: if $F' \in \mathcal{F}$ is a proper face and $F \subseteq F'$, then $F = F'$.

Any defining linear system for P must contain a distinct facet-inducing inequality for each facet. A defining system of inequalities is *minimal* if there exists a bijection between the set of inequalities and the facets of P . P always has a unique (up to positive scalar multiple) minimal defining system. The word facet will often be used to refer to both the face itself and the inequality which induces it.

2.3 Independence Systems

Let S be a finite ground set and \mathcal{I} a family of subsets which are closed under set inclusion. More precisely, $J' \subseteq J \in \mathcal{I}$ implies that $J' \in \mathcal{I}$. The pair (S, \mathcal{I}) defines an *independence system*. The elements in \mathcal{I} are known as independent sets. Each element $J \in \mathcal{I}$ has an associated incidence vector $x^J \in \mathbf{R}^{|S|}$, where $x_v^J = 1$ if $v \in J$ and $x_v^J = 0$ otherwise. The convex hull of all such incidence vectors defines an independence system polytope.

A *normal* independence system has the property that all singletons $v \in S$ are independent, i.e. $v \in S$ implies $\{v\} \in \mathcal{I}$. The polyhedra associated with normal independence systems are full-dimensional subsets of the unit hypercube in $R^{|S|}$. Independence systems are well-studied (22; 29; 53).

Finding an independent set of maximum cardinality is an NP-hard problem in general. One notable exception occurs when all maximal independent sets have the same cardinality. An independence system with this property is called a *matroid*. Matroids and the associated greedy algorithm have been well-studied (27; 28; 45; 55; 59; 67).

It is possible to define many independence systems over a finite graph G . This thesis studies a family of independence systems defined over V . In particular, for any integer $k \geq 1$, let \mathcal{I}_k denote the set of co- k -plexes in G . Notice that if S is a co- k -plex and $S' \subseteq S$, then S' is also a co- k -plex. In other words, any induced subgraph of a degree-bounded graph is also degree-bounded. Thus, \mathcal{I}_k is closed under set inclusion, and (V, \mathcal{I}_k) defines an independence system. The associated independence system polytope is studied in Chapter 4. The enumerative structure of (V, \mathcal{I}_k) is analyzed in Chapter 6.

2.4 Independence Polynomials and Enumeration

In enumerative combinatorics, a sequence of integers $(a_i)_{i \geq 0}$ is often represented as the coefficients of a *formal power series*. The reason for this is best explained

through an example. Let S be a set of n objects and suppose a_i denotes the number of subsets $T \subseteq S$ such that $|T| = i$. Following the convention that $\binom{n}{i} = 0$ for $i > n$, the elements of the sequence satisfy $a_i = \binom{n}{i}$ for all $i \geq 0$.

The sequence $(a_i)_{i \geq 0}$ can be stored as the coefficients of the following power series:

$$A(x) = \sum_{i \geq 0} a_i x^i = \sum_{i \geq 0} \binom{n}{i} x^i.$$

Observe that a_i is the coefficient of x^i in the polynomial $A(x)$. In this context, $A(x)$ is called a *generating function*. This construction is a form of book-keeping, and there is no claim made on the convergence properties of $A(x)$. Moreover, the analysis of $A(x)$ will focus on its properties as an object subject to operations such as multiplication and addition. Although $A(1)$ happens to give the total number of subsets of S , the evaluation of $A(x)$ need not have combinatorial significance in general.

Notice that the Binomial Theorem allows for an elegant representation of this sequence. $A(x)$ can be described as follows:

$$A(x) = \sum_{i \geq 0} \binom{n}{i} x^i = \sum_{i \geq 0}^n \binom{n}{i} x^i = (1+x)^n.$$

Thus, the value of a_i is stored as the coefficient of x^i in the polynomial $(1+x)^n$. One purpose of this representation is that performing an operation on $A(x)$ can correspond to an operation on the set S . For example, let S' be a set of m objects such that $S \cap S' = \emptyset$. Define $(b_i)_{i \geq 0}$ accordingly. The sequence $(b_i)_{i \geq 0}$ can be represented as

the polynomial $B(x) = (1 + x)^m$. Consider the product of generating functions:

$$C(x) = A(x)B(x) = (1 + x)^n(1 + x)^m = (1 + x)^{n+m}.$$

The coefficient c_i of x^i in $C(x)$ now represents the number of subsets $T \subseteq S \cup S'$ such that $|T| = i$. Therefore, taking the product of generating functions corresponded to taking the union of the underlying sets. Generating functions are also useful for developing recursive relationships and analyzing asymptotic behavior. It would have been easy to derive these results directly for this particular sequence, but generating functions are powerful tools for gaining insight into the behavior of more complicated combinatorial structures.

Given a graph $G = (V, E)$, let \mathcal{I}^G denote the set of stable sets in G . Gutman and Harary (33) associated the following polynomial with G :

$$I(G; x) = \sum_{I \in \mathcal{I}^G} x^{|I|}.$$

This is the *independence polynomial* of G . Now the coefficient a_i of x^i is the number of stable sets of cardinality i in G . The *independence polynomial* has been studied in a number of papers (2; 12; 13; 14; 20; 34; 35; 37; 40; 41; 42). Levit and Mandrescu offer a survey (43). Chapter 6 introduces the *co- k -plex polynomial* and generalizes some properties of the independence polynomial.

The definitions and notation discussed in this chapter will be used throughout this

thesis. In-depth treatments of these concepts can be found in the references listed at the beginning of this chapter.

Chapter 3

Composition of Stable Set Polyhedra

Barahona and Mahjoub found a defining system of the stable set polytope for a graph with a cut-set of cardinality 2. This chapter extends this result to cut-sets composed of a complete graph minus an edge and uses the new theorem to derive a class of facets.

3.1 Introduction

Let $G = (V, E)$ be a simple undirected graph. Let $\mathcal{S} := \{S \subseteq V \mid S \text{ is a stable set}\}$. Each $S \in \mathcal{S}$ has an incidence vector $x^S \in \mathbf{R}^{|V|}$, where $x^S(v) = 1$ if $v \in S$ and $x^S(v) = 0$ otherwise. Let $P(G)$ be the convex hull of all x^S such that $S \in \mathcal{S}$. $P(G)$ is a full-dimensional polytope and has a unique (up to positive scalar multiples) minimal defining system. A vertex set $K \subseteq V$ is complete whenever $G[K]$ is a complete subgraph. A maximal complete subgraph defines a clique. A vertex $v \in V$ is *simplicial* if $G[N(v)]$ is complete.

A cut-set $C \subset V$ decomposes G into a pair of proper subgraphs (G_1, G_2) such that $C = V(G_1) \cap V(G_2)$ and all paths from G_1 to G_2 intersect C . Chvátal (21) showed

that the union of defining systems of $P(G_1)$ and $P(G_2)$ defines $P(G)$ when $G[C]$ is a clique. Barahona and Mahjoub (8) defined $P(G)$ based on systems related to $P(G_1)$ and $P(G_2)$ when $|C| \leq 2$. We extend this result to the case where $G[C]$ is a complete graph minus an edge.

Section 3.2 contains results necessary to extend Barahona and Mahjoub's theorem. Section 3.3 generalizes their theorem. Section 3.3 refers to results from (8). Section 3.4 applies the new theorem to derive a class of facets for the stable set polytope called diamonds. Section 3.5 uses techniques similar to Barahona and Mahjoub's method to prove a theorem of Chvátal. Section 3.6 summarizes the results.

3.2 Support Graphs

Suppose G has a cut-set C consisting of a nonadjacent pair of vertices. To obtain a defining system for $P(G)$, Barahona and Mahjoub (8) attach to C a new set of vertices $\{w_i\}$. This augmentation defines a graph \tilde{G} . $P(\tilde{G})$ has a facet which projects along the subspace of $\{w_i\}$ variables to define $P(G)$. We generalize this method to the case where $G[C]$ is a complete graph minus an edge. Section 3.3 analyzes the decomposition of \tilde{G} into the pair $(\tilde{G}_1, \tilde{G}_2)$. Here, we determine how the support graphs of facets for $P(\tilde{G}_k)$ interact with the $\{w_i\}$ vertices.

Let $a^T x \leq b$ be a nontrivial facet of $P(G)$. Nontriviality implies $b > 0$ and $a_v \geq 0$ for all $v \in V$. In this section, all facets are assumed to be nontrivial. Define the following sets:

$$V_a := \{v \in V \mid a_v > 0\} \text{ and } \mathcal{F}_a := \{S \in \mathcal{S} \mid a^T x^S = b\}.$$

The *support graph* of $a^T x \leq b$ is defined as $G_a := G[V_a]$, the subgraph induced by V_a .

Remark 1. *Given a facet $a^T x \leq b$, \mathcal{F}_a consists of maximal stable sets in G_a .*

In Section 3.3, we partition inequalities based on their intersection with the set $\{w_i\}$. Lemma 1 reduces the number of partition sets. Recall that since $P(G)$ is full-dimensional, the sets $S \in \mathcal{F}_a$ collectively satisfy no equations other than scalar multiples of $a^T x = b$.

Lemma 1. *If $a^T x \leq b$ is a non-clique facet, then G_a contains no simplicial vertex.*

Proof. Suppose $v \in V_a$ is simplicial in G_a . Then $K := \bar{N}_{G_a}(v)$ is a clique and there exists an $S \in \mathcal{F}_a$ such that $S \cap K = \emptyset$. Otherwise, $\sum_{v \in K} x^{S'}(v) = 1$ for all $S' \in \mathcal{F}_a$, a contradiction because $a^T x \leq b$ is not a clique inequality. Observe that S is not a maximal stable set in G_a , since $S \cup \{v\}$ is a feasible stable set. This contradicts Remark 1. □

Suppose $G = (G_1, G_2)$ has a cut-set C where $G[C]$ is a complete graph minus an edge. Notice $G[C]$ has a stable set $\{u, v\}$. For $k \in \{1, 2\}$, add the $\{w_i\}$ vertices to G_k such that $N_{\tilde{G}_k}(w_1) = \{w_2\} \cup (C \setminus \{u\})$, $N_{\tilde{G}_k}(w_2) = \{w_1, u\}$, and $N_{\tilde{G}_k}(w_3) = C$. See Figure 3.1 for the augmented graph \tilde{G}_k . The heavy edges denote joins (see (71)). For example, the edge between u and $C \setminus \{u, v\}$ indicates that u is adjacent to every vertex in $C \setminus \{u, v\}$.

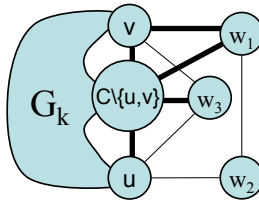


Figure 3.1: The augmented graph \tilde{G}_k .

$$\begin{bmatrix} 1 & \vec{0}^T & 1 & 0 & 0 \\ 0 & \vec{1}^T & 0 & 1 & 0 \\ 0 & \vec{0}^T & 1 & 1 & 0 \\ 1 & \vec{0}^T & 0 & 0 & 1 \\ \vec{0} & I^{(|C|-1) \times (|C|-1)} & \vec{0} & \vec{0} & \vec{1}_v \end{bmatrix}$$

Figure 3.2: The matrix A.

Lemma 2. *Let $u, v \in C$ be nonadjacent and $\tilde{C} := C \cup \{w_1, w_2, w_3\}$. For $k \in \{1, 2\}$,*

$$F_k := \{x \in P(\tilde{G}_k) \mid \sum_{z \in \tilde{C}} x(z) = 2\}$$

is a facet for $P(\tilde{G}_k)$. Moreover, no other facet contains all the vertices of \tilde{C} in its support.

Proof. We show that F_k is a facet for $P(\tilde{G}_k[\tilde{C}])$ by building a full-rank $|\tilde{C}| \times |\tilde{C}|$ matrix whose columns are incidence vectors of all stable sets which lie on F_k . See Figure 3.2. The first three rows correspond to w_1, w_2 , and w_3 . The last rows correspond to u and $C \setminus \{u\}$, respectively. Let $\vec{1}_v$ be the $(|C|-1)$ -dimensional column vector with a 1 in row v and 0's elsewhere.

We now lift the inequality $\sum_{z \in \tilde{C}} x(z) \leq 2$ to a facet of $P(\tilde{G}_k)$. Since all maximal stable sets J in \tilde{G}_k satisfy $|J \cap \tilde{C}| = 2$, the lifting coefficients for vertices in $V(\tilde{G}_k) \setminus \tilde{C}$

are zero. Thus, the inequality is a facet of $P(\tilde{G}_k)$. Suppose another facet $a^T x \leq b$ contains all vertices of \tilde{C} in its support. By Remark 1, $\sum_{z \in \tilde{C}} x^{S'}(z) = 2$ for all $S' \in \mathcal{F}_a$. It follows that F_k coincides with the face induced by $a^T x \leq b$. \square

Given a defining system for a polytope, the process of projecting along a subspace of variables, say w_1 and w_2 , is less complicated if the coefficients of w_1 and w_2 are binary. The following lemma allows the defining systems encountered in Section 3.3 to be put in this form.

Lemma 3 (Mahjoub (47)). *Given a facet $a^T x \leq b$, let $w_1, w_2 \in V_a$ be adjacent vertices in G_a . If w_1 is simplicial in $G_a - w_2$ and w_2 is simplicial in $G_a - w_1$, then $a_{w_1} = a_{w_2}$.*

Lemma 3 implies that $a_{w_1} = a_{w_2}$ in any nontrivial facet containing both w_1 and w_2 in its support. As a result, scaling these inequalities by $(1/a_{w_1}) = (1/a_{w_2})$ will produce inequalities where both variables have binary coefficients.

3.3 Composition of Stable Set Polyhedra

This section offers a straightforward extension of techniques developed by Barahona and Mahjoub. We will refer to results from (8). Let $G = (G_1, G_2)$ have a cut-set C where $G[C]$ is a complete graph minus an edge. Construct the augmented graph \tilde{G} by adding a new set of vertices $\{w_i\}$ to C , as in Section 3.2. Define $\tilde{C} := C \cup \{w_i\}$.

$P(\tilde{G})$ has a facet $F = \{x \in P(\tilde{G}) \mid \sum_{z \in \tilde{C}} x(z) = 2\}$ such that

$$P(G) = \text{proj}_{w_1, w_2, w_3} \{F\} = \{x \in \mathbf{R}^{|\tilde{G}|} \mid \exists w \in \mathbf{R}^3 \text{ s.t. } (x, w) \in F\}.$$

The set \tilde{C} decomposes \tilde{G} into the pair $(\tilde{G}_1, \tilde{G}_2)$. In Section 3.2, it was shown that $P(\tilde{G}_k)$ has a facet F_k for $k \in \{1, 2\}$.

Lemma 4 (Barahona and Mahjoub (8)). *The facet F is defined by the union of the systems that define F_1 and F_2 .*

Lemma 4 relies on the existence of a full-rank, square matrix of all incidence vectors for stable sets on F , F_1 , and F_2 . The matrix A constructed in the proof of Lemma 2 (see Figure 3.2) implies that this lemma holds for the class of cut-sets C we are analyzing. In order to find a defining system for F , consider the defining system for $P(\tilde{G}_k)$ (other than clique inequalities involving the $\{w_i\}$ variables). Recall from Section 3.2 that the support of $a^T x \leq b$ is denoted by V_a . Lemma 1 and Lemma 2 imply that the facet-defining inequalities can be partitioned into three sets I_1^k, I_2^k, I_3^k defined as follows:

$$I_1^k := \{a_i^T x \leq b_i \mid V_{a_i} \cap \{w_1, w_2, w_3\} = \emptyset\}$$

$$I_2^k := \{a_i^T x \leq b_i \mid V_{a_i} \cap \{w_1, w_2, w_3\} = \{w_1, w_2\}\}$$

$$I_3^k := \{a_i^T x \leq b_i \mid V_{a_i} \cap \{w_1, w_2, w_3\} = \{w_3\}\}.$$

Let $V_k = V(G_k)$. Lemma 3 and Lemma 4 imply that the defining system of F can be written as follows, $k \in \{1, 2\}$:

$$\sum_{j \in V_k} a_{ij}^k x(j) \leq b_i^k, \text{ for all } i \in I_1^k$$

$$\sum_{j \in V_k} a_{ij}^k x(j) + x(w_1) + x(w_2) \leq b_i^k, \text{ for all } i \in I_2^k$$

$$\sum_{j \in V_k} a_{ij}^k x(j) + x(w_3) \leq b_i^k, \text{ for all } i \in I_3^k$$

$$\sum_{j \in C \setminus u} x(j) + x(w_1) \leq 1$$

$$\sum_{j \in C \setminus u} x(j) + x(w_3) \leq 1$$

$$\sum_{j \in C \setminus v} x(j) + x(w_3) \leq 1$$

$$x(u) + x(w_2) \leq 1$$

$$x(w_1) + x(w_2) \leq 1$$

$$\sum_{j \in \tilde{C}} x(j) = 2$$

$$x(j) \geq 0, \text{ for all } j \in \tilde{V}_k.$$

The projection of this system along the subspace of the $\{w_i\}$ variables is the polytope $P(G)$. To define $P(G)$, we proceed exactly as in (8).

Theorem 1. *The polytope $P(G)$ is defined by the union of defining systems for $P(G_1)$ and $P(G_2)$, the non-negativity constraints, and the following facet-defining mixed inequalities:*

$$\sum_{j \in V_k} a_{ij}^k x(j) + \sum_{j \in V_l} a_{rj}^l x(j) - \sum_{j \in C} x(j) \leq b_i^k + b_r^l - 2 \quad \text{for } k = 1, 2; l = 1, 2; k \neq l; i \in I_2^k; r \in I_3^l.$$

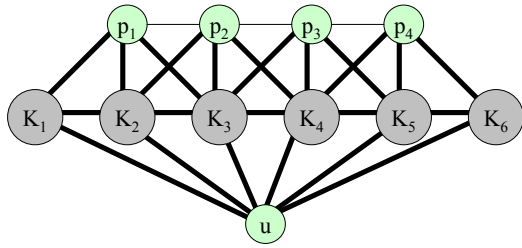


Figure 3.3: A diamond of size 6.

Proof. See Theorem 3.5 and Corollary 3.7 in (8). □

3.4 Diamonds

This section uses Theorem 1 to derive a class of facets for $P(G)$. Let K_1, \dots, K_6 be sets of vertices such that each K_i is nonempty and complete. The graph G shown in Figure 3.3 is a member of a class of graphs which we call diamonds. The heavy edges denote joins. For example, an edge between K_i and K_j indicates that $G[K_i \cup K_j]$ is complete. The size of the diamond is equal to the number of sets K_i . The diamond in Figure 3.3 has size 6, and $\sum_{z \in V} x(z) \leq 3$ induces a facet for $P(G)$. In general, facet-inducing diamonds have size $2n$ (where $n > 1$), a vertex u such that $N_G(u) = \bigcup_{i=1}^{2n} K_i$, and a path $P = p_1 p_2 \dots p_{2n-2}$ attached to the sets K_1, \dots, K_{2n} as shown in Figure 3.3.

Theorem 2. *Let $n > 1$. If a diamond G has size $2n$, then $\sum_{z \in V} x(z) \leq n$ induces a facet for $P(G)$.*

Proof. The proof is by induction on n .

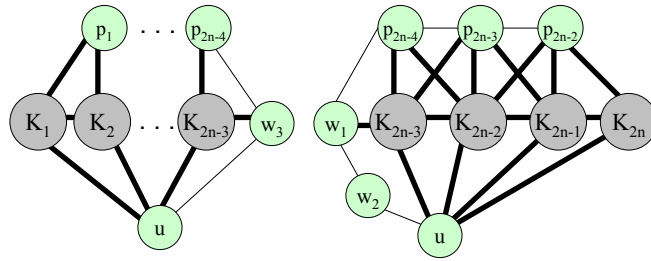


Figure 3.4: Subgraphs of \tilde{G}_1 and \tilde{G}_2 .

Base case ($n = 2$): Choose $v \in K_1$ and $w \in K_4$. The diamond of size 4 has a 5-hole on the vertex set $\{p_1, p_2, w, u, v\}$. Moreover, the odd-hole inequality can be lifted to include all vertices in $\bigcup_{i=1}^4 K_i$. This implies that $\sum_{z \in V} x(z) \leq 2$ induces a facet for $P(G)$ as claimed.

Induction step ($n > 2$): Suppose the theorem holds for all diamonds of even size less than $2n$. The diamond of size $2n$ has a cut-set $C = K_{2n-3} \cup \{u, p_{2n-4}\}$ which can be constructed by removing an edge from a complete graph. Therefore, we apply Theorem 1. Figure 3.4 shows subgraphs of the pair $(\tilde{G}_1, \tilde{G}_2)$. Let $V'_1 = V(\tilde{G}_1) \setminus \{w_1, w_2\}$ and $V'_2 = V(\tilde{G}_2) \setminus \{w_3\}$. The graph on the left is a diamond of size $2n - 2$. By induction,

$$\sum_{z \in V'_1} x(z) \leq n - 1 \quad (3.1)$$

is a facet for $P(\tilde{G}_1)$. \tilde{G}_2 has an odd-hole inequality which lifts to obtain that

$$\sum_{z \in V'_2} x(z) \leq 3 \quad (3.2)$$

is a facet for $P(\tilde{G}_2)$.

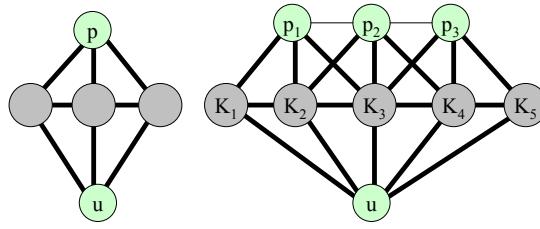


Figure 3.5: Diamonds with odd size.

Notice that inequality (3.1) $\in I_3^1$ and inequality (3.2) $\in I_2^2$. Theorem 1 gives the following facet-defining mixed inequality for $P(G)$:

$$\sum_{z \in V(G_1)} x(z) + \sum_{z \in V(G_2)} x(z) - \sum_{z \in C} x(z) \leq n - 1 + 3 - 2$$

Upon simplifying, we obtain that $\sum_{z \in V} x(z) \leq n$ is a facet for $P(G)$ as claimed. □

Theorem 2 fails when the diamond has size that is odd and at least three. To see this, let G be the diamond of size 3 shown in Figure 3.5. G is perfect and not a clique, so G is not a support graph for any facet of $P(G)$. Now let G be the diamond of size 5 also shown in Figure 3.5. If G is the support graph of a facet, then there must exist $4 + \sum_{i=1}^5 |K_i|$ affinely independent maximal stable sets satisfying some equation. However, no such set exists. It follows by induction that a diamond of odd size is not a support graph for any facet of $P(G)$.

3.5 A Theorem of Chvátal

This section uses techniques from the previous sections to obtain a theorem of Chvátal. Let $G = (G_1, G_2)$ be a graph with cut-set C , where C is a clique. Define \tilde{G} by adding a new vertex w such that $N_{\tilde{G}}(w) = C$. The maximal clique inequality $\sum_{j \in C} x(j) + x(w) \leq 1$ is a facet F for $P(\tilde{G})$ and a facet F_k for $P(\tilde{G}_k)$. Moreover, $P(G)$ is the projection of F along the w variable. Partition the defining system for $P(\tilde{G}_k)$ into the sets $I_1^k := \{\alpha^T x \leq \beta \mid w \notin V_\alpha\}$ and $I_2^k := \{\alpha^T x \leq \beta \mid w \in V_\alpha\}$. Lemma 1 implies $I_2^k = \{\sum_{j \in C} x(j) + x(w) \leq 1\}$ since w is simplicial. Therefore, F is defined by the following system $k \in \{1, 2\}$:

1. $\sum_{j \in V_k} a_{ij}^k x(j) \leq \beta_i^k$, for all $i \in I_1^k$
2. $\sum_{j \in C} x(j) + x(w) = 1$
3. $x(j) \geq 0$, for all $j \in \tilde{V}_k$

The projection of which is simply the union of defining systems for $P(G_1)$ and $P(G_2)$.

3.6 Conclusions

This chapter generalizes a theorem of Barahona and Mahjoub concerning the composition of stable set polyhedra. The main theorem extends Barahona and Mahjoub's theorem to the case where the separating set consists of a complete graph minus an edge. The new result is applied to derive a class of facets called diamonds. It is also

shown that similar techniques can be used to prove Chvátal's theorem on complete separating sets.

Chapter 4

The Co- k -plex Polyhedra and Integral Systems

k -plexes are cohesive subgraphs which were introduced to relax the structure of cliques. A co- k -plex is the complement of a k -plex and is therefore similar to a stable set. This chapter derives the co-2-plex analogue for certain properties of the stable set polytope. We also describe a class of 0-1 matrices A for which the polytope $\{x \in \mathbf{R}_+^n \mid Ax \leq 2, x \leq 1\}$ is integral. This characterization leads to the concept of k -plex perfection.

4.1 Introduction

Given a graph $G = (V, E)$, the problem of finding a maximum cardinality stable set in G is a fundamental topic in combinatorial optimization. The Maximum Stable Set Problem (MSSP) has been the subject of extensive research, much of which has focused on analyzing the convex hull of stable set incidence vectors $P(G)$. If a system of linear inequalities which define $P(G)$ is at hand, MSSP can be solved using linear programming methods. However, such defining systems can be difficult to obtain because MSSP is NP-hard in general.

The Maximum Clique Problem (MCP) is intimately related to MSSP. The search for cohesive subgraphs has applications in ad hoc wireless networks (19), data mining (69), social network analysis (70), and biochemistry and genomics (16). For a discussion of these applications, the reader is referred to Balasundaram et al.(6). Using MCP to detect cohesive subgraphs can be overly restrictive. MCP will find only extremely cohesive subgraphs. This approach can fail to detect much of the structure present in a graph. Seidman and Foster (62) introduced k -plexes to address this issue.

Recall that a co- k -plex is the complement of a k -plex. This chapter focuses on the co-2-plex polytope and a related class of matrices. We derive the co-2-plex analogue for certain properties of the stable set polytope.

This chapter is organized as follows. Section 4.2 discusses some preliminary definitions. Section 4.3 derives four classes of facets for the co-2-plex polytope and a class of facets for the general co- k -plex polytope. The facets are related to 2-plexes, cycles, wheels, webs, and the claw. Section 4.4 analyzes the clutter of maximal 2-plexes in 2-plexes, paths, cycles, and co-2-plexes. Note, Section 4.4 uses definitions and theorems found in Cornuéjols (24). Section 4.5 characterizes 2-claw-free graphs (2-claws are defined in Section 4.3). The results of Section 4.4 and Section 4.5 allow us to characterize the maximal 2-plex clutter matrices for which the polytope $\{x \in \mathbf{R}_+^n \mid Ax \leq 2, x \leq 1\}$ is integral. This characterization leads to the concept of k -plex perfection, which is the topic of Section 4.6.

4.2 Preliminaries

Let $G = (V, E)$ be a finite, simple graph. Fix $k \geq 1$, recall that a subset $K \subseteq V$ induces a k -plex if the following condition holds:

$$\deg_{G[K]}(v) \geq |K| - k \quad \forall v \in K.$$

Notice that 1-plexes are cliques. k -plexes were introduced by Seidman and Foster (62) in the context of social network analysis. Balasundaram et al.(6) provided an integer programming formulation for the maximum k -plex problem and established the NP-hardness of the k -plex decision problem.

A co- k -plex is the complement of a k -plex. Each vertex in a co- k -plex S has at most $(k - 1)$ neighbors in S . Notice that co-1-plexes are stable sets. The NP-hardness of the co- k -plex decision problem follows directly from the result for k -plexes.

Define $\alpha_k(G)$ as the size of a largest co- k -plex in G and refer to $\alpha_k(G)$ as the co- k -plex number of G . Let $\mathcal{I} := \{I \subseteq V \mid I \text{ induces a co-}k\text{-plex}\}$. Each co- k -plex $I \in \mathcal{I}$ has an associated incidence vector $x^I \in R^{|V|}$, where $x_v^I = 1$ if $v \in I$ and $x_v^I = 0$ otherwise. Let $P_k(G)$ denote the convex hull of all x^I such that $I \in \mathcal{I}$. $P_k(G)$ is a full-dimensional polytope and therefore has a unique (up to positive scalar multiples) minimal defining system of inequalities. The maximal faces of $P_k(G)$ and their corresponding inequalities are both called facets. A positive scalar multiple of every facet must appear in any defining system for $P_k(G)$.

4.3 Facets of the co-2-plex polytope

Co-2-plexes and stable sets are both induced subgraphs of low maximum degree. Stable sets are induced subgraphs consisting of isolated vertices. Co-2-plexes are induced subgraphs consisting of isolated vertices and matched pairs. In this section, we shall see that the associated polytopes share similar properties.

We will first determine when a 2-plex inequality induces a facet for $P_2(G)$. The result is analogous to the maximal clique facets of the stable set polytope. The search for facets then continues with four familiar classes of graphs: cycles, wheels, webs, and the claw. It is well-known that the presence of these subgraphs can complicate the facial structure of the stable set polytope (50; 52; 56; 66). It turns out that similar graphs affect the structure of the co-2-plex polytope as well.

Our first result gives a useful equivalent characterization of 2-plexes. Define the neighbor set of v as follows:

$$N(v) := \{u \in V \mid (u, v) \in E\}.$$

Lemma 5. $G = (V, E)$ is a 2-plex if and only if $\alpha_2(G) = \min\{2, |V|\}$.

Proof. To show necessity, let G be a 2-plex. $|V| = 1$ clearly implies that $\alpha_2(G) = 1$. Otherwise, we have $\alpha_2(G) \geq 2$ since any pair of vertices induce a co-2-plex. Suppose $\alpha_2(G) > 2$. Then there exists an $S \subseteq V$ such that $G[S]$ is a co-2-plex of cardinality 3, and we must have $\deg_{G[S]}(v) = 0$ for some $v \in S$. $G[S]$ is a vertex-induced subgraph

of G which is not a 2-plex. However, Seidman and Foster (62) showed that if G is a 2-plex, then any vertex-induced subgraph of G is also a 2-plex. This contradiction implies the result.

To show sufficiency, let $\alpha_2(G) = \min\{2, |V|\}$. If $\alpha_2(G) = 1$, then $|V| = 1$ and hence G is a 2-plex. Suppose $\alpha_2(G) = 2$. All graphs on 2 vertices are 2-plexes, so we may assume $|V| \geq 3$. If G is not a 2-plex, then there exists $v \in V$ such that $\deg_G(v) \leq |V| - 3$. Let $w, u \in V \setminus N(v)$. The set $\{v, u, w\}$ induces a co-2-plex and $\alpha_2(G) \geq 3$, a contradiction. \square

Lemma 5 fails for general k . For example, let $k = 3$ and consider the chordless cycle on five vertices. Cycles are 2-regular, so C^5 is both a co-3-plex and a 3-plex. Thus

$$\alpha_3(C^5) = 5 \neq \min\{3, |V|\}.$$

4.3.1 2-plexes

This subsection offers the co-2-plex analogue of the maximal clique inequalities for the stable set polytope. Let $G = (V, E)$ and $|V| = n$. Given a 2-plex K , define

$$\sum_{v \in K} x_v \leq \alpha_2(K)$$

to be the associated 2-plex inequality.

We first examine the case when $K = \{v\}$. By Lemma 5, the 2-plex inequality

becomes $x_v \leq 1$. Consider the vectors

$$x^{\{v\}}, x^{\{u_1, v\}}, \dots, x^{\{u_{n-1}, v\}}$$

where $\{u_1, \dots, u_{n-1}\} = V \setminus v$. These n affinely independent vectors satisfy the 2-plex inequality at equality. Moreover, they are the incidence vectors of co-2-plexes in G . Therefore, $x_v \leq 1$ is a facet for $P_2(G)$.

Notice that if $|K| > 1$, then the right hand side of the 2-plex inequality increases. Consequently, any 2-plex properly containing $\{v\}$ will not induce $x_v \leq 1$. In other words, $x_v \leq 1$ is a facet regardless of whether or not $\{v\}$ is maximal.

Consider the case where $K = \{w, u\}$. The 2-plex inequality $x_w + x_u \leq 2$ does not induce a facet. This is because $x_w + x_u \leq 2$ is a linear combination of the inequalities $x_w \leq 1$ and $x_u \leq 1$. In contrast, when $|K| > 2$, we have the following result.

Theorem 3. *If K is maximal and $|K| > 2$, then the 2-plex inequality induces a facet for $P_2(G)$.*

Proof. Lemma 5 implies that $\alpha_2(K) = 2$, so the 2-plex inequality becomes $\sum_{v \in K} x_v \leq 2$. Let $\gamma^T x \leq \gamma_0$ be a valid inequality for $P_2(G)$ and define the following sets:

$$F = \{x \in P_2(G) \mid \sum_{v \in K} x_v = 2\}, \quad F_\gamma = \{x \in P_2(G) \mid \gamma^T x = \gamma_0\}.$$

Suppose that $F \subseteq F_\gamma$, and that F_γ is a proper face (i.e. γ nonzero). We will show that $F = F_\gamma$. This implies that F is maximal and that the 2-plex inequality is a facet

for $P_2(G)$. Notice that we may assume γ has nonnegative components. For if $\gamma_v < 0$, then F_γ is contained in the face induced by $x_v \geq 0$, and $\gamma^T x \leq \gamma_0$ can be replaced by $x_v \geq 0$ without loss of generality.

Let $u, w, z \in K$ and note that $x^{\{u,w\}}, x^{\{u,z\}}, x^{\{w,z\}} \in F$. Since $F \subseteq F_\gamma$, we have

$$\gamma_u + \gamma_w = \gamma_u + \gamma_z = \gamma_w + \gamma_z = \gamma_0 \quad \Rightarrow \quad \gamma_u = \gamma_z = \gamma_w.$$

u, w , and z were arbitrary, so there exists a scalar $t > 0$ such that $\gamma_w = t$ for all $w \in K$. It also follows that $\gamma_0 = 2t$.

Suppose there exists $s \notin K$. By the maximality of K , there exists $u, z \in K \setminus N(s)$. Moreover, $x^{\{u,z\}}, x^{\{s,u,z\}} \in F \subseteq F_\gamma$. Hence

$$\gamma_s + \gamma_u + \gamma_z = \gamma_u + \gamma_z = \gamma_0 \quad \Rightarrow \quad \gamma_s = 0.$$

Thus $\gamma_s = 0$ for all $s \notin K$. We have shown that $\gamma^T x \leq \gamma_0$ represents an inequality of the form $t \sum_{v \in K} x_v \leq 2t$. It follows that $F = F_\gamma$. \square

An independent proof of Theorem 3 appears in Balasundaram et al.(6).

4.3.2 Paths, cycles, and wheels

Let P^n denote the path with n vertices and C^n the chordless cycle on n vertices. The following lemmas will be useful as we determine which cycles and wheels induce facets for the co-2-plex polytope.

Lemma 6. $\alpha_2(P^n) = \lceil \frac{2n}{3} \rceil, \quad \forall n \geq 1.$

Proof. Given a path P^n , label $V(P^n)$ with $\{1, \dots, n\}$ such that:

$$N(1) = \{2\}, \quad N(n) = \{n-1\}, \quad N(i) = \{i-1, i+1\} \quad 2 \leq i \leq n-1.$$

Define $S \subseteq V(P^n)$, where $i \in S \Leftrightarrow i \not\equiv 0 \pmod{3}$. S is a co-2-plex, and $|S| = n - \lfloor \frac{n}{3} \rfloor = \lceil \frac{2n}{3} \rceil$. Any larger set $S' \subseteq V(P^n)$ must have a subset of the form $\{i, i+1, i+2\}$ and is thus not a co-2-plex. The result follows. \square

Lemma 7. $\alpha_2(C^n) = \lfloor \frac{2n}{3} \rfloor, \quad \forall n \geq 3.$

Proof. C^3 is a 2-plex, so Lemma 5 implies that $\alpha_2(C^3) = 2 = \lfloor \frac{2*3}{3} \rfloor$. Suppose $n \geq 4$.

Given a cycle C^n , label $V(C^n)$ with $\{1, \dots, n\}$ such that:

$$N(1) = \{n, 2\}, \quad N(n) = \{n-1, 1\}, \quad N(i) = \{i-1, i+1\} \quad 2 \leq i \leq n-1.$$

For all $j \in V(C^n)$ define $K_j = \{j, j+1, j+2\} \subseteq V$ (written mod n). K_j is a 2-plex for $1 \leq j \leq n$. Therefore, Lemma 5 implies that $\sum_{v \in K_j} x_v \leq 2$ is a valid inequality for $1 \leq j \leq n$. In addition, since $n \geq 4$, each vertex belongs to exactly three of the K_j sets. We now sum these n inequalities and derive a Chvátal-Gomory cut.

$$\sum_{j=1}^n \sum_{v \in K_j} x_v \leq 2n$$

$$\sum_{v \in V(C^n)} 3x_v \leq 2n$$

$$\sum_{v \in V(C^n)} x_v \leq \frac{2n}{3}$$

$$\sum_{v \in V(C^n)} x_v \leq \left\lfloor \frac{2n}{3} \right\rfloor.$$

This valid inequality implies that $\alpha_2(C^n) \leq \lfloor \frac{2n}{3} \rfloor$.

Define $S \subseteq V$, where $i \in S \Leftrightarrow i \not\equiv 0 \pmod{3}$ and $i \neq n-1$. S is a co-2-plex, and $|S| = \lfloor \frac{2n}{3} \rfloor$. Thus $\alpha_2(C^n) \geq \lfloor \frac{2n}{3} \rfloor$ and the result follows. \square

An edge $e \in E(G)$ is co- k -plex critical if $\alpha_k(G - e) = \alpha_k(G) + 1$. The following is a variation of a theorem and proof originally given by Chvátal (21).

Theorem 4. *Let $G = (V, E)$ be a graph and $E^* \subseteq E$ the set of co- k -plex critical edges. If $G^* = (V, E^*)$ is connected then the inequality*

$$\sum_{v \in V} x_v \leq \alpha_k(G)$$

is a facet of $P_k(G)$.

Proof. Let G satisfy the hypothesis and let $P_k(G) = \{x \in R_+^{|V|} \mid \sum_{v \in V} a_{iv} x_v \leq b_i, i \in I\}$, where I is the index set of facets other than the nonnegativity constraints.

Consider the dual linear programs given by

$$\max \left\{ \sum_{v \in V} x_v \mid x \geq 0, \sum_{v \in V} a_{iv} x_v \leq b_i, i \in I \right\}$$

$$\min \left\{ \sum_{i \in I} \lambda_i b_i \mid \lambda \geq 0, \sum_{i \in I} \lambda_i a_{iv} \geq 1, v \in V \right\}.$$

An optimal dual solution λ^* satisfies $\sum_{i \in I} \lambda_i^* b_i = \alpha_k(G)$. Let $s \in V$, and notice by dual feasibility, there exists $j \in I$ such that $\lambda_j^*, a_{js} > 0$.

Choose $(u, w) \in E^*$. There exist co- k -plex incidence vectors y and z such that

$$\sum_{v \in V} y_v = \sum_{v \in V} z_v = \alpha_k(G), \quad (4.1)$$

$$y_u = z_w = 1, \quad y_w = z_u = 0, \quad y_v = z_v \quad \forall v \in V \setminus \{u, w\}. \quad (4.2)$$

It follows that

$$\sum_{v \in V} a_{jv} y_v = \sum_{v \in V} a_{jv} z_v = b_j. \quad (4.3)$$

For if not, then without loss of generality, we have $\sum_{v \in V} a_{jv} z_v < b_j$ and hence

$$\sum_{v \in V} z_v \leq \sum_{v \in V} \left(\sum_{i \in I} \lambda_i^* a_{iv} \right) z_v = \sum_{i \in I} \lambda_i^* \left(\sum_{v \in V} a_{iv} z_v \right) < \sum_{i \in I} \lambda_i^* b_i = \alpha_k(G),$$

thus contradicting (4.1). Now (4.2) and (4.3) imply $a_{ju} = a_{jw}$. Recall that $(u, w) \in E^*$ was arbitrary and G^* is connected, so we have

$$a_{jv} = a_{js} > 0 \quad \forall v \in V.$$

Therefore, (4.1) and (4.3) imply

$$b_j = \sum_{v \in V} a_{jv} z_v = a_{js} \sum_{v \in V} z_v = a_{js} \alpha_k(G).$$

The facet indexed by j was a positive scalar multiple of $\sum_{v \in V} x_v \leq \alpha_k(G)$. \square

As a corollary we obtain the co-2-plex analogue of odd holes and wheels.

Corollary 1. *Let $n \geq 4$. If $n \not\equiv 0 \pmod{3}$, then the inequality*

$$\sum_{v \in V(C^n)} x_v \leq \left\lfloor \frac{2n}{3} \right\rfloor$$

is a facet of $P_2(C^n)$.

Proof. Lemmas 6 and 7 imply that every edge in C^n is co-2-plex critical whenever $n \not\equiv 0 \pmod{3}$. The result follows from Theorem 4. \square

It seems possible that for larger values of k , a certain class of cycles might induce facets for $P_k(C^n)$. However, for $k \geq 3$, C^n is a co- k -plex and $\alpha_k(C^n) = n$. Therefore, any cycle inequality would be implied by summing the $x_i \leq 1$ constraints.

A wheel W_n is the cycle C^n with an additional vertex u such that $N(u) = V(C^n)$.

Corollary 2. *Let $n \geq 4$. If $n \not\equiv 0 \pmod{3}$, then the inequality*

$$\left(\left\lfloor \frac{2n}{3} \right\rfloor - 1 \right) x_u + \sum_{v \in V(C^n)} x_v \leq \left\lfloor \frac{2n}{3} \right\rfloor$$

is a facet of $P_2(W_n)$.

Proof. Corollary 1 implies that $\sum_{v \in V(C^n)} x_v \leq \left\lfloor \frac{2n}{3} \right\rfloor$ is a facet for $P_2(C^n)$. Therefore, we can lift the cycle inequality to a facet of $P_2(W_n)$. We need only calculate the lifting

coefficient β_u of x_u .

$$\beta_u = \max\left\{\left\lfloor\frac{2n}{3}\right\rfloor - \sum_{v \in V(C^n)} x_v \mid x_u = 1, x \in P_2(W_n)\right\} = \left\lfloor\frac{2n}{3}\right\rfloor - 1.$$

□

4.3.3 Webs

Trotter (66) showed that a class of graphs called webs can induce facets for the stable set polytope. We now show that webs can induce facets for the co-2-plex polytope as well. In this section, all sums are written mod n . For integers $n \geq 2$ and p , $1 \leq p \leq \frac{n}{2}$, let $W(n, p)$ denote the graph on vertices $V = \{1, \dots, n\}$ and edges

$$E = \{(i, j) \mid j = i + p, \dots, i + n - p; \forall i \in V\}.$$

The web $W(n, p)$ is regular of degree $n - 2p + 1$ and has independence number p . In particular, any set of p pairwise nonadjacent vertices must form a dominating set in $W(n, p)$, and every vertex i satisfies $|N(i) \cap N(j)| = n - 2p$ for $j \in \{i - 1, i + 1\}$. We refer to such a pair i, j as *consecutive*. Notice that $\deg_{W(n, p)}(v) \geq 3 \forall v \in V$ whenever $p < \lfloor \frac{n}{2} \rfloor$.

Lemma 8. *If $p < \lfloor \frac{n}{2} \rfloor$, then $\alpha_2(W(n, p)) = p + 1$.*

Proof. $\alpha_2(W(n, p)) \geq p + 1$ follows from the fact that $\{i, i + 1, \dots, i + p\}$ is a co-2-plex of size $p + 1$ for all $i \in V$. We show that no larger co-2-plex exists. Since $W(n, p)$

has independence number p , any subset S of $p + 2$ vertices satisfies $|E(G[S])| \geq 2$. Suppose for contradiction that S is a co-2-plex of cardinality $p + 2$ such that $|E(G[S])|$ is minimum. Let $(e_1, e_2), (v_1, u_1) \in E(G[S])$.

Define $u_2, \dots, u_{p+1} \in V$ such that $u_2 \in N(v_1) \setminus \{u_1\}$ and u_i, u_{i+1} are consecutive for $1 \leq i \leq p$. Observe $u_2 \notin S$ since S is a co-2-plex and $(v_1, u_1) \in E(G[S])$. In addition, $|N(u_{i+1}) \setminus N(u_i)| = 1$ because u_i, u_{i+1} are consecutive. Define $v_{i+1} = N(u_{i+1}) \setminus N(u_i)$. By construction, we have that

$$u_i, u_{i+1}, u_{i+2} \in N(v_i) \quad 2 \leq i \leq p - 1. \quad (4.4)$$

The set $\{u_1, \dots, u_p\}$ is a maximum independent set and hence dominating. Therefore $e_1 = v_j$ for some $2 \leq j \leq p$. Let j' be the smallest index such that either $v_{j'} \notin S$ or $v_{j'} \in S$ is not isolated in $G[S]$. We have $v_{j'-1} \in S$ is isolated in $G[S]$, and (4.4) implies that $\{u_2, \dots, u_{j'+1}\} \subseteq V \setminus S$. If $v_{j'} \notin S$, let $S' = (S \setminus \{v_1, \dots, v_{j'-1}\}) \cup \{u_2, \dots, u_{j'}\}$. If $v_{j'} \in S$ is not isolated in $G[S]$, let $S' = (S \setminus \{v_1, \dots, v_{j'}\}) \cup \{u_2, \dots, u_{j'+1}\}$. In either case, S' is a $p + 2$ co-2-plex with $|E(G[S'])| < |E(G[S])|$, a contradiction. \square

Consider the case where $p = \lfloor \frac{n}{2} \rfloor$. If n is even, then $W(n, p)$ is a perfect matching and $\alpha_2(W(n, p)) = n$. If n is odd, then $W(n, p)$ is a cycle and $\alpha_2(W(n, p)) = \lfloor \frac{2n}{3} \rfloor$ by Lemma 7.

Theorem 5. Let $p < \lfloor \frac{n}{2} \rfloor$. When n and $p + 1$ are relatively prime, the inequality

$$\sum_{v \in V} x_v \leq p + 1$$

is a facet of $P_2(W(n, p))$.

Proof. Lemma 8 implies that the inequality is valid. For $n \geq 1$ and $1 \leq p < n$ define $A(n, p)$ as the $n \times n$ binary matrix where $a_{ij} = 1$ if $j \in \{i, i + 1, \dots, i + p\}$ and $a_{ij} = 0$ otherwise.

In Trotter (66), it was shown that $A(n, p)$ is nonsingular whenever n and $p + 1$ are relatively prime. Notice that $A(n, p)$ is an incidence matrix of n maximum co-2-plexes given by $\{i, i + 1, \dots, i + p\}$ for all $i \in V$. These maximum co-2-plexes satisfy the web inequality at equality. Thus, the web inequality induces a facet of $P_2(W(n, p))$. \square

For completeness, we mention that $W(2s + 1, s)$ is facet-inducing by Corollary 1 whenever $2s + 1 \not\equiv 0 \pmod{3}$. We also obtain the co-2-plex analogue to odd antiholes. An antihole \bar{C}^n is the complement of the chordless cycle C^n .

Corollary 3. Let $n \geq 4$. If $n \not\equiv 0 \pmod{3}$, then the inequality

$$\sum_{v \in V(\bar{C}^n)} x_v \leq 3$$

is a facet of $P_2(\bar{C}^n)$.

Proof. The antihole \bar{C}^n is the web $W(n, 2)$. By Theorem 5, $\sum_{v \in V(\bar{C}^n)} x_v \leq 3$ is a facet whenever n and 3 are relatively prime. \square

4.3.4 k -claws

Our next goal is to show that a class of graphs similar to the claw can induce facets for the co- k -plex polytope. This motivates the definition of a k -claw. Given an integer $k \geq 1$, the graph H is a k -claw if there exists a vertex $u \in V(H)$ such that $V(H) \setminus u = N(u)$, $N(u)$ is a co- k -plex, and $|N(u)| \geq \max\{3, k\}$. We refer to u as the *center* of the k -claw.

Theorem 6. *Fix $k \geq 2$. Let $H = (V, E)$ be a k -claw with center u and $|V| = n$. The inequality*

$$(n - k)x_u + \sum_{v \in N(u)} x_v \leq n - 1$$

is a facet of $P_k(H)$.

Proof. Let S be a co- k -plex in H . If $u \in S$, then $|N(u) \cap S| \leq k - 1$ by definition of co- k -plex. If $u \notin S$, then $|N(u) \cap S| \leq |N(u)| = n - 1$. In either case, the k -claw inequality is valid. Let $\gamma^T x \leq \gamma_0$ be a valid inequality for $P_k(H)$ and define the following sets:

$$F_k = \{x \in P_k(H) \mid (n-k)x_u + \sum_{v \in N(u)} x_v = n-1\}, \quad F_\gamma = \{x \in P_k(H) \mid \gamma^T x = \gamma_0\}.$$

Suppose that $F_k \subseteq F_\gamma$, and that F_γ is a proper face. We will show that $F_k = F_\gamma$.

This implies that F_k is maximal and the k -claw inequality is a facet for $P_k(H)$. As in

the proof of Theorem 3, we assume that γ has nonnegative components.

Given a subset of vertices I , let x^I be the associated incidence vector. Define

$$\mathcal{S} = \{u \cup S \mid S \subset N(u), |S| = k - 1\}.$$

Notice that $F_k = \{x^S \mid S \in \mathcal{S}\} \cup \{x^{N(u)}\}$. Now choose $i, j \in N(u)$ and observe that there exist $S_i, S_j \in \mathcal{S}$ such that

$$i \in S_i, \quad j \in S_j, \quad i \notin S_j, \quad j \notin S_i, \quad |S_i \cap S_j| = k - 1.$$

Since $F_k \subseteq F_\gamma$, we have $\gamma^T x^{S_i} = \gamma^T x^{S_j} = \gamma_0$. It follows that $\gamma_i = \gamma_j$. So for some constant $t > 0$, $\gamma_i = \gamma_j = t \quad \forall i, j \in N(u)$.

Moreover, we know that $\gamma^T x^{N(u)} = \gamma_0$. This implies that $\gamma_0 = t(n - 1)$. Finally, take $S \in \mathcal{S}$. Notice that $\gamma^T x^S = \gamma_0 = t(n - 1)$. We can now deduce that $\gamma_u = t(n - 1) - t(k - 1) = t(n - k)$. Therefore, the inequality $\gamma^T x^S \leq \gamma_0$ can be written as

$$t(n - k)x_u + \sum_{v \in N(u)} tx_v \leq t(n - 1).$$

Thus it was a scalar multiple of the k -claw inequality and $F_k = F_\gamma$. □

A k -claw subgraph can properly contain other k -claws which give rise to distinct facet-inducing inequalities. In other words, a k -claw need not be maximal to produce a facet. For our purposes, 2-claws will be of special interest in Section 4.5. See Figure 4.1 for examples of 2-claws.

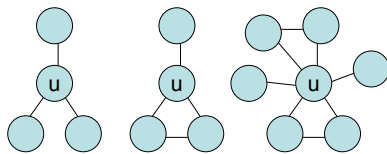


Figure 4.1: Three examples of 2-claws.

4.4 $P_2(G)$ for 2-plexes, paths, cycles, and co-2-plexes

The purpose of this section is to show that the 2-plex inequalities suffice to describe the co-2-plex polytope of 2-plexes, paths, certain cycles, and co-2-plexes. This is analogous to a property of perfect graphs. These results provide a class of 0-1 matrices A for which the polytope $\{x \in \mathbf{R}_+^n \mid Ax \leq 2, x \leq 1\}$ is integral. We will analyze the clutter of maximal 2-plexes. The definitions and theorems used in this section can be found in Cornuéjols (24).

A *clutter* is a pair $\mathcal{C} = (V, E)$ where V is a finite set and E is a family of subsets of V none of which is included in another. We refer to elements of V as vertices and elements of E as edges. Given a graph $G = (V, E)$, let \mathcal{C} be the clutter whose vertices are V and whose edges are the maximal 2-plexes of G . Denote by M_G the edge-vertex incidence matrix of \mathcal{C} .

The clutter matrix M_G is *totally unimodular* (TU) if every square submatrix has determinant $0, \pm 1$. Hoffman and Kruskal (38) showed that M_G is TU if and only if the polyhedron

$$\{x \in \mathbf{R}_+^n \mid M_G x \leq w\}$$

is integral for all integral vectors w .

Suppose K is a 2-plex. The clutter matrix M_K of maximal 2-plexes in K consists of a single row of 1's. In this case, M_K is clearly TU. It is well known that appending the identity matrix to M_K preserves total unimodularity. Therefore, Lemma 5 implies that the set

$$\{x \in \mathbf{R}_+^n \mid M_K x \leq 2, x \leq 1\}$$

is in fact the co-2-plex polytope of K . Thus, the 2-plex inequalities suffice to describe the co-2-plex polytope of any 2-plex.

A matrix is minimally nontotally unimodular (*mntu*) if it is not totally unimodular, but every submatrix satisfies total unimodularity. If a matrix is not TU, then it must contain an *mntu* submatrix. Camion (17) and Gomory (cited in (17)) showed that an *mntu* matrix has determinant equal to ± 2 , and each row and column of an *mntu* matrix has an even number of nonzeros. Let P^n be the path on n vertices.

Theorem 7. *Let $n \geq 1$. The clutter matrix M_{P^n} of maximal 2-plexes in P^n is TU.*

Proof. We show by induction that M_{P^n} contains no *mntu* submatrix. For $n \leq 3$, P^n is a 2-plex and M_{P^n} is TU. Let $n \geq 4$ and suppose $M_{P^{n'}}$ is TU for all $n' < n$. Label the vertices of P^n as in Lemma 6. The maximal 2-plexes in P^n are of the form $K_j := \{j, j+1, j+2\}$ for $1 \leq j \leq n-2$. We can permute the rows of M_{P^n} so that row j corresponds to K_j . It follows that there are three 1's in every row of M_{P^n} . In addition, M_{P^n} has a single 1 in columns 1 and n and exactly two 1's in columns 2 and $n-1$. See Figure 4.2 for an example.

We attempt to construct an *mntu* submatrix M' by examining which elements

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 \end{bmatrix}$$

Figure 4.2: M_{P^7} .

from the first row can contribute to M' . If we are able to show that no element from the first row contributes, it follows by a symmetric argument that no element from the last row contributes. Removing the first and last rows from M_{P^n} creates an $M_{P^{n-2}}$ which contains no $mntu$ submatrix by induction.

The first and last columns of M_{P^n} have an odd number of nonzero entries, so we restrict the search to columns 2 through $n - 1$. Denote by m_{ij} the element in the i^{th} row and j^{th} column of M . Let $m_{ij} \in M'$ denote that m_{ij} contributes a nonzero entry to the $mntu$ submatrix M' . Suppose $m_{12} \in M'$. Notice that $m_{12} \in M'$ if and only if $m_{13} \in M'$ since these are the only nonzero candidates from the first row. Moreover, if $m_{12} \in M'$, we also know $m_{22} \in M'$ as it is the only other nonzero entry in the second column. It follows that $m_{23} \in M'$ as well. Now $m_{24} \notin M'$ since the corresponding row in M' would have three nonzeros. Thus M' has two identical rows and $\det(M') = 0$, a contradiction. Therefore, M' contains no elements from the first or last rows, and M_{P^n} is TU by the induction hypothesis. \square

Once again, we can append the identity matrix and preserve total unimodularity.

Consequently, Theorem 7 and Lemma 5 imply that the set

$$\{x \in \mathbf{R}_+^n \mid M_{P^n}x \leq 2, x \leq 1\}$$

is the co-2-plex polytope of P^n . In other words, the 2-plex inequalities suffice to describe the co-2-plex polytope of any path.

We now turn our attention to the clutter of 2-plexes in chordless cycles. C^n is a 2-plex when $n \leq 4$. Let $n \geq 5$. Corollary 1 implies that the 2-plex inequalities will not suffice to describe $P_2(C^n)$ for $n \not\equiv 0 \pmod{3}$. Even when $n \equiv 0 \pmod{3}$, the 2-plex clutter matrix M_{C^n} is not TU since it contains an odd-hole submatrix. We deal with this case directly by showing that $P(C^n)$ has no facets other than the 2-plex inequalities.

Given an inequality $\alpha^T x \leq \beta$, define $\text{supp}_\alpha = \{v \in V \mid \alpha_v > 0\}$ and $G_\alpha = G[\text{supp}_\alpha]$.

Lemma 9. *If $\alpha^T x \leq \beta$ is a facet for $P_k(G)$, then G_α is connected.*

Proof. Let $F_\alpha = \{x \in P_k(G) \mid \alpha^T x = \beta\}$, and suppose for contradiction that G_α has distinct components H_1 and H_2 . Since $\alpha^T x \leq \beta$ is a valid inequality, we must have

$$\max\left\{\sum_{v \in H_1} \alpha_v x_v \mid x \in P_k(G)\right\} + \max\left\{\sum_{v \in H_2} \alpha_v x_v \mid x \in P_k(G)\right\} = \beta_1 + \beta_2 = \beta.$$

In addition, every $x \in F_\alpha$ satisfies $\sum_{v \in H_1} \alpha_v x_v = \beta_1$. Otherwise, $\sum_{v \in H_1} \alpha_v x_v < \beta_1$ and $\sum_{v \in H_2} \alpha_v x_v > \beta_2$, a contradiction. Let $F'_\alpha = \{x \in P_k(G) \mid \sum_{v \in H_1} \alpha_v x_v = \beta_1\}$.

We have that $F_\alpha \subset F'_\alpha$. This is a contradiction since F_α must be maximal whenever $\alpha^T x \leq \beta$ is a facet. \square

Theorem 8. *If $n \geq 5$ and $n \equiv 0 \pmod{3}$, then $P_2(C^n) = \{x \in \mathbf{R}_+^n \mid M_{C^n}x \leq 2, x \leq 1\}$.*

Proof. Suppose $P_2(C^n) \neq \{x \in \mathbf{R}_+^n \mid M_{C^n}x \leq 2, x \leq 1\}$. Then there exists a facet $\alpha^T x \leq \beta$ of $P_2(C^n)$ such that G_α is not a 2-plex. We know that C^n does not induce a facet, so $G_\alpha \subset G$. Lemma 9 implies that G_α is connected, so G_α must be a path P^m with at least four vertices. Since $\alpha^T x \leq \beta$ is a facet, there exist m co-2-plexes S_1, \dots, S_m in P^m such that x^{S_1}, \dots, x^{S_m} are affinely independent and satisfy the facet at equality. Thus $\alpha^T x \leq \beta$ also induces a facet of the co-2-plex polytope for P^m . This contradicts the fact that $\{x \in \mathbf{R}_+^n \mid M_{P^n}x \leq 2, x \leq 1\}$ defines the co-2-plex polytope for P^m . \square

Thus far, we have shown that the 2-plex inequalities suffice to define the co-2-plex polytope of 2-plexes, paths, and chordless cycles of length $n \equiv 0 \pmod{3}$. We also have that co-2-plexes satisfy this property. This is because the associated polytope is the entire n -dimensional hypercube which is defined by the system of $0 \leq x_i \leq 1$ inequalities. As a result, the polytope $\{x \in \mathbf{R}_+^n \mid Ax \leq 2, x \leq 1\}$ is integral whenever A is the maximal 2-plex clutter matrix of a 2-plex, co-2-plex, path, or chordless cycle of length $n \equiv 0 \pmod{3}$.

4.5 2-claw-free graphs and integral systems

The purpose of this section is to show that each component of a 2-claw-free graph must be a co-2-plex, 2-plex, path, or chordless cycle. We use this result to completely characterize the 2-plex clutter matrices A for which the polytope $\{x \in \mathbf{R}_+^n \mid Ax \leq 2, x \leq 1\}$ is integral.

Theorem 9. *Let $G = (V, E)$. If G contains a component other than a path, chordless cycle, co-2-plex, or 2-plex, then G contains an induced 2-claw.*

Proof. If G is not connected, simply apply the proof to each component. Hence, we may assume G is connected. Suppose G is not a path, chordless cycle, co-2-plex, or 2-plex. We will find an induced 2-claw subgraph. Every graph on 3 or less vertices is a co-2-plex or a 2-plex. Thus, we may assume $|V| \geq 4$.

If G is acyclic, then $\exists v \in V$ such that $\deg(v) \geq 3$ since G is connected and not a path. The set $v \cup N(v)$ induces a 2-claw with v as the center vertex. If G is not acyclic, let $C^m \subset G$ be a largest induced cycle. Label $V(C^m)$ using $\{1, 2, \dots, m\}$ as in Lemma 7. G is connected and not a cycle, so

$$N_C := \{u \in V \setminus V(C^m) \mid \exists v \in V(C^m) \text{ s.t. } (u, v) \in E\} \neq \emptyset.$$

Suppose $m \geq 4$ and let $u \in N_C$ satisfy $V(C^m) \not\subseteq N(u)$. Then there exists $i \in V(C^m)$ such that $i \in N(u), i+1 \notin N(u)$. The set $\{u, i-1, i, i+1\}$ induces a 2-claw

with i as the center vertex. Therefore, whenever $m \geq 4$, we assume that

$$V(C^m) \subseteq N(u) \quad \forall u \in N_C.$$

Notice that if $m \geq 5$, then this implies that the set $\{u, 1, 3, 4\}$ induces a 2-claw with center vertex u for any $u \in N_C$. We now have $m \leq 4$ left to consider. When $m = 3$, we exclude the case where $u \in N_C$ and $V(C^3) \cap N(u) = \{i\}$. This is because $u \cup V(C^3)$ induces a 2-claw with i as the center vertex.

Furthermore, if $N_C \cup V(C^m) \neq V$, then there exist $u \in N_C$ and $v \in V \setminus \{N_C \cup V(C^m)\}$ such that $(u, v) \in E$. For any $i, j \in V(C^m) \cap N(u)$, the set $\{u, v, i, j\}$ induces a 2-claw with u as the center vertex. Thus, for both of the following cases, we assume

$$N_C \cup V(C^m) = V.$$

Notice that this implies $|V| = |N_C| + |V(C^m)|$.

Case 1 ($m = 4$). Recall that we may assume $V(C^4) \subseteq N(u) \forall u \in N_C$. If $G[N_C]$ is a 2-plex, then $\deg_{G[N_C]}(u) \geq |N_C| - 2 \forall u \in N_C$. Hence

$$\deg_G(u) \geq |V(C^4)| + (|N_C| - 2) = |V| - 2 \quad \forall u \in N_C.$$

Moreover, $\deg_G(v) = |N_C| + 2 = |V| - 2 \forall v \in V(C^4)$. This implies that G is a 2-plex, a contradiction. Thus $G[N_C]$ is not a 2-plex, so Lemma 5 implies that there exists a

co-2-plex $S \subseteq N_C$ such that $|S| = 3$. The set $i \cup S$ is a 2-claw for any $i \in V(C^4)$.

Case 2 ($m = 3$). Recall that we may assume $|N(u) \cap V(C^3)| \geq 2 \forall u \in N_C$. If $G[N_C]$ is not a 2-plex, then Lemma 5 implies that there exists a co-2-plex $S \subseteq N_C$ such that $|S| = 3$. If $\exists i \in \bigcap_{v \in S} N(v)$, then the set $i \cup S$ induces a 2-claw with center vertex i .

Now suppose $\bigcap_{v \in S} N(v) = \emptyset$. Observe that $\deg_{G[N_C]}(w) = 0$ for some vertex w in S . Let $\{v, z\} = S \setminus w$ and $i \in N(w) \cap N(v) \cap V(C^3)$. The latter set is nonempty since $|N(u) \cap V(C^3)| \geq 2 \forall u \in N_C$. For either $j \in V(C^3) \cap N(z)$, the set $\{w, v, i, j\}$ induces a 2-claw with i as the center vertex.

Suppose $G[N_C]$ is a 2-plex. Recall that G is not a 2-plex, so there exists a co-2-plex $S \subset V$ such that $|S| = 3$ by Lemma 5. All vertices in N_C have at least two neighbors in $V(C^3)$ and $\alpha_2(G[N_C]) = 2$, so we must have $S \cap V(C^3) = \{i\}$. Let $S \cap N_C = \{u, v\}$ and $j \in N(u) \cap N(v) \cap V(C^3)$. The set $\{j, i, u, v\}$ induces a 2-claw with center vertex j . This completes the proof. \square

Define \mathcal{H} to be the set of all graphs whose components are co-2-plexes, 2-plexes, paths, or chordless cycles C^n such that $n \equiv 0 \pmod{3}$. We refer to any chordless cycle $C^n \notin \mathcal{H}$ as an *odd-mod 3-hole*. Let A be the 2-plex clutter matrix for a graph G . Consider the polytope

$$P'(G) = \{x \in \mathbf{R}_+^n \mid Ax \leq 2, x \leq 1\}.$$

Theorem 10. $P'(G)$ is integral if and only if $G \in \mathcal{H}$.

Proof. The results of Section 4.4 imply that $P'(G)$ is integral whenever $G \in \mathcal{H}$. For the converse, suppose $G \notin \mathcal{H}$. If G contains an induced 2-claw $H = (u \cup N(u), E')$, then Theorem 6 implies that the 2-claw inequality can be lifted to a facet of $P_2(G)$. Since H is not a 2-plex, the defining system for $P'(G)$ is missing the lifted 2-claw inequality. We can deduce that $P'(G) \neq P_2(G)$. In particular, the optimal solution to

$$\max\{(n-2)x_u + \sum_{v \in N(u)} x_v \mid x \in P'(G)\}$$

is a fractional vertex of $P'(G)$.

If $G \notin \mathcal{H}$ is 2-claw-free, then Theorem 9 implies that G has a component which is an odd-mod 3-hole. In this case, the defining system for $P'(G)$ is missing the cycle inequality which is a facet by Corollary 1. If C^n is an odd-mod 3-hole component of G , then the optimal solution to

$$\max\left\{\sum_{v \in V(C^n)} x_v \mid x \in P'(G)\right\}$$

is a fractional vertex of $P'(G)$. □

Theorem 10 implies that G is 2-claw-free for all $G \in \mathcal{H}$, otherwise the defining system for $P'(G)$ would be missing the 2-claw facet from Theorem 6.

We have shown that when A is the 2-plex clutter matrix of a graph G , the polytope $P'(G)$ is integral if and only if $G \in \mathcal{H}$. When $G \notin \mathcal{H}$, then either G contains an induced

$$\begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \end{bmatrix}$$

Figure 4.3: M_{2-claw} .

2-claw or G has an odd-mod 3-hole component. Whenever G contains an induced 2-claw of any size, it must contain an induced 2-claw $H = (u \cup S, E')$ such that $|S| = 3$. In this case, A contains the submatrix shown in Figure 4.3. If G has an odd-mod 3-hole component, we mention that A contains the circulant clutter matrix \mathcal{C}_n^3 . The matrix \mathcal{C}_n^3 has vertex set $\{1, \dots, n\}$ and edges $\{i, i + 1, i + 2\}$ for $1 \leq i \leq n$ (written mod n).

Corollary 4. *Given a 2-plex clutter matrix A , there exists a polynomial-time algorithm to determine if the polytope $\{x \in \mathbf{R}_+^n \mid Ax \leq 2, x \leq 1\}$ is integral.*

Proof. A is a 2-plex clutter matrix for some graph $G = (V, E)$. By Theorem 10, it suffices to test if $G \in \mathcal{H}$. We first test A for the submatrix in Figure 4.3. This can be done in polynomial time since we check every triplet of rows. If A contains no M_{2-claw} submatrix, then $G \in \mathcal{H}$ unless there exists a component of G which is an odd-mod 3-hole. However, if G has an odd-mod 3-hole component, then the optimal solution to the linear program $\max\{\sum_{v \in C} x_v \mid Ax \leq 2, 0 \leq x \leq 1\}$ will be fractional by Corollary 1 for some component C . □

4.6 k -plex Perfection

Chvátal (21) showed that the maximal clique inequalities suffice to describe the stable set polytope of any perfect graph. Section 4.4 characterizes the graphs for which the 2-plex inequalities suffice to describe the co-2-plex polytope. This characterization can be seen as a generalization of Chvátal's theorem on perfect matrices. In other words, Theorem 10 can be interpreted as a polyhedral characterization of 2-plex perfection. It is natural to ask for a combinatorial characterization of k -plex perfection in general. The purpose of this section is to develop a characterization in analogy with graph perfection.

The first step is to find an upper bound on $\omega_k(G)$. The bound will generalize the concept of graph coloring. A coloring of G is a function $c_m : V \mapsto \{1, \dots, m\}$ such that $c_m(u) \neq c_m(v)$ whenever $uv \in E$. The *chromatic number*, $\chi(G)$, of G is the smallest m for which there exists a valid coloring c_m . Notice that $c_m(u) \neq c_m(v)$ for all $u, v \in K$ whenever K induces a clique in G . It follows that the chromatic number is an upper bound for $\omega(G)$. Hence,

$$\omega(G) \leq \chi(G). \tag{4.5}$$

A graph G is perfect if every vertex induced subgraph of G satisfies (4.5) at equality. We are interested in generalizing (4.5) to bound $\omega_k(G)$. To that end, suppose the vertex set V partitions into co- k -plexes C_1, \dots, C_m . Let K be a maximum

k -plex in G . We have

$$\omega_k(G) = |K| = |K \cap V| = \sum_{i=1}^m |K \cap C_i| \leq \sum_{i=1}^m \omega_k(G[C_i]), \quad (4.6)$$

where the inequality follows from the fact that k -plexes are closed under set inclusion (62). Now let Π be the set of all partitions of V into co- k -plexes and define the graph invariant

$$\chi_k(G) := \min\left\{\sum_{C \in \mathcal{C}} \omega_k(G[C]) : \mathcal{C} \in \Pi\right\}. \quad (4.7)$$

The elements of Π are *co- k -plex colorings*, and $\chi_k(G)$ is the *co- k -plex chromatic number* of G . Section 5.2 discusses heuristics for computing $\chi_k(G)$. Notice that (4.6) reduces to (4.5) when $k = 1$ and C_1, \dots, C_m are the color classes of an optimal coloring. It follows that $\chi_1(G) = \chi(G)$. Moreover, (4.6) and (4.7) together imply the bound

$$\omega_k(G) \leq \chi_k(G). \quad (4.8)$$

Definition. A k -plex perfect graph G satisfies $\omega_k(G') = \chi_k(G')$ for all vertex induced subgraphs $G' \subseteq G$.

Graphs which satisfy this definition have some nice algorithmic properties. Mainly, $\chi_k(G)$ can provide tight bounds on $\omega_k(G)$ in a branch and bound scheme. However, many properties of perfect graphs do not generalize to k -plex perfect graphs. The next section provides some examples of k -plex perfect graphs.

Lemma 10. *If G has at least k vertices, then there exists an optimal co- k -plex coloring*

S_1, \dots, S_m of G such that $|S_j| \geq k$ for some j .

Proof. Suppose the lemma is false. Choose an optimal coloring S_1, \dots, S_m with $|S_1|$ maximum. Notice that $m \geq 2$ since $|V| \geq k$ and $|S_i| < k$ for all i . Moreover, $|S_i| < k$ implies that $\omega_k(G[S_i]) = |S_i|$. Choose $v \in S_2$. Define $S'_1 := S_1 \cup \{v\}$ and $S'_2 := S_2 \setminus \{v\}$.

Notice that

$$\chi_k(G) = \sum_{i=1}^m \omega_k(G[S_i]) = \sum_{i=1}^m |S_i| = |S'_1| + |S'_2| + \sum_{i=3}^m |S_i|,$$

so S'_1, S'_2, \dots, S_m is an optimal co- k -plex coloring such that $|S'_1| > |S_1|$. This contradicts the maximality of S_1 . □

4.6.1 Examples

This subsection contains examples of k -plex perfect graphs. It is clear that any co- k -plex S is k -plex perfect since $\chi_k(S) = \omega_k(S)$ by definition. Therefore, k -plex perfection follows from the fact that every vertex-induced subgraph of a co- k -plex is also a co- k -plex (62). Recall that a finite set X and a family \mathcal{I} of subsets of X define a *matroid* if the following axioms hold:

1. $\emptyset \in \mathcal{I}$
2. $I' \subseteq I \in \mathcal{I}$ implies $I' \in \mathcal{I}$
3. Every maximal set in \mathcal{I} has the same cardinality

Given a graph $G = (V, E)$, define

$$\mathcal{K} = \{K \subseteq V : \delta(G[K]) \geq |K| - k\}.$$

\mathcal{K} is the set of k -plexes in G , and (V, \mathcal{K}) satisfies the first two matroid axioms for any graph.

Theorem 11. *If $M := (V, \mathcal{K})$ defines a matroid, then G is k -plex perfect.*

Proof. Given any vertex-induced subgraph $G' = (V', E')$, define $D := V \setminus V'$ and $\mathcal{K}' = \{K \subseteq V' : \delta(G[K]) \geq |K| - k\}$. Observe that

$$(V', \mathcal{K}') = (V \setminus D, \mathcal{K}') =: M \setminus D$$

is again a matroid known as a deletion matroid, so it suffices to show $\chi_k(G) = \omega_k(G)$.

Define $x(A) = \sum_{a \in A} x_a$, $\mathcal{S} = \{S \subseteq V : \Delta(G[S]) \leq k - 1\}$, and $\mathcal{S}_v = \{S \in \mathcal{S} : v \in S\}$. Consider the following dual pair of linear programs:

$$\max\{x(V) : x \geq 0, x(S) \leq \omega_k(G[S]) \text{ for all } S \in \mathcal{S}\} \quad (4.9)$$

$$\min\left\{\sum_{S \in \mathcal{S}} \omega_k(G[S]) y_S : y \geq 0, y(\mathcal{S}_v) \geq 1 \text{ for all } v \in V\right\}. \quad (4.10)$$

Since M is a matroid, a theorem of Edmonds (27) implies that optimal solutions for (4.9) and (4.10) are integral. Observe that $\omega_k(G)$ and $\chi_k(G)$ are the optimal objective values for (4.9) and (4.10), respectively. Moreover, $\omega_k(G) = \chi_k(G)$ by

strong duality. □

Corollary 5. *If G is a k -plex, then G is k -plex perfect.*

Proof. Given any $K' \subset V$ and $v \in V \setminus K'$, $K' \cup \{v\}$ defines a k -plex. It follows that all maximal k -plexes have cardinality $\omega_k(G) = |V|$, so G is k -plex perfect by Theorem 11. □

Recall that an r -partite graph is r -colorable. The complete r -partite graphs have all possible edges between distinct color classes.

Theorem 12. *If G is the complete r -partite graph K_{n_1, \dots, n_r} , then G is k -plex perfect.*

Proof. Let K be a maximal k -plex in G and S_i the i^{th} partition class. Clearly, $|K \cap S_i| \leq |S_i| = n_i$. In addition, $|K \cap S_i| \leq k$. For if not, let $v \in K \cap S_i$, and notice that $N_G(v) \cap S_i = \emptyset$ implies

$$\deg_{G[K]}(v) = |K| - |K \cap S_i| < |K| - k,$$

which contradicts that K is a k -plex. Therefore, $|K \cap S_i| \leq \min\{k, n_i\}$ for each S_i .

Suppose for contradiction that $|K| = \sum_{i=1}^r |K \cap S_i| < \sum_{i=1}^r \min\{k, n_i\}$. Then there exists a j such that $|K \cap S_j| < \min\{k, n_j\}$, and $|K \cap S_j| < n_j$ implies that there exists a vertex $v \in S_j \setminus K$. Consider the set $K' := K \cup \{v\}$ and a vertex $u \in K' \setminus S_j$. Since $uv \in E$,

$$\deg_{G[K']}(u) = \deg_{G[K]}(u) + 1 \geq (|K| - k) + 1 = |K'| - k.$$

Now suppose $u \in K \cap S_j$. Observe that $\deg_{G[K']}(u) = \deg_{G[K]}(u) = |K| - |K \cap S_j| > |K| - k$ since $uv \notin E$ and $|K \cap S_j| < k$. It follows that

$$\deg_{G[K']}(u) \geq |K| - k + 1 = |K'| - k.$$

Thus, since $\deg_{G[K']}(u) = \deg_{G[K']}(v)$, K' is a k -plex in G , which contradicts the maximality of K . It follows that all maximal k -plexes in G have cardinality $\sum_{i=1}^r \min\{k, n_i\}$, so G is k -plex perfect by Theorem 11. \square

The final two examples are classes of 2-plex perfect graphs.

Theorem 13. *The complement of a path \bar{P}^n is 2-plex perfect.*

Proof. This theorem follows from Theorem 7 and the fact that $\omega_2(\bar{P}^n) = \alpha_2(P^n)$.

More precisely, since the clutter matrix M_{P^n} is totally unimodular, we know that

$$\omega_2(\bar{P}^n) = \alpha_2(P^n) = \max\left\{ \sum_{v \in V(P^n)} x_v \mid M_{P^n} x \leq 2, 0 \leq x \leq 1 \right\}.$$

Let $K_j = \{j, j+1, j+2\}$. Notice that the dual linear program

$$\min\left\{ \sum_{i=1}^{n-2} 2y_{K_i} + \sum_{i=1}^n \lambda_i \mid yM_{P^n}^T + \lambda \geq 1, y, \lambda \geq 0 \right\}$$

also has an integral optimal solution. Letting \mathcal{S} denote the set of all co- k -plexes in \bar{P}^n

and performing a change of variables allows us to rewrite the previous LP as follows:

$$\min\left\{\sum_{C \in \mathcal{S}} \omega_2(C) z_C \mid \sum_{C: v \in C} z_C \geq 1 \text{ for all } v, z \geq 0\right\} = \chi_2(\bar{P}^n).$$

Now $\chi_2(\bar{P}^n) = \omega_2(\bar{P}^n)$ follows from LP duality. Moreover, this same proof holds for any vertex induced subgraph of \bar{P}^n because all submatrices of M_{P^n} are also totally unimodular. \square

Recall that for integers $n \geq 2$ and p , $1 \leq p \leq \frac{n}{2}$, $W(n, p)$ denotes the graph on vertices $V = \{1, \dots, n\}$ and edges

$$E = \{(i, j) \mid j = i + p, \dots, i + n - p; \forall i \in V\}.$$

Theorem 14. *Let $m \geq 2$. The web $W(3m, 2)$ is 2-plex perfect.*

Proof. Notice that $W(3m, 2)$ is the complement of the cycle C^{3m} . Any proper induced subgraph of $W(3m, 2)$ is also an induced subgraph of \bar{P}^{3m} and hence 2-plex perfect by Theorem 13. Therefore, it suffices to show $\chi_2(W(3m, 2)) = \omega_2(W(3m, 2))$. Observe that $\{v_1, v_2, v_3\}, \dots, \{v_{3m-2}, v_{3m-1}, v_{3m}\}$ is a co-2-plex coloring of $W(3m, 2)$, so we can deduce

$$\chi_2(W(3m, 2)) \leq \omega_2(\{v_1, v_2, v_3\}) + \dots + \omega_2(\{v_{3m-2}, v_{3m-1}, v_{3m}\}) = 2 + \dots + 2 = 2m.$$

Consider the set $K = \{v_i \in V : i \not\equiv 0 \pmod{3}\}$. First observe that $|K| = |V| - m =$

$2m$. We claim that K is a 2-plex. This is because every vertex v_i has exactly two non-neighbors $v_{i-1}, v_{i+1} \in V$. However, the definition of K implies that for each v_i exactly one of the non-neighbors is also in K . In other words,

$$\deg_{W(3m,2)[K]}(v) \geq |K| - 2 \quad \text{for all } v \in V,$$

and K is a k -plex. Finally,

$$\chi_2(W(3m, 2)) \leq 2m = |K| \leq \omega_2(W(3m, 2)) \leq \chi_2(W(3m, 2)),$$

and equality holds throughout. □

4.6.2 Graph Perfection and k -plex Perfection

It turns out that many properties of perfect graphs do not have k -plex analogues. Consider the complement $\overline{K}_{r,r}$ of a complete bipartite graph. Both components H_1 and H_2 of $\overline{K}_{r,r}$ are complete subgraphs.

Lemma 11. *Let $k \geq 1$. If $r = 2k - 1$, then $\alpha_k(\overline{K}_{r,r}) = 2k$ and $\omega_k(\overline{K}_{r,r}) = 2k - 1$.*

Proof. In the proof of Theorem 12, it was shown that

$$\omega_k(K_{r,r}) = \sum_{i=1}^2 \min\{k, r\} = 2k.$$

Thus, $\alpha_k(\overline{K}_{r,r}) = \omega_k(K_{r,r}) = 2k$.

Now $\omega_k(\overline{K}_{r,r}) \geq 2k - 1$ because each component H_i is complete and hence a k -plex of cardinality $2k - 1$. Suppose for contradiction that $\omega_k(\overline{K}_{r,r}) > 2k - 1$. Then there exists a k -plex $K \subseteq V$ such that $|K| = 2k$. If $|K \cap H_i| \leq k$, then

$$\deg_{\overline{K}_{r,r}[K]}(v) \leq k - 1 < k = |K| - k \text{ for all } v \in K \cap H_i.$$

This contradicts the definition of k -plex. Therefore, $|K \cap H_1| > k$ and $|K \cap H_2| > k$, which contradicts $|K| = 2k$. \square

Theorem 15. *Let $k > 1$. If $r = 2k - 1$, then $\overline{K}_{r,r}$ is not k -plex perfect.*

Proof. By Lemma 11, it suffices to show that $\chi_k(\overline{K}_{r,r}) \geq 2k$. Clearly, $\chi_k(\overline{K}_{r,r}) \geq \omega_k(\overline{K}_{r,r}) = 2k - 1$. Suppose for contradiction that $\chi_k(\overline{K}_{r,r}) = 2k - 1$. Lemma 10 implies the existence of an optimal co- k -plex coloring S_1, \dots, S_m of $\overline{K}_{r,r}$ such that $|S_1| \geq k$. Therefore, $\omega_k(\overline{K}_{r,r}[S_1]) \geq k$. Furthermore, $\chi_k(\overline{K}_{r,r}) < 2k$ implies that all other sets S_i satisfy $|S_i| < k$. Notice that

$$2k - 1 = \chi_k(\overline{K}_{r,r}) = \sum_{i=1}^m \omega_k(\overline{K}_{r,r}[S_i]) \geq k + \sum_{i=2}^m \omega_k(\overline{K}_{r,r}[S_i]) = k + \sum_{i=2}^m |S_i|.$$

Consequently, $k - 1 \geq \sum_{i=2}^m |S_i|$. Now since the sets S_i partition V and $|V| = 4k - 2$,

$$|S_1| = |V| - \sum_{i=2}^m |S_i| \geq 3k - 1.$$

Therefore, $k > 1$ implies that $|S_1| \geq 3k - 1 > 2k$. This contradicts Lemma 11 because

S_1 is a co- k -plex and $\alpha_k(\overline{K}_{r,r}) = 2k$. □

Lovász's (46) replication lemma is a well-known result from the theory of perfect graphs. Replication of a vertex $v \in V$ corresponds to the following operation: create a new vertex v' and join it to v and all the neighbors of v . The replication lemma states that replication of a vertex in a perfect graph produces another perfect graph. However, for $k \geq 2$, replication of a vertex in a k -plex perfect graph does not necessarily produce another k -plex perfect graph.

Fix $k > 1$. Consider the edgeless graph G on two vertices v_1 and v_2 . G is a co- k -plex since $\Delta(G) = 0$. It follows that G is k -plex perfect. Construct G' by performing $2k - 2$ replication operations on each of v_1 and v_2 . This construction implies that $G' = \overline{K}_{r,r}$, which is not k -plex perfect by Theorem 15. Therefore, vertex replication does not preserve k -plex perfection.

Theorem 15 also illustrates the following interesting property: G might not be k -plex perfect even if all components of G are k -plex perfect. This statement follows from Corollary 5 and Theorem 15.

The final topic of this section is a k -plex version of the Weak Perfect Graph Theorem (46). The Weak Perfect Graph Theorem states that G is perfect if and only if \overline{G} is perfect. Theorems 12 and 15 together provide counterexamples for k -plex analogues of the Weak Perfect Graph Theorem for any $k \geq 2$.

We now show that k -plex perfection does not imply that the co- k -plex polytope is described by the k -plex inequalities. To see this, fix integers $k \geq 2$ and $n \geq \min\{3, k\}$.

Consider the complete bipartite graph $K_{1,n}$. Theorem 12 implies that $K_{1,n}$ is k -plex perfect. Observe that $K_{1,n}$ is also a k -claw. Theorem 6 states that the k -claw inequality is a facet and hence necessary for any linear description of the co- k -plex polytope $P_k(K_{1,n})$. However, the k -claw inequality is not implied by the k -plex inequalities. Therefore, the k -plex inequalities do not suffice to describe the co- k -plex polytope of the k -plex perfect graph $K_{1,n}$. Thus, the polyhedral characterization of k -plex perfection differs from the combinatorial characterization whenever $k \geq 2$.

4.7 Conclusions

This chapter derives four classes of facets for the co-2-plex polytope and a class of facets for the co- k -plex polytope. The facets are related to 2-plexes, cycles, wheels, webs, and the claw. Two sections of this chapter are devoted to a characterization of 2-plex clutter matrices A for which the polytope $\{x \in \mathbf{R}_+^n \mid Ax \leq 2, x \leq 1\}$ is integral. We show that 2-plex clutter matrices can be tested for this property in polynomial time. The final section of this chapter is devoted to the development of a combinatorial concept of k -plex perfection. We give examples of k -plex perfect graphs and discussed some difficulties in generalizing certain properties of graph perfection.

Chapter 5

Detecting Cohesive Subgraphs

The Maximum Clique Problem provides a classic framework for detecting cohesive subgraphs. However, this approach can fail to detect much of the cohesive structure in a graph. To address this issue, Seidman and Foster introduced k -plexes by relaxing the definition of graph completeness. This chapter describes methods for finding maximum k -plexes.

5.1 Introduction

The problem of finding maximum cardinality cliques is a classic NP-complete problem and is of fundamental importance in combinatorial optimization. The Maximum Clique Problem (MCP) has applications in ad hoc wireless networks (19), data mining (69), social network analysis (70), and biochemistry and genomics (16). MCP is also related to the derivation of a class of inequalities for general integer programs (3).

Cliques provide a useful framework for detecting *cohesion*, or mutual adjacency among a set of vertices, but they can be overly restrictive. For example, consider the

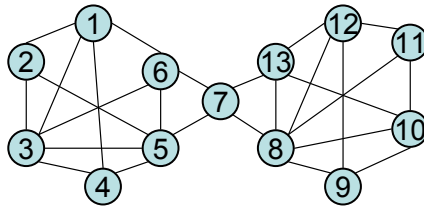


Figure 5.1: A graph G such that $\omega(G)=3$.

graph G in Figure 5.1. A maximum cardinality clique in G has three vertices, denoted by $\omega(G) = 3$. However, G has multiple subgraphs which are one edge short of defining a larger clique. Furthermore, G itself consists of two fairly cohesive subgraphs. The maximum clique approach fails to detect this cohesive structure because MCP can only detect subgraphs with the highest possible level of cohesion. Seidman and Foster (62) introduced k -plexes to address this issue. Recall the following definitions.

Definition (Seidman and Foster (62)). $K \subseteq V$ induces a k -plex if $\delta(G[K]) \geq |K| - k$.

The term k -plex refers to both the set K and the subgraph $G[K]$. The definition of k -plex formalizes a general notion of cohesion. Let $\omega_k(G)$ denote the cardinality of a largest k -plex in G . Consider the graph G in Figure 5.1. The set $\{1, 2, 3, 4, 5\}$ is a maximum 2-plex. The set $\{8, 9, 10, 11, 12, 13\}$ is a maximum 3-plex. In this example, $\omega_2(G) = 5$ and $\omega_3(G) = 6$.

Definition (Seidman and Foster (62)). $C \subseteq V$ induces a co- k -plex if $\Delta(G[C]) \leq k - 1$.

Seidman and Foster (62) introduced k -plexes and analyzed them from a graph-theoretic perspective. More recently, Balasundaram et al. (6) provided an integer programming formulation for the Maximum k -plex Problem, derived inequalities for

the k -plex polytope, and established the NP-completeness of the k -plex decision problem.

The purpose of this chapter is to develop algorithms for finding maximum k -plexes. Sections 5.2 and 5.3 describe heuristics for bounding the size of k -plexes in a graph. Section 5.2 contains upper bounds. Section 5.3 contains a lower bound. Section 5.4 develops the exact k -plex algorithms. The exact algorithms are based either on a standard clique algorithm (1; 18) or an algorithm of Östergård (54). Section 5.5 summarizes the results. The algorithms in Sections 5.2, 5.3, and 5.4 were tested on the DIMACS benchmark graphs. All implementations were run on a 2.2 GHz Dual-Core AMD Opteron processor with 3 GB of memory.

5.2 Co- k -plex Coloring

This section contains heuristics for finding an upper bound on $\omega_k(G)$. The heuristics are based on the concept of co- k -plex coloring developed in Section 4.6. Let Π be the set of all co- k -plex colorings of V , and recall the definition of the co- k -plex coloring number

$$\chi_k(G) = \min\left\{\sum_{C \in \mathcal{C}} \omega_k(G[C]) : \mathcal{C} \in \Pi\right\}. \quad (5.1)$$

In Section 4.6, it was shown that

$$\omega_k(G) \leq \chi_k(G). \quad (5.2)$$

In practice, determining the exact value of $\chi_k(G)$ can be computationally prohibitive, so we must approximate $\chi_k(G)$. Our co- k -plex coloring heuristics fall into two categories: integral and fractional. To see the distinction, let \mathcal{S} be the set of all co- k -plexes in G , and let \mathcal{S}_v denote the set of co- k -plexes containing v . Define $x(A) := \sum_{a \in A} x_a$. Consider the following dual pair of integer programs:

$$\max\{x(V) : x \in \{0, 1\}, x(S) \leq \omega_k(G[S]) \text{ for all } S \in \mathcal{S}\} \quad (5.3)$$

$$\min\left\{\sum_{S \in \mathcal{S}} \omega_k(G[S]) y_S : y \in \{0, 1\}, y(\mathcal{S}_v) \geq 1 \text{ for all } v \in V\right\}. \quad (5.4)$$

Notice that the optimal objective value for (5.3) is $\omega_k(G)$ and the optimal objective value for (5.4) is $\chi_k(G)$. Moreover, by strong duality, the optimal objective values for the respective linear relaxations are equal. We can deduce that any feasible solution to the linear relaxation of (5.4) produces an upper bound on the optimal objective value for (5.3).

Integer Co- k -plex Coloring Heuristics (ICCH) find feasible solutions to (5.4). Fractional Co- k -plex Coloring Heuristics (FCCH) find feasible solutions to the linear relaxation of (5.4). In either case, the result is an upper bound on $\omega_k(G)$. Before presenting these heuristics, we begin with three results bounding the k -plex number of a graph.

Lemma 12. *Every graph G satisfies $\omega_k(G) \leq \Delta(G) + k$.*

Proof. Suppose that there exists a k -plex K in G such that $|K| > \Delta(G) + k$. Choose

a vertex $v \in K$. Observe that $\deg_{G[K]}(v) \geq |K| - k$ by the definition of k -plex. Therefore, $\deg_{G[K]}(v) \geq |K| - k > \Delta(G)$, a contradiction since $G[K] \subseteq G$. \square

Lemma 13. *Given a graph G and an integer $m \geq 0$, let a_m denote the number of vertices $v \in V$ such that $\deg_G(v) \geq m$. If $j := \max\{m : a_m \geq k + m\}$, then*

$$\omega_k(G) \leq k + j.$$

Proof. Suppose for contradiction that G contains a k -plex K such that $|K| \geq k + j + 1$.

By definition of k -plex,

$$\deg_{G[K]}(v) \geq |K| - k \geq j + 1 \quad \text{for all } v \in K.$$

In other words, K contains at least $k + j + 1$ vertices v such that $\deg_G(v) \geq j + 1$. It follows that $a_{j+1} \geq k + j + 1$, contradicting the definition of j . \square

Lemma 14 (Balasundaram et al. (6)). *Every co- k -plex C satisfies*

$$\omega_k(G[C]) \leq 2k - 2 + k \pmod{2},$$

and this bound is tight for all $k \geq 1$.

The co- k -plex coloring heuristics in this section apply Lemmas 12, 13, and 14 to bound the k -plex number of a co- k -plex. Notice that $a_i = 0$ for all $i \geq k$ whenever Lemma 13 is applied to a co- k -plex. Therefore, $j \leq k - 1$ and Lemma 13 gives the

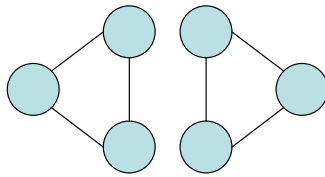


Figure 5.2: Lemmas 12-14 are not exact.

bound $\omega(G[C]) \leq 2k - 1$ for any co- k -plex C . Thus, Lemma 13 implies Lemma 14 when k is odd. For k even, Lemma 14 can give a better for co- k -plexes. However, in practice, one would expect Lemma 13 to outperform Lemma 14 because the latter is valid for all co- k -plexes while the former is derived for a given co- k -plex.

The co-3-plex C shown in Figure 5.2 shows that these bounds are not exact. Notice that $\omega_3(C) = 4$. However, each bound implies $\omega_3(C) \leq 5$.

5.2.1 Integer Co- k -plex Coloring Heuristics

This subsection contains two Integer Co- k -plex Coloring Heuristics for approximating $\chi_k(G)$. Figure 5.3 shows the first: **ICCH1**. Lines 1-5 produce a valid co- k -plex coloring \mathcal{C} of G . Line 7 uses Lemmas 12, 13, and 14 to bound $\omega_k(G[C])$. The result is an upper bound on $\omega_k(G)$. Each execution of Line 4 can be used to store the degree of every vertex in C_m . Lines 3, 4, 6, and 7 can each be accomplished in linear time using an adjacency matrix. It follows that **ICCH1** is an $\mathcal{O}(|V|^2)$ algorithm. Table 5.1 contains computational results obtained by running **ICCH1** on the DIMACS benchmark graphs with an arbitrary initial vertex ordering.

We can alter **ICCH1** by adding a feature modeled after the DSATUR graph coloring heuristic (11). Define the *saturation degree* of a vertex v to be the number

Table 5.1: ICCH1 Results

G	$\chi_2(G)$	seconds	$\chi_3(G)$	seconds	$\chi_4(G)$	seconds
brock200-1	93	0.0	151	0.0	169	0.0
brock200-2	55	0.0	95	0.0	118	0.0
brock200-4	78	0.0	131	0.0	151	0.0
brock400-2	172	0.1	285	0.1	332	0.1
brock400-4	168	0.1	286	0.1	330	0.1
brock800-2	248	0.3	442	0.3	570	0.3
brock800-4	247	0.3	440	0.3	557	0.3
c-fat200-1	18	0.0	20	0.0	21	0.0
c-fat200-2	34	0.0	37	0.0	38	0.0
c-fat200-5	82	0.0	89	0.0	90	0.0
c-fat500-1	19	0.0	23	0.0	24	0.0
c-fat500-2	36	0.0	41	0.0	42	0.0
c-fat500-5	85	0.1	98	0.0	99	0.0
c-fat500-10	172	0.1	191	0.1	192	0.1
C125.9	95	0.0	122	0.0	123	0.0
C250.9	176	0.0	230	0.0	240	0.0
C1000.9	525	0.7	897	0.7	929	0.7
gen400-p0.9-55	242	0.1	365	0.1	379	0.1
gen400-p0.9-65	243	0.1	369	0.1	382	0.1
gen400-p0.9-75	235	0.1	368	0.1	384	0.1
hamming6-2	32*	0.0	48	0.0	56	0.0
hamming6-4	8	0.0	12	0.0	16	0.0
hamming8-2	128*	0.0	192	0.0	224	0.0
hamming8-4	32	0.0	48	0.0	64	0.0
hamming10-2	512*	0.7	768	0.7	896	0.7
hamming10-4	128	0.5	192	0.5	256	0.5
johnson8-2-4	12	0.0	16	0.0	19	0.0
johnson8-4-4	28	0.0	42	0.0	48	0.0
johnson16-2-4	30	0.0	63	0.0	73	0.0
johnson32-2-4	72	0.1	122	0.1	171	0.1
keller4	54	0.0	100	0.0	128	0.0
keller5	235	0.3	450	0.3	554	0.3
MANN-a9	38	0.0	44	0.0	45	0.0
MANN-a27	324	0.1	369	0.1	378	0.1
MANN-a45	833	1.0	1032	0.8	1035	0.8
p-hat300-1	39	0.0	69	0.0	90	0.0
p-hat300-2	76	0.0	135	0.0	173	0.0
p-hat300-3	129	0.0	210	0.0	245	0.0
p-hat700-1	76	0.1	135	0.1	184	0.1
p-hat700-2	165	0.2	289	0.1	375	0.2
p-hat700-3	267	0.3	451	0.2	556	0.2
p-hat1500-1	136	0.5	251	0.6	349	0.6
p-hat1500-2	302	0.9	553	1.0	758	1.0
p-hat1500-3	508	1.5	908	1.5	1100	1.6
san200-0.7-2	105	0.0	147	0.0	159	0.0
san200-0.9-1	133	0.0	184	0.0	193	0.0
san200-0.9-2	136	0.0	189	0.0	192	0.0
san200-0.9-3	140	0.0	189	0.0	191	0.0
san400-0.9-1	249	0.1	374	0.1	378	0.1
sanr200-0.9	130	0.0	192	0.0	193	0.0

* optimal

```

function ICCH1( $V$ )
1.   $C_i = \emptyset$  for  $1 \leq i \leq |V|$ 
2.  for all  $u \in V$ 
3.     $m = \min\{i : C_i \cup \{u\} \text{ is a co-}k\text{-plex in } G\}$ 
4.     $C_m = C_m \cup \{u\}$ 
5.  end
6.  Compute  $j_i := \max\{m : a_m \geq k + m\}$  for each  $C_i$ 
7.   $bound = \sum_{i=1}^{|V|} \min\{2k - 2 + k \bmod 2, k + j_i, \Delta(G[C_i]) + k, |C_i|\}$ 
8.  return  $bound$ 

```

Figure 5.3: Co- k -plex Coloring Heuristic **ICCH1**

of distinct partition sets C such that $C \cup \{v\}$ is not a co- k -plex. At each step in the algorithm, color the vertex with the largest saturation degree. The resulting algorithm is shown in Figure 5.4. Lines 4-8 can all be accomplished in linear time, so **ICCH2** is another $\mathcal{O}(|V|^2)$ algorithm. Table 5.2 contains computational results obtained by running **ICCH2** on the DIMACS benchmark graphs with an arbitrary initial vertex ordering.

The results show that **ICCH1** and **ICCH2** give similar estimations of $\chi_k(G)$ on the DIMACS graphs and that no significant gain is realized by considering saturation degrees. Both heuristics tend to run in under a second.

5.2.2 Fractional Co- k -plex Coloring Heuristics

This subsection adapts the fractional coloring procedure of Balas and Xue (5) in order to obtain a bound on $\omega_k(G)$. The resulting FCCH defines a set of co- k -plexes $C_1, \dots, C_h \subseteq V$ with the property that after p iterations, each vertex $v \in V$ belongs to exactly p distinct co- k -plex sets. We can then construct a feasible solution y to the

Table 5.2: ICCH2 Results

G	$\chi_2(G)$	seconds	$\chi_3(G)$	seconds	$\chi_4(G)$	seconds
brock200-1	94	0.0	148	0.0	169	0.0
brock200-2	55	0.0	96	0.0	118	0.0
brock200-4	80	0.0	129	0.0	151	0.0
brock400-2	172	0.1	284	0.1	332	0.1
brock400-4	169	0.1	288	0.1	330	0.1
brock800-2	250	0.5	436	0.3	563	0.3
brock800-4	249	0.8	440	0.3	569	0.4
c-fat200-1	18	0.0	20	0.0	21	0.0
c-fat200-2	33	0.0	37	0.0	38	0.0
c-fat200-5	82	0.0	89	0.0	90	0.0
c-fat500-1	22	0.1	23	0.0	24	0.0
c-fat500-2	37	0.1	41	0.0	42	0.0
c-fat500-5	90	0.1	98	0.0	99	0.1
c-fat500-10	173	0.2	191	0.1	192	0.1
C125.9	96	0.0	119	0.0	123	0.0
C250.9	168	0.1	237	0.0	240	0.0
C1000.9	527	1.1	872	0.9	929	0.9
gen400-p0.9-55	238	0.1	371	0.1	379	0.1
gen400-p0.9-65	238	0.1	364	0.1	382	0.1
gen400-p0.9-75	230	0.1	372	0.1	384	0.1
hamming6-2	32*	0.0	59	0.0	61	0.0
hamming6-4	10	0.0	25	0.0	26	0.0
hamming8-2	128*	0.0	235	0.0	251	0.0
hamming8-4	49	0.0	116	0.0	154	0.0
hamming10-2	512*	1.0	939	0.9	1017	0.9
hamming10-4	260	0.7	556	0.8	755	0.8
johnson8-2-4	12	0.0	18	0.0	19	0.0
johnson8-4-4	38	0.0	55	0.0	57	0.0
johnson16-2-4	48	0.0	81	0.0	95	0.0
johnson32-2-4	133	0.1	236	0.1	332	0.1
keller4	57	0.0	101	0.0	115	0.0
keller5	220	0.4	430	0.3	576	0.3
MANN-a9	37	0.0	42	0.0	45	0.0
MANN-a27	306	0.1	351	0.1	378	0.1
MANN-a45	814	1.1	990	0.9	1035	0.9
p-hat300-1	38	0.0	69	0.0	89	0.0
p-hat300-2	76	0.0	138	0.0	169	0.0
p-hat300-3	125	0.1	203	0.0	237	0.0
p-hat700-1	77	0.1	136	0.1	178	0.1
p-hat700-2	158	0.2	290	0.2	373	0.2
p-hat700-3	263	0.3	449	0.3	554	0.3
p-hat1500-1	140	0.9	251	0.9	352	0.9
p-hat1500-2	302	1.6	555	1.7	764	1.7
p-hat1500-3	503	2.3	905	2.4	1113	2.4
san200-0.7-2	66	0.0	113	0.0	155	0.0
san200-0.9-1	131	0.0	183	0.0	194	0.0
san200-0.9-2	134	0.0	185	0.0	192	0.0
san200-0.9-3	135	0.0	190	0.0	191	0.0
san400-0.9-1	229	0.1	346	0.1	378	0.1
sanr200-0.9	131	0.0	188	0.0	193	0.0

* optimal

function ICCH2(V)

1. $C_i = \emptyset$ for $1 \leq i \leq |V|$
2. $sat(v) = 0$ for all $v \in V$
3. **while** $V \neq \emptyset$
4. Let $u \in \{v \in V : sat(v) \geq sat(w) \text{ for all } w \in V\}$
5. $V = V \setminus \{u\}$
6. $m = \min\{i : C_i \cup \{u\} \text{ is a co-}k\text{-plex in } G\}$
7. $C_m = C_m \cup \{u\}$
8. Update $sat(v)$ for all uncolored $v \in N(u)$
9. **end**
10. Compute $j_i := \max\{m : a_m \geq k + m\}$ for each C_i
11. $bound = \sum_{i=1}^{|V|} \min\{2k - 2 + k \bmod 2, k + j_i, \Delta(G[C_i]) + k, |C_i|\}$
12. **return** $bound$

Figure 5.4: Co- k -plex Coloring Heuristic **ICCH2**

linear relaxation of (5.4) as follows:

$$y := \frac{1}{p} \sum_{i=1}^h y_{C_i}.$$

From this solution, we deduce

$$\omega_k(G) \leq \frac{1}{p} \sum_{i=1}^h \omega_k(G[C_i]) y_{C_i}.$$

Figure 5.5 contains the FCCH. The set \mathcal{C} consists of the co- k -plexes $C_1 \cup \dots \cup C_h$. At each iteration, a vertex is either added to an existing $C_i \in \mathcal{C}$ in Line 7 or to a new partition set in Line 10. When the algorithm reaches Line 12, every vertex belongs to exactly p partition sets, so t_{new} is a valid upper bound on $\omega_k(G)$.

The FCCH can be run using either **ICCH1** or **ICCH2**. Tables 5.3 and 5.4 contain computational results obtained by running **FCCH1** and **FCCH2**, which use

```

function FCCH( $V$ )
1.   $t_{old} = \infty; p = 1$ 
2.   $t_{new} = \text{ICCH}(V)$ ; store the partition sets in  $\mathcal{C}$ 
3.  while  $t_{new} < t_{old}$ 
4.     $U = V; t_{old} = t_{new}; p = p + 1$ 
5.    for all  $v \in U$ 
6.      if  $\exists C_i \in \mathcal{C}$  such that  $v \notin C_i$  and  $C_i \cup \{v\}$  is a co- $k$ -plex
7.         $C_i = C_i \cup \{v\}; U = U \setminus \{v\}$ 
8.      end
9.    end
10.   $\text{ICCH}(U)$ ; append new partition sets in  $\mathcal{C}$ 
11.  Compute  $j_i := \max\{m : a_m \geq k + m\}$  for each  $C_i \in \mathcal{C}$ 
12.   $t_{new} = \frac{1}{p} \cdot \sum_{C_i \in \mathcal{C}} \min\{2k - 2 + k \bmod 2, k + j_i, \Delta(G[C_i]) + k, |C_i|\}$ 
13. end
14. return  $t_{old}$ 

```

Figure 5.5: Fractional Co- k -plex Coloring Heuristic **FCCH**

ICCH1 and **ICCH2**, respectively. The **FCCH** shown in Figure 5.5 has an ill-defined termination condition. To bound the runtime, we bound the number iterations and the number of partition sets in \mathcal{C} to be $\mathcal{O}(|V|)$. For these runs, the bound was set at $5 \cdot |V|$.

Theorem 16. *If the number of iterations and the number of partition sets are $\mathcal{O}(|V|)$, then **FCCH** can be executed in $\mathcal{O}(|V|^4)$ time.*

Proof. At every iteration, for each vertex $v \in V$, we must test if $C_i \cup \{v\}$ is a co- k -plex. This can be done by counting the number of $u \in N(v) \cap C_i$, which requires $\mathcal{O}(\min\{\deg_G(v), \alpha_k(G)\}) = \mathcal{O}(|V|)$ time. Since there are $\mathcal{O}(|V|)$ partition sets, there can be $\mathcal{O}(|V|^2)$ possible pairs (C_i, v) . Thus, after $\mathcal{O}(|V|)$ iterations, this step has complexity $\mathcal{O}(|V|^4)$. Lines 2 and 10 execute a $\mathcal{O}(|V|^2)$ **ICCH** algorithm. Since there are at most $\mathcal{O}(|V|)$ iterations, these steps have complexity $\mathcal{O}(|V|^3)$. All other

operations contribute $\mathcal{O}(|V|^2)$ to the complexity. Therefore, the overall complexity of **FCCH** is $\mathcal{O}(|V|^4)$. \square

Clearly, the FCCH algorithms offer a better approximation of $\chi_k(G)$ than the ICCH algorithms. **FCCH2** appears to be slightly slower **FCCH1**, but both heuristics tend to run in under five seconds.

5.3 A k -plex Heuristic

For a lower bound on $\omega_k(G)$, we search for feasible k -plexes. Recall from Section 5.1 that the Maximum k -plex Problem is NP-complete. Consequently, the worst-case runtime of any algorithm which finds an optimal solution is most likely exponential with respect to the size of the input parameters. The guarantee of an optimal solution comes at the price of a potentially enormous runtime. Heuristics, on the other hand, sacrifice all guarantees on solution quality in order to obtain efficient runtimes. We will now describe a heuristic for finding k -plexes. The heuristic indirectly searches for cohesive subgraphs in G and extends them to maximal k -plexes.

There has been extensive research on heuristics for finding large complete subgraph (15; 30; 32; 48). We are interested in designing a combinatorial heuristic for finding k -plexes. A typical combinatorial heuristic systematically searches a set of neighborhoods in the feasible solution space for local optima (36). When a local optimum is obtained, we compare it to the incumbent solution, store its value if necessary, and continue searching in other neighborhoods. Obviously, the solution

Table 5.3: FCCH1 Results

G	$\chi_2(G)$	seconds	$\chi_3(G)$	seconds	$\chi_4(G)$	seconds
brock200-1	82	0.0	139	0.1	164	0.0
brock200-2	48	0.0	89	0.0	118	0.0
brock200-4	68	0.0	122	0.0	151	0.0
brock400-2	151	0.2	267	0.2	320	0.2
brock400-4	151	0.2	265	0.3	320	0.1
brock800-2	221	1.4	401	1.7	535	1.3
brock800-4	223	2.4	410	0.8	537	1.2
c-fat200-1	16	0.0	20	0.0	21	0.0
c-fat200-2	30	0.0	37	0.0	38	0.0
c-fat200-5	76	0.0	89	0.0	90	0.0
c-fat500-1	18	0.1	23	0.0	24	0.0
c-fat500-2	33	0.1	41	0.0	42	0.0
c-fat500-5	82	0.2	98	0.1	99	0.1
c-fat500-10	166	0.4	191	0.1	192	0.2
C125.9	83	0.0	120	0.0	123	0.0
C250.9	146	0.1	230	0.0	240	0.1
C1000.9	491	3.3	826	5.8	929	3.0
gen400-p0.9-55	216	0.3	357	0.2	379	0.2
gen400-p0.9-65	210	0.6	362	0.1	382	0.1
gen400-p0.9-75	213	0.4	353	0.3	384	0.3
hamming6-2	32*	0.0	48	0.0	56	0.0
hamming6-4	8	0.0	12	0.0	16	0.0
hamming8-2	128*	0.0	192	0.0	224	0.1
hamming8-4	32	0.0	48	0.0	64	0.0
hamming10-2	512*	1.3	768	1.3	896	2.0
hamming10-4	128	0.7	192	0.6	256	0.6
johnson8-2-4	10	0.0	16	0.0	18	0.0
johnson8-4-4	28	0.0	42	0.0	46	0.0
johnson16-2-4	27	0.0	63	0.0	73	0.0
johnson32-2-4	68	0.1	118	0.2	152	0.2
keller4	45	0.0	88	0.0	113	0.0
keller5	172	0.9	376	1.0	517	1.7
MANN-a9	36	0.0	44	0.0	45	0.0
MANN-a27	321	0.2	366	0.1	378	0.1
MANN-a45	803	5.9	1028	1.8	1035	1.1
p-hat300-1	34	0.0	62	0.0	85	0.0
p-hat300-2	71	0.1	129	0.0	161	0.1
p-hat300-3	115	0.2	201	0.1	240	0.1
p-hat700-1	68	0.3	123	0.3	168	0.3
p-hat700-2	146	0.7	272	0.3	349	0.5
p-hat700-3	243	1.4	428	0.8	532	0.6
p-hat1500-1	126	2.6	233	1.9	323	4.3
p-hat1500-2	282	4.8	518	3.9	705	3.5
p-hat1500-3	472	10.4	849	19.0	1071	7.4
san200-0.7-2	79	0.0	140	0.0	159	0.0
san200-0.9-1	127	0.0	177	0.1	191	0.1
san200-0.9-2	123	0.1	183	0.0	192	0.0
san200-0.9-3	121	0.0	186	0.0	191	0.1
san400-0.9-1	231	0.2	360	0.2	378	0.2
sanr200-0.9	119	0.0	187	0.0	193	0.0

* optimal

Table 5.4: FCCH2 Results

G	$\chi_2(G)$	seconds	$\chi_3(G)$	seconds	$\chi_4(G)$	seconds
brock200-1	83	0.1	139	0.1	167	0.0
brock200-2	48	0.1	87	0.0	115	0.0
brock200-4	68	0.1	121	0.0	151	0.0
brock400-2	152	0.7	272	0.1	320	0.2
brock400-4	150	0.7	269	0.3	319	0.3
brock800-2	224	1.7	400	2.6	535	1.6
brock800-4	220	3.1	402	1.0	544	1.2
c-fat200-1	15	0.0	20	0.0	21	0.0
c-fat200-2	30	0.0	37	0.0	38	0.0
c-fat200-5	75	0.1	89	0.0	90	0.0
c-fat500-1	22	0.1	23	0.0	24	0.0
c-fat500-2	34	0.1	41	0.1	42	0.1
c-fat500-5	81	0.1	98	0.1	99	0.1
c-fat500-10	164	0.3	191	0.2	192	0.3
C125.9	84	0.0	116	0.0	122	0.0
C250.9	143	0.1	230	0.1	240	0.1
C1000.9	489	4.6	828	4.3	929	2.8
gen400-p0.9-55	209	0.6	350	0.3	379	0.2
gen400-p0.9-65	207	0.4	352	0.2	382	0.4
gen400-p0.9-75	208	0.6	353	0.4	384	0.2
hamming6-2	32*	0.0	59	0.0	61	0.0
hamming6-4	8	0.0	20	0.0	26	0.0
hamming8-2	128*	0.1	231	0.1	251	0.1
hamming8-4	47	0.0	105	0.0	145	0.0
hamming10-2	512*	2.1	939	23.4	1017	2.4
hamming10-4	212	2.0	449	3.3	673	8.8
johnson8-2-4	10	0.0	18	0.0	19	0.0
johnson8-4-4	28	0.0	51	0.0	57	0.0
johnson16-2-4	34	0.0	76	0.0	95	0.0
johnson32-2-4	75	1.0	224	0.5	299	0.3
keller4	44	0.1	90	0.0	111	0.0
keller5	174	2.3	378	2.1	536	1.5
MANN-a9	37	0.0	42	0.0	45	0.0
MANN-a27	301	0.4	351	0.2	378	0.1
MANN-a45	755	7.2	990	2.6	1035	1.3
p-hat300-1	35	0.0	63	0.0	89	0.0
p-hat300-2	72	0.1	126	0.1	162	0.1
p-hat300-3	118	0.1	200	0.1	237	0.1
p-hat700-1	68	0.4	124	0.3	169	0.5
p-hat700-2	149	0.5	267	0.6	348	0.6
p-hat700-3	243	1.2	422	2.0	528	1.5
p-hat1500-1	125	4.0	230	6.3	326	4.4
p-hat1500-2	277	9.3	515	7.6	700	7.5
p-hat1500-3	470	14.5	854	12.0	1074	12.1
san200-0.7-2	57	0.0	113	0.0	144	0.1
san200-0.9-1	125	0.1	170	0.1	190	0.1
san200-0.9-2	113	0.1	173	0.1	192	0.1
san200-0.9-3	119	0.1	181	0.1	191	0.0
san400-0.9-1	208	0.4	315	0.5	378	0.2
sanr200-0.9	115	0.1	183	0.1	193	0.0

* optimal

quality heavily depends on both the choice of neighborhoods and the local search method.

Recall that if \mathcal{I}_G denotes the set of all complete subgraphs in G , then \mathcal{I}_G also denotes the set of all stable sets in \bar{G} . The remainder of this section focuses on finding stable sets in \bar{G} which we extend to maximal k -plexes in G . This approach is valid because every element in \mathcal{I}_G is extendible to a maximal k -plex in G . To find stable sets in \bar{G} , we will construct sets $K \notin \mathcal{I}_G$ and alter them to obtain elements $K' \in \mathcal{I}_G$. Without loss of generality, assume G is connected. For if not, simply run the heuristic on each component.

For $u, v \in V$, let $d(u, v)$ be the length of a shortest path from u to v in G . Our concept of neighborhood is based on the parity of shortest path lengths from some root node s . Given a root $s \in V$, define the following sets:

$$K_0 := \{v \in V \mid d(s, v) \text{ even}\} \quad \text{and} \quad K_1 := \{v \in V \mid d(s, v) \text{ odd}\}.$$

For example, suppose that we are searching for k -plexes in some graph H and that \bar{H} is shown in Figure 5.6. The vertex set $V(H)$ partitions into the sets $K_0 = \{s, 5, 6, 7, 8, 12, 13\}$ and $K_1 = \{1, 2, 3, 4, 9, 10, 11\}$. For $i \in \{0, 1\}$, notice that $u, v \in K_i$ and $uv \in E(\bar{H})$ together imply $d(u, s) = d(v, s)$. Otherwise, $d(u, s)$ and $d(v, s)$ would have different parities. Therefore, for every $v \in K_i$,

$$N_{\bar{H}}(v) \cap \{u \in K_i \setminus \{v\} : d(u, s) \neq d(v, s)\} = \emptyset.$$

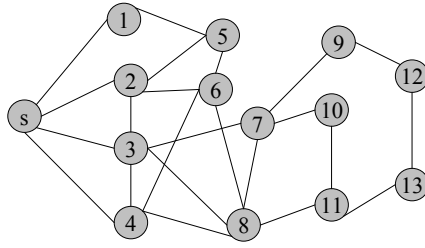


Figure 5.6: \bar{H} with root s .

We hope this property causes K_i to contain large stable sets.

Now $K_i \notin \mathcal{I}_H$ in general, but there will typically exist many subsets $K'_i \subseteq K_i$ such that $K'_i \in \mathcal{I}_H$. In order to examine a variety of these subsets, we construct elements in \mathcal{I}_H from K_i by removing one end of every edge in $\bar{H}[K_i]$. To summarize, we have two sets K_1 and K_2 such that $\bar{H}[K_1]$ and $\bar{H}[K_2]$ can have edges. For $i = 1, 2$, we will scan $E(\bar{H}[K_i])$ and remove one end of each edge. We construct four sets from K_i . Each set is defined by applying only one of the following rules to every edge:

Rule 1. If $\deg_{\bar{H}[K_i]}(v) \leq \deg_{\bar{H}[K_i]}(u)$, remove u . Otherwise, remove v .

Rule 2. If $\deg_{\bar{H}}(v) \leq \deg_{\bar{H}}(u)$, remove u . Otherwise, remove v .

Rule 3. Always remove v .

Rule 4. Always remove u .

Let K_i^j be the subset obtained from K_i by applying only Rule j to every edge in $E(\bar{H}[K_i])$. Rules 1 and 2 are greedy metrics. Rules 3 and 4 are included to diversify the search space.

We can now extend each set K_i^j to a maximal k -plex in H . All k -plexes that can be constructed from a set K_i in this way constitute a neighborhood. Therefore,

```

function lbound( $\mathcal{R}$ )
1.  for all  $s \in \mathcal{R}$ 
2.      define  $K_0$  and  $K_1$  with respect to root  $s$ 
3.      construct sets  $K_i^j \subseteq K_i$ 
4.      extend sets  $K_i^j$  to maximal  $k$ -plexes in  $H$ 
5.      for all  $j$  and  $i$ 
6.          kick( $K_i^j$ )
7.      end
8.      update incumbent  $I$  if necessary
9.  end

```

Figure 5.7: k -plex Heuristic **lbound**.

```

function kick( $K$ )
1.  construct set  $S := \{v \in V \setminus K : |N_{\bar{H}}(v) \cap K| \leq 1\}$ 
2.  let  $K = K \cup S$ 
3.  construct sets  $K^j \subseteq K$ 
4.  extend sets  $K^j$  to maximal  $k$ -plexes in  $H$ 

```

Figure 5.8: The **kick** function.

the search space is essentially a function of the root nodes, and specifying a set of neighborhoods is equivalent to specifying a set of root nodes \mathcal{R} . The k -plex heuristic **lbound** is shown in Figure 5.7. The incumbent solution I is initially empty and stored as a global variable.

To find a k -plex in H , we arbitrarily choose a set of vertices to define \mathcal{R} . Line 2 builds a breadth-first-search tree in \bar{H} rooted at s to determine $d(v, s)$ for all $v \in V$. The breadth-first-search tree is also used to define $deg_{\bar{H}[K_i]}(v)$ for all v . Line 3 applies Rules 1-4, and Line 4 uses a greedy heuristic. Line 6 passes the sets K_i^j to the new function **kick**. The function **kick** is shown in Figure 5.8. Its purpose is to help the heuristic escape local optima. Figure 5.7 is our basic k -plex heuristic.

Line 3 in the function **kick** scans the edges of $G[K_i]$, so the function requires

$\mathcal{O}(|E|)$ time. The function **lbound** makes $\mathcal{O}(|\mathcal{R}|)$ calls to **kick**. It follows that **lbound** is an $\mathcal{O}(|E| \cdot |\mathcal{R}|)$ algorithm. Table 5.5 contains computational results obtained by running **lbound** on the DIMACS benchmark graphs. **LB1** corresponds to choosing an arbitrary set of $\frac{|V|}{40}$ vertices to define \mathcal{R} . **LB2** corresponds to setting $\mathcal{R} = V$.

This section described a heuristic for finding k -plexes in a graph G . The results of this section will serve as a lower bound in an exact k -plex algorithm described in Section 5.4.

5.4 Exact k -plex Algorithms

This section describes exact algorithms for finding maximum k -plexes in a graph $G = (V, E)$. The first type is based on a standard clique algorithm (1; 18). The second type adapts an algorithm of Östergård (54).

5.4.1 Algorithm Type 1

Our first type of k -plex algorithms are an adaptation of the basic clique algorithm shown in Figure 5.9. At any point in the basic clique algorithm, we are constructing a complete graph K . The candidate set, $U \subseteq V \setminus K$, contains all vertices v such that $K \cup \{v\}$ is complete. In other words, $U := \bigcap_{v \in K} N(v)$. The global variable max stores the cardinality of the largest clique found. To find a maximum clique in G , we initialize $max = 0$ and make the function call **basicClique**(V, \emptyset).

Table 5.5: lbound Results

G	LB1		LB2		LB1		LB2		LB1		LB2	
	$\omega_2(G)$	sec.	$\omega_2(G)$	sec.	$\omega_3(G)$	sec.	$\omega_3(G)$	sec.	$\omega_4(G)$	sec.	$\omega_4(G)$	sec.
brock200-1	25	1	25	3	27	1	28	3	31	1	32	3
brock200-2	12	1	13*	5	15	1	15	6	17	1	17	5
brock200-4	18	1	19	4	22	1	23	4	24	1	25	4
brock400-2	27	2	28	23	31	2	32	23	35	2	36	23
brock400-4	33	2	33	23	33	2	33	23	36	2	37	23
brock800-2	22	15	23	299	26	15	26	298	29	15	30	299
brock800-4	22	15	23	301	25	15	26	301	29	15	30	301
c-fat200-1	12*	2	12*	10	12*	2	12*	10	12*	2	12*	10
c-fat200-2	24*	2	24*	9	24*	2	24*	9	24*	2	24*	10
c-fat200-5	58*	2	58*	7	58*	2	58*	7	58*	2	58*	7
c-fat500-1	14*	20	14*	225	14*	19	14*	226	14*	19	14*	226
c-fat500-2	26*	19	26*	210	26*	18	26*	210	26*	19	26*	212
c-fat500-5	64*	16	64*	191	64*	16	64*	185	64*	16	64*	194
c-fat500-10	126*	13	126*	146	126*	13	126*	150	126*	13	126*	152
C125.9	42	0	42	0	47	0	48	0	54	0	54	0
C250.9	50	0	50	3	58	0	59	3	66	1	67	3
C1000.9	69	7	74	165	80	7	83	168	91	7	92	173
gen400-p0.9-55	59	2	61	12	71	1	72	11	80	1	81	12
gen400-p0.9-65	66	1	67	11	78	1	87	11	86	1	86	12
gen400-p0.9-75	75	1	75	11	84	1	91	11	91	1	98	12
hamming6-2	32*	0	32*	0	32*	0	32*	0	32	0	32	0
hamming6-4	4	0	4	0	8*	0	8*	0	8	0	8	0
hamming8-2	128*	0	128*	2	128*	0	128*	2	128	0	128	2
hamming8-4	16*	1	16*	8	16	1	16	8	16	1	16	8
hamming10-2	512*	3	512*	65	512	3	512	67	512	3	512	74
hamming10-4	43	12	43	281	64	12	64	288	63	12	64	297
johnson8-2-4	4	0	4	0	8*	0	8*	0	9*	0	9*	0
johnson8-4-4	14	0	14	0	14	0	14	0	14	0	14	0
johnson16-2-4	8	0	8	1	16	0	16	1	18	0	18	1
johnson32-2-4	16	2	16	21	32	2	32	25	36	2	36	26
keller4	15*	1	15*	3	18	1	18	2	20	1	20	2
keller5	31	10	31	176	37	9	39	176	42	10	42	180
MANN-a9	22	0	22	0	30	0	30	0	36*	0	36*	0
MANN-a27	218	2	218	14	258	3	260	29	250	2	257	17
MANN-a45	646	35	646	859	762	76	762	1748	756	21	756	540
p-hat300-1	9	4	9	28	11	4	11	28	12	4	13	28
p-hat300-2	30	3	30	20	34	3	34	19	39	3	39	20
p-hat300-3	42	1	43	10	49	1	49	10	53	2	55	11
p-hat700-1	10	33	12	537	13	33	14	555	16	32	16	529
p-hat700-2	50	19	51	316	58	19	58	320	65	19	66	321
p-hat700-3	70	8	71	140	82	9	84	140	92	9	95	141
p-hat1500-1	13	202	13	7318	14	204	16	7320	16	204	18	7414
p-hat1500-2	73	124	75	4516	86	120	89	4504	98	121	99	4433
p-hat1500-3	107	48	108	1716	122	48	124	1719	137	48	139	1723
san200-0.7-2	26	1	26	3	36	1	36	4	48	1	48	4
san200-0.9-1	90	0	90	2	125*	0	125*	2	125	0	125	2
san200-0.9-2	71	0	71	2	105	0	105	2	105	0	105	2
san200-0.9-3	50	0	52	1	62	0	67	2	65	0	65	2
san400-0.9-1	102	2	102	15	150	2	150	18	200	2	200	16
sanr200-0.9	48	0	48	1	56	0	56	2	63	0	64	2

* optimal


```

function basicClique( $U, K$ )
1.  while  $U \neq \emptyset$ 
2.    if  $|K| + |U| \leq \mathit{max}$ 
3.      return
4.    end
5.     $U = U \setminus \{v\}$  for some  $v \in U$ 
6.    basicClique( $U \cap N(v), K \cup \{v\}$ )
7.  end
8.  if  $|K| > \mathit{max}$ 
9.     $\mathit{max} = |K|$ 
10. end
11. return

```

Figure 5.9: Basic Clique Algorithm

The basic clique algorithm can be generalized to find maximum k -plexes. The main difference is that given a k -plex K , the candidate set U can no longer be defined as $\bigcap_{v \in K} N(v)$. The candidate set is now defined as

$$U = \{v \in V \setminus K : K \cup \{v\} \text{ is a } k\text{-plex}\}.$$

The basic k -plex algorithm is shown in Figure 5.10. To find a maximum k -plex in G , we initialize $\mathit{max} = 0$ and make the function call **basicPlex**(V, \emptyset). Table 5.6 contains computational results obtained by running **basicPlex** on the DIMACS benchmark graphs.

Without Lines 2-4, the function **basicClique** examines every clique in G . Recall that G can contain an exponential, with respect to $|V|$, number of cliques (Moon and Moser 1965). Lines 2-4 are an attempt to avoid total enumeration of an exponential number of subgraphs. This is known as pruning the search tree. Unfortunately, there

Table 5.6: basicPlex Results

G	$\omega_2(G)$	seconds	BBN	$\omega_3(G)$	seconds	BBN	$\omega_4(G)$	seconds	BBN
brock200-1	25	≥ 3600	172822699	28	≥ 3600	182056437	31	≥ 3600	180633250
brock200-2	13*	166	9759381	15	≥ 3600	199178608	17	≥ 3600	192281927
brock200-4	20	≥ 3600	193074734	22	≥ 3600	199289654	25	≥ 3600	193677120
brock400-2	27	≥ 3600	169761253	31	≥ 3600	162264447	34	≥ 3600	155153487
brock400-4	27	≥ 3600	160979618	32	≥ 3600	146807899	36	≥ 3600	145283598
brock800-2	23	≥ 3600	134201916	25	≥ 3600	139748190	28	≥ 3600	124918468
brock800-4	23	≥ 3600	133857528	24	≥ 3600	144247348	27	≥ 3600	127834010
c-fat200-1	12*	0	975	12*	4	58324	12*	170	2025883
c-fat200-2	24*	0	7308	24*	5	115832	24*	226	3827925
c-fat200-5	58*	3112	86024721	58	≥ 3600	104935293	58	≥ 3600	108945815
c-fat500-1	14*	1	2712	14*	115	364617	14	≥ 3600	6098258
c-fat500-2	26*	1	31068	26*	126	818322	26	≥ 3600	14272751
c-fat500-5	64	≥ 3600	84968699	64	≥ 3600	94102915	64	≥ 3600	92359122
c-fat500-10	126	≥ 3600	39813170	126	≥ 3600	45937780	126	≥ 3600	45046647
C125.9	40	≥ 3600	165580704	49	≥ 3600	159562046	56	≥ 3600	172499878
C250.9	49	≥ 3600	131071734	59	≥ 3600	121221452	67	≥ 3600	118891127
C1000.9	63	≥ 3600	86340711	73	≥ 3600	95156344	81	≥ 3600	89623119
gen400-p0.9-55	57	≥ 3600	107671535	66	≥ 3600	104998011	77	≥ 3600	104332374
gen400-p0.9-65	57	≥ 3600	123654827	65	≥ 3600	105148691	75	≥ 3600	100728355
gen400-p0.9-75	56	≥ 3600	115238978	69	≥ 3600	92913241	79	≥ 3600	109864417
hamming6-2	32*	506	26461612	32	≥ 3600	244753572	37	≥ 3600	261840105
hamming6-4	6*	0	4709	8*	1	71069	10*	9	849851
hamming8-2	128	≥ 3600	39716014	128	≥ 3600	43138327	128	≥ 3600	50079738
hamming8-4	16	≥ 3600	237558610	18	≥ 3600	222683938	22	≥ 3600	230542048
hamming10-2	512	≥ 3600	3595516	512	≥ 3600	3790553	512	≥ 3600	3877853
hamming10-4	32	≥ 3600	146893539	43	≥ 3600	132802297	64	≥ 3600	54961531
johnson8-2-4	5*	0	1666	8*	0	12837	9*	0	104984
johnson8-4-4	14*	110	11542436	18	≥ 3600	350491163	22	≥ 3600	342248079
johnson16-2-4	10	≥ 3600	625712305	15	≥ 3600	480893056	17	≥ 3600	497459524
johnson32-2-4	21	≥ 3600	318645985	27	≥ 3600	270404308	32	≥ 3600	267621112
keller4	15	≥ 3600	247583422	20	≥ 3600	207711375	22	≥ 3600	258859895
keller5	29	≥ 3600	122027776	39	≥ 3600	95885696	46	≥ 3600	89880382
MANN-a9	26*	66	5585820	36*	2	106834	36*	278	25470013
MANN-a27	234	≥ 3600	79044110	351	≥ 3600	7146812	351	≥ 3600	10158168
MANN-a45	660	≥ 3600	19339018	990	≥ 3600	1022834	990	≥ 3600	1283088
p-hat300-1	10*	14	665249	12*	1111	40704167	14	≥ 3600	128042727
p-hat300-2	29	≥ 3600	167764775	35	≥ 3600	162883168	41	≥ 3600	154569677
p-hat300-3	42	≥ 3600	145501695	51	≥ 3600	145528614	57	≥ 3600	139965092
p-hat700-1	13*	1887	55769755	14	≥ 3600	110462323	16	≥ 3600	98797915
p-hat700-2	49	≥ 3600	116066244	58	≥ 3600	116785628	65	≥ 3600	117405227
p-hat700-3	69	≥ 3600	105454118	81	≥ 3600	105553105	93	≥ 3600	97553599
p-hat1500-1	14	≥ 3600	83137273	16	≥ 3600	77843491	17	≥ 3600	71616718
p-hat1500-2	74	≥ 3600	82521849	86	≥ 3600	83606200	96	≥ 3600	80774894
p-hat1500-3	98	≥ 3600	81882477	119	≥ 3600	77654872	133	≥ 3600	72234293
san200-0.7-2	24	≥ 3600	441219398	36	≥ 3600	395072520	48	≥ 3600	330336652
san200-0.9-1	90	≥ 3600	107493877	125	≥ 3600	35590748	125	≥ 3600	39843163
san200-0.9-2	62	≥ 3600	101186509	73	≥ 3600	95434310	70	≥ 3600	118663294
san200-0.9-3	49	≥ 3600	151525669	54	≥ 3600	135610532	63	≥ 3600	136277860
san400-0.9-1	59	≥ 3600	82032873	62	≥ 3600	98221391	71	≥ 3600	106470241
sanr200-0.9	47	≥ 3600	138079311	54	≥ 3600	145898461	60	≥ 3600	132831001

* optimal

```

function basicPlex( $U, K$ )
1.  while  $U \neq \emptyset$ 
2.    if  $|K| + |U| \leq \mathit{max}$ 
3.      return
4.    end
5.     $K = K \cup \{v\}; U = U \setminus \{v\}$  for some  $v \in U$ 
6.     $U' := \{u \in U : K \cup \{u\} \text{ is } ak\text{-plex}\}$ 
7.    basicPlex( $U', K$ )
8.  end
9.  if  $|K| > \mathit{max}$ 
10.    $\mathit{max} = |K|$ 
11. end
12. return

```

Figure 5.10: Basic k -plex Algorithm

may exist graphs which require the algorithm to examine an exponential number of cliques. In practice, though, pruning can dramatically reduce the runtime.

The basic clique algorithm has many variants (60; 63; 65; 72). Many researchers have focused on improving the pruning strategy using the coloring bound. In particular, a coloring heuristic provides an upper bound on $\omega(G[U])$. The coloring bound has the potential to prune a larger portion of the search tree because $\chi(G[U]) \leq |U|$. This approach generalizes to improve **basicPlex** by using the heuristics in Sections 5.2 to bound $\omega_k(G[U])$. Figure 5.11 shows a function which uses co- k -plex coloring to prune the search tree.

In Section 5.2.1 we described two Integer Co- k -plex Coloring Heuristics, **ICCH1** and **ICCH2**, for approximating $\chi_k(G[U])$. Let **k -plex1a** denote the function obtained by using **ICCH1** to execute Line 2 of **k -plex1**. The function **ICCH1** is shown in Figure 5.3. Let **k -plex1b** denote the function obtained by using **ICCH2** to execute Line 2 of **k -plex1**. The function **ICCH2** is shown in Figure 5.4.

```

function  $k$ -plex1( $U, K$ )
1.  while  $U \neq \emptyset$ 
2.    Compute  $\tilde{\chi}_k(G[U]) \geq \chi_k(G[U])$ 
3.    if  $|K| + \tilde{\chi}_k(G[U]) \leq \mathit{max}$ 
4.      return
5.    end
6.     $K = K \cup \{v\}$ ;  $U = U \setminus \{v\}$  for some  $v \in U$ 
7.     $U' := \{u \in U : K \cup \{u\} \text{ is a } k\text{-plex}\}$ 
8.     $k$ -plex1( $U', K$ )
9.  end
10. if  $|K| > \mathit{max}$ 
11.    $\mathit{max} = |K|$ 
12. end
13. return

```

Figure 5.11: k -plex Algorithm

In Section 5.2.2 we described two Fractional Co- k -plex Coloring Heuristics, **FCCH1** and **FCCH2**, for approximating $\chi_k(G[U])$. Let **k -plex1c** denote the function obtained by using **FCCH1** to execute Line 2 of **k -plex1**. Let **k -plex1d** denote the function obtained by using **FCCH2** to execute Line 2 of **k -plex1**.

To find a maximum k -plex in G , we run the **LB1** heuristic on G to obtain an initial value for the global variable max . Next we make the function call to **k -plex1a**(V, \emptyset), **k -plex1b**(V, \emptyset), **k -plex1c**(V, \emptyset), or **k -plex1d**(V, \emptyset). Tables 5.7 - 5.10 contain computational results obtained by running these algorithms on the DIMACS benchmark graphs. Each algorithm was run for one hour.

5.4.2 Algorithm Type 2

This subsection describes a second type of exact algorithm for finding maximum k -plexes. The algorithm is based on the following idea of Östergård (54). Let $V =$

Table 5.7: k -plex1a Results

G	$\omega_2(G)$	seconds	BBN	$\omega_3(G)$	seconds	BBN	$\omega_4(G)$	seconds	BBN
brock200-1	25	≥ 3600	86030174	28	≥ 3600	95147581	31	≥ 3600	97664910
brock200-2	13*	289	8663613	15	≥ 3600	100542983	17	≥ 3600	90143057
brock200-4	19	≥ 3600	102282008	22	≥ 3600	106907189	25	≥ 3600	98966956
brock400-2	27	≥ 3600	95110220	31	≥ 3600	88619566	35	≥ 3600	81344425
brock400-4	33	≥ 3600	51472394	33	≥ 3600	74724985	36	≥ 3600	80938337
brock800-2	23	≥ 3600	94857693	26	≥ 3600	81559009	29	≥ 3600	71154628
brock800-4	23	≥ 3600	96369941	25	≥ 3600	90097273	29	≥ 3600	72735746
c-fat200-1	12*	2	873	12*	27	57730	12*	922	1960167
c-fat200-2	24*	3	5269	24*	28	109070	24*	909	3385277
c-fat200-5	58	≥ 3600	19298000	58	≥ 3600	24247513	58	≥ 3600	28799458
c-fat500-1	14*	32	2293	14*	1580	357420	14	≥ 3600	545917
c-fat500-2	26*	33	20601	26*	1617	787649	26	≥ 3600	1224327
c-fat500-5	64	≥ 3600	14631858	64	≥ 3600	21078075	64	≥ 3600	24930408
c-fat500-10	126	≥ 3600	5104395	126	≥ 3600	7643111	126	≥ 3600	9068983
C125.9	42	≥ 3600	63076397	49	≥ 3600	79939042	56	≥ 3600	86375809
C250.9	50	≥ 3600	55392820	59	≥ 3600	60836513	67	≥ 3600	62347611
C1000.9	69	≥ 3600	31155586	80	≥ 3600	30906202	91	≥ 3600	25238173
gen400-p0.9-55	59	≥ 3600	49418395	71	≥ 3600	36435391	80	≥ 3600	46290499
gen400-p0.9-65	66	≥ 3600	26145966	78	≥ 3600	25302636	86	≥ 3600	28527938
gen400-p0.9-75	75	≥ 3600	16646961	84	≥ 3600	24505892	91	≥ 3600	27923471
hamming6-2	32*	0	0	32	≥ 3600	92535097	37	≥ 3600	119263227
hamming6-4	6*	0	3668	8*	1	59533	10*	15	701425
hamming8-2	128*	0	0	128	≥ 3600	14422543	128	≥ 3600	20007766
hamming8-4	16	≥ 3600	158903409	18	≥ 3600	149846604	22	≥ 3600	157055208
hamming10-2	512*	1	0	512	≥ 3600	434296	512	≥ 3600	456014
hamming10-4	43	≥ 3600	44661342	64	≥ 3600	21254123	64	≥ 3600	33084666
johnson8-2-4	5*	0	1585	8*	0	12378	9*	1	104804
johnson8-4-4	14*	138	7755953	18	≥ 3600	191111049	22	≥ 3600	172931195
johnson16-2-4	10	≥ 3600	418302911	16	≥ 3600	275029061	18	≥ 3600	280703595
johnson32-2-4	21	≥ 3600	323578720	32	≥ 3600	127870041	36	≥ 3600	139455728
keller4	15	≥ 3600	147002319	20	≥ 3600	128108327	22	≥ 3600	169102280
keller5	31	≥ 3600	86174831	39	≥ 3600	98084379	46	≥ 3600	93468119
MANN-a9	26*	123	4111457	36*	6	102896	36*	739	25470013
MANN-a27	234	≥ 3600	78820556	351	≥ 3600	383569	351	≥ 3600	781334
MANN-a45	660	≥ 3600	18866263	990	≥ 3600	18029	990	≥ 3600	53068
p-hat300-1	10*	33	562727	12*	2827	39631513	14	≥ 3600	54618899
p-hat300-2	30	≥ 3600	77146967	35	≥ 3600	84162645	41	≥ 3600	84779804
p-hat300-3	42	≥ 3600	73906134	50	≥ 3600	70787196	57	≥ 3600	70408792
p-hat700-1	13*	3186	46290951	14	≥ 3600	56967864	16	≥ 3600	43437614
p-hat700-2	50	≥ 3600	51487369	58	≥ 3600	56760785	65	≥ 3600	61159187
p-hat700-3	70	≥ 3600	42921661	82	≥ 3600	46670755	92	≥ 3600	48056462
p-hat1500-1	14	≥ 3600	64200197	16	≥ 3600	54760864	17	≥ 3600	46539732
p-hat1500-2	74	≥ 3600	40645458	86	≥ 3600	47106186	98	≥ 3600	37702129
p-hat1500-3	107	≥ 3600	16720124	122	≥ 3600	30607204	137	≥ 3600	25319618
san200-0.7-2	26	≥ 3600	247380139	36	≥ 3600	368232192	48	≥ 3600	301494773
san200-0.9-1	90	≥ 3600	64534714	125	≥ 3600	5514998	125	≥ 3600	6899702
san200-0.9-2	71	≥ 3600	28455841	105	≥ 3600	7916622	105	≥ 3600	9512515
san200-0.9-3	50	≥ 3600	60230554	62	≥ 3600	36447308	65	≥ 3600	52422167
san400-0.9-1	102	≥ 3600	5427342	150	≥ 3600	2818053	200	≥ 3600	1606559
sanr200-0.9	48	≥ 3600	57674935	56	≥ 3600	62350486	63	≥ 3600	48460533

* optimal

Table 5.8: k -plex1b Results

G	$\omega_2(G)$	seconds	BBN	$\omega_3(G)$	seconds	BBN	$\omega_4(G)$	seconds	BBN
brock200-1	25	≥ 3600	69161245	28	≥ 3600	74047699	31	≥ 3600	76443907
brock200-2	13*	347	8655872	15	≥ 3600	78758942	17	≥ 3600	77611816
brock200-4	19	≥ 3600	83379665	22	≥ 3600	84435853	25	≥ 3600	81410084
brock400-2	27	≥ 3600	79503226	31	≥ 3600	72526576	35	≥ 3600	67993634
brock400-4	33	≥ 3600	41435291	33	≥ 3600	63082448	36	≥ 3600	68610667
brock800-2	23	≥ 3600	76380258	26	≥ 3600	62187146	29	≥ 3600	59527523
brock800-4	23	≥ 3600	77313428	25	≥ 3600	70818151	29	≥ 3600	60106034
c-fat200-1	12*	3	865	12*	30	57730	12*	1020	1960167
c-fat200-2	24*	3	5029	24*	32	109143	24*	1050	3385287
c-fat200-5	58	≥ 3600	14304248	58	≥ 3600	17982184	58	≥ 3600	21121009
c-fat500-1	14*	33	2308	14*	1701	357500	14	≥ 3600	522142
c-fat500-2	26*	34	20682	26*	1781	783956	26	≥ 3600	1162013
c-fat500-5	64	≥ 3600	10796547	64	≥ 3600	15457652	64	≥ 3600	18009810
c-fat500-10	126	≥ 3600	3977561	126	≥ 3600	5712426	126	≥ 3600	6343703
C125.9	42	≥ 3600	48114789	49	≥ 3600	62425904	56	≥ 3600	67231585
C250.9	50	≥ 3600	44235096	59	≥ 3600	47320128	67	≥ 3600	47691224
C1000.9	69	≥ 3600	26979405	80	≥ 3600	24032891	91	≥ 3600	19359650
gen400-p0.9-55	59	≥ 3600	41787235	71	≥ 3600	29644490	80	≥ 3600	40201337
gen400-p0.9-65	66	≥ 3600	21715889	78	≥ 3600	20199799	86	≥ 3600	23625879
gen400-p0.9-75	75	≥ 3600	13498174	84	≥ 3600	19004764	91	≥ 3600	22944583
hamming6-2	32*	0	0	32	≥ 3600	73053164	36	≥ 3600	96335439
hamming6-4	6*	0	3650	8*	2	59787	10*	17	699306
hamming8-2	128*	0	0	128	≥ 3600	6833516	128	≥ 3600	13907811
hamming8-4	16	≥ 3600	124321999	18	≥ 3600	119121603	22	≥ 3600	129103474
hamming10-2	512*	1	0	512	≥ 3600	145167	512	≥ 3600	348239
hamming10-4	43	≥ 3600	35220491	64	≥ 3600	15056227	64	≥ 3600	27378559
johnson8-2-4	5*	0	1584	8*	0	12385	9*	1	104810
johnson8-4-4	14*	176	8018473	18	≥ 3600	150199235	22	≥ 3600	151926832
johnson16-2-4	10	≥ 3600	382064672	16	≥ 3600	231091629	18	≥ 3600	239417405
johnson32-2-4	21	≥ 3600	293812276	32	≥ 3600	104729724	36	≥ 3600	113914581
keller4	15	≥ 3600	119019307	20	≥ 3600	100734057	22	≥ 3600	138097548
keller5	31	≥ 3600	69020984	39	≥ 3600	84262597	46	≥ 3600	84210063
MANN-a9	26*	156	3935491	36*	4	46660	36*	915	25470013
MANN-a27	234	≥ 3600	70015613	351	≥ 3600	219473	351	≥ 3600	524874
MANN-a45	660	≥ 3600	21797551	990	≥ 3600	12475	990	≥ 3600	35814
p-hat300-1	10*	41	562708	12*	3238	39638895	14	≥ 3600	46803014
p-hat300-2	30	≥ 3600	61132951	35	≥ 3600	68747655	41	≥ 3600	68314947
p-hat300-3	42	≥ 3600	58400176	50	≥ 3600	55985983	57	≥ 3600	54496873
p-hat700-1	13	≥ 3600	44795502	14	≥ 3600	48920440	16	≥ 3600	37009440
p-hat700-2	50	≥ 3600	43620842	58	≥ 3600	48534119	65	≥ 3600	52567570
p-hat700-3	70	≥ 3600	37660188	82	≥ 3600	41443956	92	≥ 3600	41606985
p-hat1500-1	14	≥ 3600	46650067	16	≥ 3600	43939635	17	≥ 3600	36602990
p-hat1500-2	74	≥ 3600	39134197	86	≥ 3600	35705377	98	≥ 3600	29410335
p-hat1500-3	107	≥ 3600	11583397	122	≥ 3600	22363784	137	≥ 3600	17768382
san200-0.7-2	26	≥ 3600	212477345	36	≥ 3600	309410312	48	≥ 3600	288909214
san200-0.9-1	90	≥ 3600	54941877	125	≥ 3600	3496383	125	≥ 3600	4838807
san200-0.9-2	71	≥ 3600	22006508	105	≥ 3600	5041182	105	≥ 3600	6842531
san200-0.9-3	50	≥ 3600	46924868	62	≥ 3600	26131072	65	≥ 3600	43126175
san400-0.9-1	102	≥ 3600	3922872	150	≥ 3600	1909788	200	≥ 3600	1085227
sanr200-0.9	48	≥ 3600	46925391	56	≥ 3600	48282533	63	≥ 3600	39527458

* optimal

Table 5.9: k -plex1c Results

G	$\omega_2(G)$	seconds	BBN	$\omega_3(G)$	seconds	BBN	$\omega_4(G)$	seconds	BBN
brock200-1	25	≥ 3600	10054924	28	≥ 3600	9610060	31	≥ 3600	11595841
brock200-2	13*	1778	7722362	15	≥ 3600	15728716	17	≥ 3600	15883075
brock200-4	19	≥ 3600	12056663	22	≥ 3600	11842251	24	≥ 3600	13308843
brock400-2	27	≥ 3600	3298972	31	≥ 3600	2506819	35	≥ 3600	3084792
brock400-4	33	≥ 3600	2879018	33	≥ 3600	2769768	36	≥ 3600	3339363
brock800-2	22	≥ 3600	847946	26	≥ 3600	687075	29	≥ 3600	719475
brock800-4	22	≥ 3600	846155	25	≥ 3600	708185	29	≥ 3600	771036
c-fat200-1	12*	3	802	12*	41	57612	12*	1397	1958425
c-fat200-2	24*	3	2050	24*	60	96754	24	≥ 3600	1586893
c-fat200-5	58*	836	444241	58	≥ 3600	3960477	58	≥ 3600	5319030
c-fat500-1	14*	34	2060	14*	1796	356744	14	≥ 3600	427000
c-fat500-2	26*	39	10177	26*	2368	754350	26	≥ 3600	797974
c-fat500-5	64*	1579	557081	64	≥ 3600	2800459	64	≥ 3600	3453142
c-fat500-10	126	≥ 3600	327032	126	≥ 3600	974543	126	≥ 3600	1193712
C125.9	42	≥ 3600	10708047	49	≥ 3600	17227347	56	≥ 3600	18474262
C250.9	50	≥ 3600	4488455	59	≥ 3600	6659440	67	≥ 3600	6746445
C1000.9	69	≥ 3600	298746	80	≥ 3600	159248	91	≥ 3600	378692
gen400-p0.9-55	59	≥ 3600	2474705	71	≥ 3600	1657601	80	≥ 3600	2755943
gen400-p0.9-65	66	≥ 3600	1909277	78	≥ 3600	2027657	86	≥ 3600	2433789
gen400-p0.9-75	75	≥ 3600	1438210	84	≥ 3600	1214538	91	≥ 3600	2274896
hamming6-2	32*	0	0	32	≥ 3600	6160422	36	≥ 3600	44987310
hamming6-4	6*	0	3380	8*	3	58663	10*	33	693982
hamming8-2	128*	0	0	128	≥ 3600	636791	128	≥ 3600	2835717
hamming8-4	16	≥ 3600	9945892	18	≥ 3600	9748498	18	≥ 3600	10199713
hamming10-2	512*	1	0	512	≥ 3600	7508	512	≥ 3600	29602
hamming10-4	43	≥ 3600	323816	64	≥ 3600	370717	64	≥ 3600	236250
johnson8-2-4	5*	0	1585	8*	0	12337	9*	2	104679
johnson8-4-4	14*	475	6389736	18	≥ 3600	48544486	22	≥ 3600	52307238
johnson16-2-4	10	≥ 3600	37768568	16	≥ 3600	34069665	18	≥ 3600	34721894
johnson32-2-4	21	≥ 3600	1976217	32	≥ 3600	1911159	36	≥ 3600	1913056
keller4	15	≥ 3600	18263136	20	≥ 3600	17714412	22	≥ 3600	20281149
keller5	31	≥ 3600	766363	37	≥ 3600	741184	45	≥ 3600	818500
MANN-a9	26*	395	3240597	36*	15	100969	36*	1733	25470013
MANN-a27	234	≥ 3600	3053292	351	≥ 3600	78758	351	≥ 3600	253074
MANN-a45	660	≥ 3600	28446	990	≥ 3600	7035	990	≥ 3600	20406
p-hat300-1	10*	139	500766	12	≥ 3600	12816637	14	≥ 3600	12577276
p-hat300-2	30	≥ 3600	7335988	35	≥ 3600	6439794	40	≥ 3600	8083792
p-hat300-3	42	≥ 3600	5279160	50	≥ 3600	5693325	57	≥ 3600	5957872
p-hat700-1	12	≥ 3600	2617164	13	≥ 3600	2557821	16	≥ 3600	2516929
p-hat700-2	50	≥ 3600	1176955	58	≥ 3600	1407568	65	≥ 3600	1459008
p-hat700-3	70	≥ 3600	750652	82	≥ 3600	1007772	92	≥ 3600	1001573
p-hat1500-1	13	≥ 3600	418932	14	≥ 3600	407346	16	≥ 3600	418855
p-hat1500-2	73	≥ 3600	198544	86	≥ 3600	246326	98	≥ 3600	245532
p-hat1500-3	107	≥ 3600	127330	122	≥ 3600	169405	137	≥ 3600	167369
san200-0.7-2	26	≥ 3600	12473403	36	≥ 3600	16047112	48	≥ 3600	16009322
san200-0.9-1	90	≥ 3600	9748246	125	≥ 3600	970390	125	≥ 3600	1705032
san200-0.9-2	71	≥ 3600	4524615	105	≥ 3600	1196715	105	≥ 3600	2153725
san200-0.9-3	50	≥ 3600	7414271	62	≥ 3600	5709518	65	≥ 3600	8130115
san400-0.9-1	102	≥ 3600	440889	150	≥ 3600	398976	200	≥ 3600	231849
sanr200-0.9	48	≥ 3600	6400789	56	≥ 3600	7604646	63	≥ 3600	8343819

* optimal

Table 5.10: k -plex1d Results

G	$\omega_2(G)$	seconds	BBN	$\omega_3(G)$	seconds	BBN	$\omega_4(G)$	seconds	BBN
brock200-1	25	≥ 3600	22042601	28	≥ 3600	29648861	31	≥ 3600	34480695
brock200-2	13*	724	7713075	15	≥ 3600	37753625	17	≥ 3600	37853872
brock200-4	19	≥ 3600	31441620	22	≥ 3600	32118801	25	≥ 3600	37191920
brock400-2	27	≥ 3600	26906867	31	≥ 3600	11381556	35	≥ 3600	18660437
brock400-4	33	≥ 3600	10569863	33	≥ 3600	15191176	36	≥ 3600	22886705
brock800-2	23	≥ 3600	27085224	26	≥ 3600	13448585	29	≥ 3600	20637652
brock800-4	22	≥ 3600	26435168	25	≥ 3600	18628602	29	≥ 3600	20654583
c-fat200-1	12*	3	795	12*	42	57612	12*	1526	1958425
c-fat200-2	24*	3	1950	24*	66	96819	24	≥ 3600	1625686
c-fat200-5	58*	952	451391	58	≥ 3600	3673990	58	≥ 3600	5526134
c-fat500-1	14*	36	2055	14*	2032	356784	14	≥ 3600	386900
c-fat500-2	26*	41	10065	26*	2673	750513	26	≥ 3600	763007
c-fat500-5	64*	1390	541520	64	≥ 3600	3591629	64	≥ 3600	4671016
c-fat500-10	126	≥ 3600	299492	126	≥ 3600	1170531	126	≥ 3600	1526963
C125.9	42	≥ 3600	12766210	49	≥ 3600	28041660	56	≥ 3600	33598258
C250.9	50	≥ 3600	13726640	59	≥ 3600	20668136	67	≥ 3600	25607644
C1000.9	69	≥ 3600	5633304	80	≥ 3600	8642487	91	≥ 3600	7890577
gen400-p0.9-55	59	≥ 3600	12130553	71	≥ 3600	10851682	80	≥ 3600	19362117
gen400-p0.9-65	66	≥ 3600	4687226	78	≥ 3600	6320575	86	≥ 3600	10058105
gen400-p0.9-75	75	≥ 3600	2190827	84	≥ 3600	5679756	91	≥ 3600	9510820
hamming6-2	32*	0	0	32	≥ 3600	19260671	36	≥ 3600	51079990
hamming6-4	6*	0	3318	8*	3	58844	10*	31	691944
hamming8-2	128*	0	0	128	≥ 3600	1406306	128	≥ 3600	3980741
hamming8-4	16	≥ 3600	58435201	18	≥ 3600	56389907	18	≥ 3600	66294428
hamming10-2	512*	2	0	512	≥ 3600	17456	512	≥ 3600	42844
hamming10-4	43	≥ 3600	10111165	64	≥ 3600	3458007	64	≥ 3600	1400994
johnson8-2-4	5*	0	1584	8*	0	12327	9*	2	104809
johnson8-4-4	14*	358	6615020	18	≥ 3600	66381658	22	≥ 3600	68509972
johnson16-2-4	10	≥ 3600	206213634	16	≥ 3600	118169547	18	≥ 3600	132917128
johnson32-2-4	21	≥ 3600	160322819	32	≥ 3600	41091745	36	≥ 3600	58056738
keller4	15	≥ 3600	53809489	20	≥ 3600	42595921	22	≥ 3600	69265197
keller5	31	≥ 3600	21190863	38	≥ 3600	28178139	46	≥ 3600	43147077
MANN-a9	26*	395	3069378	36*	8	32661	36*	1795	25470013
MANN-a27	234	≥ 3600	38989932	351*	1122	13811	351	≥ 3600	207346
MANN-a45	660	≥ 3600	6919084	990	≥ 3600	3340	990	≥ 3600	16406
p-hat300-1	10*	61	500713	12	≥ 3600	27407867	14	≥ 3600	27853654
p-hat300-2	30	≥ 3600	20482503	35	≥ 3600	19834902	40	≥ 3600	28555545
p-hat300-3	42	≥ 3600	21195393	50	≥ 3600	23081981	57	≥ 3600	26938876
p-hat700-1	13	≥ 3600	25801496	14	≥ 3600	27416647	16	≥ 3600	22091696
p-hat700-2	50	≥ 3600	12855694	58	≥ 3600	19662734	65	≥ 3600	27101622
p-hat700-3	70	≥ 3600	10431068	82	≥ 3600	19707826	92	≥ 3600	20137759
p-hat1500-1	14	≥ 3600	24034286	15	≥ 3600	22434996	17	≥ 3600	18534805
p-hat1500-2	74	≥ 3600	9391184	86	≥ 3600	12608953	98	≥ 3600	13499197
p-hat1500-3	107	≥ 3600	2577031	122	≥ 3600	9936541	137	≥ 3600	9480218
san200-0.7-2	26	≥ 3600	103258863	36	≥ 3600	187794647	48	≥ 3600	180647265
san200-0.9-1	90	≥ 3600	31677870	125	≥ 3600	745219	125	≥ 3600	1320173
san200-0.9-2	71	≥ 3600	6274707	105	≥ 3600	929194	105	≥ 3600	1840564
san200-0.9-3	50	≥ 3600	13959883	62	≥ 3600	8019546	65	≥ 3600	17277391
san400-0.9-1	102	≥ 3600	396823	150	≥ 3600	302872	200	≥ 3600	187270
sanr200-0.9	48	≥ 3600	15017490	56	≥ 3600	17695417	63	≥ 3600	16797344

* optimal

$\{v_1, \dots, v_n\}$ and $S_i = \{v_i, \dots, v_n\}$. The basic clique algorithm in Figure 5.9 first searches for the largest clique in S_1 which contains v_1 . It then finds the largest clique in S_2 containing v_2 , and so on. Östergård suggests reversing this order. In other words, first search S_n for the largest clique containing v_n . Then search for the largest clique in S_{n-1} containing v_{n-1} , and so on. Let $c(i)$ be the size of the largest clique in S_i . Clearly, $c(n) = 1$ and $c(1) = \omega(G)$. Moreover, $c(i) \in \{c(i+1), c(i+1) + 1\}$ for $i = 1, \dots, n-1$.

Figure 5.12 shows Östergård's maximum clique algorithm. The search order allows for the following new pruning strategy. Let U be the candidate set for an arbitrary iteration, and define $i = \min\{j : v_j \in U\}$. We can deduce that $U \subseteq S_i$ and hence $\omega_k(G[U]) \leq c(i)$. This new bound is used in Line 10 in Figure 5.12.

Östergård's algorithm adapts to find maximum k -plexes with two modifications. First, let $c_k(i)$ denote the cardinality of a largest k -plex in S_i . Second, define the candidate set associated with the k -plex K to be

$$U = \{v \in V \setminus K : K \cup \{v\} \text{ is a } k\text{-plex}\}.$$

Figure 5.13 shows the resulting k -plex algorithm ***k-plex2***. Table 5.11 contains computational results obtained by running ***k-plex2*** on the DIMACS benchmark graphs.

```

function OsterClique( $U, K$ )
1.  if  $|U| = 0$ 
2.    if  $|K| > max$ 
3.       $max = |K|$ 
4.       $found = true$ 
5.    end
6.    return
7.  end
8.  while  $U \neq \emptyset$ 
9.    if  $|K| + |U| \leq max$ 
10.     return
11.   end
12.    $i = \min\{j : v_j \in U\}$ 
13.   if  $|K| + c(i) \leq max$ 
14.     return
15.   end
16.    $U = U \setminus \{v_i\}$ 
17.   OsterClique( $U \cap N(v_i), K \cup \{v_i\}$ )
18.   if  $found = true$ 
19.     return
20.   end
21. end
22. return

function findClique
23.  $max = 0$ 
24. for  $1 = n$  down to 1
25.    $found = false$ 
26.   OsterClique( $S_i \cap N(v_i), \{v_i\}$ )
27. end
28.  $c(i) = max$ 
29. return

```

Figure 5.12: Östergård's Clique Algorithm

```

function OsterPlex( $U, K$ )
1.  if  $|U| = 0$ 
2.    if  $|K| > max$ 
3.       $max = |K|$ 
4.       $found = true$ 
5.    end
6.    return
7.  end
8.  while  $U \neq \emptyset$ 
9.    if  $|K| + |U| \leq max$ 
10.     return
11.   end
12.    $i = \min\{j : v_j \in U\}$ 
13.   if  $|K| + c_k(i) \leq max$ 
14.     return
15.   end
16.    $K = K \cup \{v_i\}; U = U \setminus \{v_i\}$ 
17.    $U' := \{u \in U : K \cup \{u\} \text{ is } ak\text{-plex}\}$ 
18.   OsterPlex( $U', K$ )
19.   if  $found = true$ 
20.     return
21.   end
22. end
23. return

function  $k$ -plex2
24.  $max = 0$ 
25. for  $1 = n$  down to 1
26.    $found = false$ 
27.   OsterPlex( $S_i, \{v_i\}$ )
28. end
29.  $c_k(i) = max$ 
30. return

```

Figure 5.13: Östergård's Algorithm Adapted for k -plexes

Table 5.11: k -plex2 Results

G	$\omega_2(G)$	seconds	BBN	$\omega_3(G)$	seconds	BBN	$\omega_4(G)$	seconds	BBN
brock200-1	23	≥ 3600	791928771	24	≥ 3600	806817406	26	≥ 3600	833090023
brock200-2	13*	64	19636411	15	≥ 3600	1075870150	16	≥ 3600	1065615731
brock200-4	19	≥ 3600	881361988	20	≥ 3600	931846630	21	≥ 3600	943179921
brock400-2	22	≥ 3600	759862798	23	≥ 3600	804857686	23	≥ 3600	781885801
brock400-4	22	≥ 3600	758652153	22	≥ 3600	794063906	24	≥ 3600	771681337
brock800-2	18	≥ 3600	702311556	20	≥ 3600	721916977	21	≥ 3600	714624762
brock800-4	19	≥ 3600	719342183	20	≥ 3600	709513722	21	≥ 3600	715586808
c-fat200-1	12*	0	3758	12*	0	124483	12*	18	4463378
c-fat200-2	24*	0	2222	24*	0	32128	24*	3	792394
c-fat200-5	58*	0	2566	58*	0	11320	58*	1	137141
c-fat500-1	14*	0	19845	14*	8	1185321	14*	1234	134916615
c-fat500-2	26*	0	10463	26*	2	270561	26*	92	12897124
c-fat500-5	64*	0	6382	64*	1	59959	64*	8	1050683
c-fat500-10	126*	0	10373	126*	0	34033	126*	4	344858
C125.9	34	≥ 3600	601019873	37	≥ 3600	607049688	39	≥ 3600	647773425
C250.9	36	≥ 3600	571490135	37	≥ 3600	643968505	38	≥ 3600	662112226
C1000.9	33	≥ 3600	491059839	37	≥ 3600	495615493	41	≥ 3600	495436467
gen400-p0.9-55	34	≥ 3600	565601499	36	≥ 3600	599925462	39	≥ 3600	617236444
gen400-p0.9-65	36	≥ 3600	557748615	38	≥ 3600	587965932	40	≥ 3600	614450751
gen400-p0.9-75	34	≥ 3600	578953836	37	≥ 3600	599770569	42	≥ 3600	562373641
hamming6-2	32*	0	1161	32*	1	203776	40*	951	226269962
hamming6-4	6*	0	4533	8*	0	37119	10*	1	395739
hamming8-2	128*	1	23244	102	≥ 3600	203665707	44	≥ 3600	556953372
hamming8-4	16*	58	7996453	16	≥ 3600	1129944679	18	≥ 3600	1014983524
hamming10-2	512*	95	461740	100	≥ 3600	193939903	44	≥ 3600	471073063
hamming10-4	22	≥ 3600	527683421	16	≥ 3600	778357773	18	≥ 3600	746764413
johnson8-2-4	5*	0	2628	8*	0	10489	9*	0	151051
johnson8-4-4	14*	0	40913	18*	35	14015342	21	≥ 3600	1246612573
johnson16-2-4	10	≥ 3600	1892276637	15	≥ 3600	1256161458	18	≥ 3600	1379453092
johnson32-2-4	21	≥ 3600	843926109	24	≥ 3600	766290563	25	≥ 3600	875412190
keller4	15*	913	284120627	21	≥ 3600	886421569	16	≥ 3600	1088296129
keller5	15	≥ 3600	835222972	22	≥ 3600	662317050	16	≥ 3600	809663179
MANN-a9	26*	0	53402	36*	2	376168	36*	141	36511981
MANN-a27	235	≥ 3600	27043381	351	≥ 3600	24808187	351	≥ 3600	55749297
MANN-a45	661	≥ 3600	4140618	990	≥ 3600	3661523	990	≥ 3600	18719092
p-hat300-1	10*	5	1561134	12*	416	128854671	13	≥ 3600	1152133728
p-hat300-2	29	≥ 3600	673936016	27	≥ 3600	696210402	27	≥ 3600	752178202
p-hat300-3	31	≥ 3600	621034466	32	≥ 3600	663097551	31	≥ 3600	720400620
p-hat700-1	13*	383	90762293	13	≥ 3600	890061519	13	≥ 3600	931592519
p-hat700-2	31	≥ 3600	537122370	30	≥ 3600	618173686	29	≥ 3600	666390060
p-hat700-3	31	≥ 3600	532975341	29	≥ 3600	601725177	29	≥ 3600	636046239
p-hat1500-1	12	≥ 3600	639194212	14	≥ 3600	637343144	13	≥ 3600	666758477
p-hat1500-2	27	≥ 3600	460519275	29	≥ 3600	477421254	31	≥ 3600	474585487
p-hat1500-3	33	≥ 3600	431618259	33	≥ 3600	459920187	33	≥ 3600	473209365
san200-0.7-2	24	≥ 3600	874307781	34	≥ 3600	722461564	46	≥ 3600	607532865
san200-0.9-1	67	≥ 3600	335935223	125*	964	121912591	39	≥ 3600	621612154
san200-0.9-2	42	≥ 3600	433667092	47	≥ 3600	468417446	43	≥ 3600	566888709
san200-0.9-3	42	≥ 3600	490907696	36	≥ 3600	655264592	38	≥ 3600	645037070
san400-0.9-1	64	≥ 3600	285116552	48	≥ 3600	439741324	36	≥ 3600	614651437
sanr200-0.9	33	≥ 3600	599788142	37	≥ 3600	617210758	40	≥ 3600	629276404

* optimal

Table 5.12: Results Summary

Algorithm	$k = 2$	$k = 3$	$k = 4$	Total
basicPlex	13	8	5	26
<i>k-plex1a</i>	14	8	5	27
<i>k-plex1b</i>	13	8	5	26
<i>k-plex1c</i>	15	7	4	26
<i>k-plex1d</i>	15	8	4	27
<i>k-plex2</i>	19	14	11	44

5.5 Conclusions

This chapter describes combinatorial algorithms for finding maximum k -plexes in a graph. Section 5.2 focuses on co- k -plex coloring heuristics which are used as an upper bound on the k -plex number. Section 5.2 contains four co- k -plex coloring heuristics, two integral and two fractional. Section 5.3 discusses a heuristic for finding maximum k -plexes. This heuristic provides a lower bound on the k -plex number.

Section 5.4 describes exact algorithms for finding maximum k -plexes. Table 5.12 summarizes the number of instances solved to optimality by each exact algorithm. The first five are based on a basic clique algorithm. These algorithms perform similarly within the hour time limit, though this type of algorithm appears to benefit from the upper and lower bound heuristics.

The final exact algorithm adapts Östergård’s clique algorithm. Clearly, ***k-plex2*** dominates all other algorithms with respect to number of optimal solutions found. Moreover, ***k-plex2*** appears to converge quickly, when it converges at all. On the other hand, when ***k-plex2*** does not converge, the final solution can be far from optimal.

k-plex2’s superior performance might be a consequence of the difficulties associated with approximating $\chi_k(G)$. While Type 1 algorithms are improved by using

heuristics, the algorithms spend time at each branch and bound node to approximate $\chi_k(G[U])$ for the candidate set U . Unfortunately, $\chi_k(G)$ could be an inaccurate bound on $\omega_k(G)$ in general. The ***k*-plex2** algorithm spends no time estimating $\chi_k(G)$ but benefits from the bound obtained using the c_k array.

Chapter 6

Co- k -plex Polynomials

This chapter generalizes the independence polynomial. The resulting family of polynomials carries combinatorial information on a class of independence systems defined over the vertex set of a finite graph.

6.1 Introduction

The graphs discussed in this chapter are finite and simple. Refer to Diestel (25) for standard graph terminology. For a graph $G = (V, E)$ and $S \subseteq V$, let $G[S]$ be the subgraph induced by S . Given $v \in V$, define $N_G(v) = \{u \in V : vu \in E\}$ and $N_G[v] = N_G(v) \cup \{v\}$. Let $\Delta(G) = \max\{|N_G(v)| : v \in V\}$. A set of pairwise nonadjacent vertices in G defines an *independent set*. Let \mathcal{I}^G denote the set of all independent sets in G . Gutman and Harary (33) associated the following polynomial with G :

$$I(G; x) = \sum_{I \in \mathcal{I}^G} x^{|I|}.$$

This *independence polynomial* carries information about the enumerative structure of independent sets in G . More precisely, the coefficient of x^i in $I(G; x)$ is exactly the

number of independent sets of cardinality i in G . The independence polynomial has been studied in a number of papers (2; 12; 13; 14; 20; 34; 35; 37; 40; 41; 42). Levit and Mandrescu offer a survey (43).

Recall that an *independence system* defined over V is a nonempty collection of subsets of V which is closed under set inclusion. Fix an integer $k \geq 1$ and let $S \subseteq V$ satisfy

$$|N_G[v] \cap S| \leq k \quad \text{for all } v \in S.$$

The set S is known as a *co- k -plex* in G . Let \mathcal{I}_k^G denote the set of co- k -plexes in G . Notice that $\mathcal{I}_1^G = \mathcal{I}^G$ and that \mathcal{I}_k^G defines an independence system on V for all integers $k \geq 1$. The graph G is associated with the family of *co- k -plex polynomials* defined as follows:

$$I_k(G; x) = \sum_{I \in \mathcal{I}_k^G} x^{|I|} \quad k = 1, 2, 3, \dots$$

Let s_i^k be the coefficient of x^i in $I_k(G; x)$; that is, s_i^k denotes the number of co- k -plexes of cardinality i in G . Clearly, $s_i^k = 0$ for all $i > \alpha_k(G)$, where $\alpha_k(G)$ denotes the size of a largest co- k -plex in G . Notice also that $S \in \mathcal{I}_k^G \Rightarrow S \in \mathcal{I}_{k+1}^G$. Consequently, $s_i^k \leq s_i^{k+1}$ for any k and $I_k(G; x) = I_{k+1}(G; x)$ whenever $k > \Delta(G)$. In fact, $I_k(G; x) = (1 + x)^{|V(G)|}$ for all $k > \Delta(G)$ because every subset of vertices is a co- k -plex in this situation.

This chapter is organized as follows. Section 6.2 explores the effect certain graph operations have on the corresponding polynomials and derives recursive relationships for the co-2-plex polynomial. Section 6.3 computes the co-2-plex polynomials for

various structured graphs. Section 6.4 summarizes the results and suggests some future research directions.

6.2 Graph Operations and Recursive Relationships

This section investigates the effect certain graph operations have on the corresponding polynomials and derives recursive relationships for the co-2-plex polynomial. The first operation we study is graph union. The graph $G_1 \cup G_2$ has vertex set $V(G_1) \cup V(G_2)$ and edge set $E(G_1) \cup E(G_2)$. The graph $G = \bigcup_{i=1}^r G_i$ is defined inductively.

Lemma 15. *Fix an integer $k \geq 1$. If $G = \bigcup_{i=1}^r G_i$, then $I_k(G; x) = \prod_{i=1}^r I_k(G_i; x)$.*

Proof. The result is trivial for $r = 1$, so we first analyze the case where $r = 2$. Notice that, given co- k -plexes $S_1 \subseteq G_1$ and $S_2 \subseteq G_2$, the set $S = S_1 \cup S_2$ is a co- k -plex in $G_1 \cup G_2$. Moreover, every co- k -plex in $G_1 \cup G_2$ can be constructed this way. It follows that the coefficient of x^i in the polynomial $I_k(G_1 \cup G_2; x)$ equals the sum of the product of all coefficients of pairs y^l in $I_k(G_1; y)$ and z^m in $I_k(G_2; z)$ such that $l + m = i$. In other words, $I_k(G_1 \cup G_2; x)$ is the product of $I_k(G_1; x)$ and $I_k(G_2; x)$. Now if $r > 2$, repeat this argument using graphs $\bigcup_{i=1}^{j-1} G_i$ and G_j for each $j = 3, \dots, r$, □

The join of graphs G_1, G_2 is the graph $G = G_1 + G_2$, where $V(G) = V(G_1) \cup V(G_2)$ and $E(G) = E(G_1) \cup E(G_2) \cup \{v_1 v_2 : v_1 \in V(G_1), v_2 \in V(G_2)\}$. It is well-known (2; 33; 37) that $I_1(G; x) = I_1(G_1; x) + I_1(G_2; x) - 1$. The following result generalizes this formula to the case where $k = 2$.

Theorem 17. *Let G_1 and G_2 be graphs with n_1 and n_2 vertices, respectively. If $G = G_1 + G_2$, then*

$$I_2(G; x) = I_2(G_1; x) + I_2(G_2; x) + \sum_{j=0}^2 \left[\binom{n_1 + n_2}{j} - \binom{n_1}{j} - \binom{n_2}{j} \right] x^j.$$

Proof. The sum $I_2(G_1; x) + I_2(G_2; x)$ accounts for all co-2-plexes entirely contained in either G_1 or G_2 . However, this sum fails to count any co-2-plex S which intersects both G_1 and G_2 . Observe that $|S| \leq 2$ for any such co-2-plex. For if not, then without loss of generality, choose $v, w \in S \cap G_1$ and $z \in S \cap G_2$. We deduce that $v, w \in N_G(z)$ from the definition of graph join. Therefore, $|N_G[z] \cap S| > 2$, which contradicts that S is a co-2-plex.

Now observe that every set of two or less vertices defines a co-2-plex. G contains $\sum_{j=0}^2 \binom{n_1+n_2}{j}$ such sets, $\sum_{j=0}^2 [\binom{n_1}{j} + \binom{n_2}{j}]$ of which are entirely contained in either G_1 or G_2 . It follows that $I_2(G; x) = I_2(G_1; x) + I_2(G_2; x) + \sum_{j=0}^2 \left[\binom{n_1+n_2}{j} - \binom{n_1}{j} - \binom{n_2}{j} \right] x^j$. We mention that the final term in the formula for $I_2(G; x)$ adjusts for double counting the empty set as a co-2-plex. \square

Given graphs G_1, G_2 with vertices $v_i \in G_i$, $i = 1, 2$, the *edge join* graph $G = (G_1, v_1) \ominus (G_2, v_2)$ is formed by adding an edge joining v_1 and v_2 .

Theorem 18. *If $G = (G_1, v_1) \ominus (G_2, v_2)$, then $I_2(G; x)$ satisfies the following recursive formula*

$$I_2(G; x) = x^2 \cdot I_2(G_1 - N[v_1]; x) \cdot I_2(G_2 - N[v_2]; x) + I_2(G_1; x) \cdot I_2(G_2 - v_2; x) +$$

$$I_2(G_2; x) \cdot I_2(G_1 - v_1; x) - I_2(G_1 - v_1; x) \cdot I_2(G_2 - v_2; x).$$

Proof. We consider three classes of co-2-plexes in G and determine the cardinality of each class separately. Let S be a co-2-plex in G , and suppose $v_1, v_2 \in S$. Since v_1v_2 is an edge in G , we know that $N_{G_i}(v_i) \cap S = \emptyset$ for $i = 1, 2$. Therefore, this class contributes

$$x^2 \cdot I_2(G - \{N[v_1] \cup N[v_2]\}; x)$$

to the total. Notice that $G - \{N[v_1] \cup N[v_2]\} = \{G_1 - N[v_1]\} \cup \{G_2 - N[v_2]\}$ so that Lemma 15 implies $x^2 \cdot I_2(G - \{N[v_1] \cup N[v_2]\}; x) = x^2 \cdot I_2(G_1 - N[v_1]; x) \cdot I_2(G_2 - N[v_2]; x)$.

The class where $v_2 \notin S$ contributes $I_2(G - v_2; x)$ to the total, and Lemma 15 implies that $I_2(G - v_2; x) = I_2(G_1; x) \cdot I_2(G_2 - v_2; x)$. Similarly, the class where $v_1 \notin S$ contributes $I_2(G - v_1; x)$ to the total, and Lemma 15 implies that $I_2(G - v_1; x) = I_2(G_2; x) \cdot I_2(G_1 - v_1; x)$. Observe that the last two classes both include the case where $v_1, v_2 \notin S$. We adjust by subtracting $I_2(G_1 - v_1; x) \cdot I_2(G_2 - v_2; x)$ from the total. \square

In Section 6.3, we use recursive relationships to compute the co-2-plex polynomials of certain families of graphs. The following result is an example of one such relationship.

Theorem 19. *If $K \subseteq G$ is complete, i.e. consists of pairwise adjacent vertices, then*

$I_2(G; x)$ satisfies the following recursion:

$$I_2(G; x) = \sum_{i=0}^2 \sum_{S \subseteq K, |S|=i} x^i \cdot I_2(G - K \cup N[S]; x) + \sum_{v \in K, w \in N(v) \setminus K} x^2 \cdot I_2(G - K \cup N[v] \cup N[w]; x).$$

Proof. We consider four classes of co-2-plexes in G and determine the cardinality of each class separately. The first class consists of those co-2-plexes S such that $S \cap K = \emptyset$. This class contributes

$$I_2(G - K; x)$$

to the total. The second class satisfies $|S \cap K| = 2$. In this case, there exists a pair $u, v \in S \cap K$. Since $uv \in E(G)$, we deduce that $N(u) \cap S = \{v\}$ and $N(v) \cap S = \{u\}$.

It follows that this class contributes

$$x^2 \cdot \sum_{u, v \in K} I_2(G - \{N[u] \cup N[v]\}; x)$$

to the total.

Since $|S \cap K| \leq 2$, it remains to consider those co-2-plexes satisfying $|S \cap K| = 1$. Let $\{v\} = S \cap K$. Notice that either $S \cap N(v) = \emptyset$ or $S \cap N(v) = \{w\}$ for some $w \in V(G) \setminus K$. There are

$$x \cdot \sum_{v \in K} I_2(G - N[v]; x)$$

of the former and

$$x^2 \cdot \sum_{v \in K, w \in N(v) \setminus K} I_2(G - \{N[v] \cup N[w]\}; x)$$

of the latter. We obtain the given formula by collecting and rearranging terms. \square

Corollary 6. *Given $v \in V(G)$, $I_2(G; x)$ satisfies the following recursion*

$$I_2(G; x) = I_2(G - v; x) + x \cdot I_2(G - N[v]; x) + x^2 \cdot \sum_{w \in N(v)} I_2(G - N[v] \cup N[w]; x).$$

Proof. Let $K = \{v\}$ and apply the previous result. \square

6.3 Examples

This section computes the co- k -plex polynomials for various structured graphs. Most of the results deal with co-2-plex polynomials. First notice that an edgeless graph G on n vertices satisfies $I_k(G; x) = (1 + x)^n$ for all $k \geq 1$. A complete graph K on n vertices satisfies $I_k(G; x) = \sum_{i=1}^k \binom{n}{i} x^i$ for all $k \geq 1$.

Given an integer $k \geq 1$, the graph H is a k -claw if there exists a vertex $u \in V(H)$ such that $V(H) \setminus u = N(u)$, $N(u)$ is a co- k -plex, and $|N(u)| \geq \max\{3, k\}$.

Example 1. *If H be a k -claw on n vertices, then*

$$I_k(H; x) = (1 + x)^{n-1} + \sum_{i=0}^{k-1} \binom{n-1}{i} x^{i+1}.$$

Proof. The term $(1+x)^{n-1}$ counts all co- k -plexes which exclude the center vertex u .

The term $\sum_{i=0}^{k-1} \binom{n-1}{i} x^{i+1}$ counts all those co- k -plexes which include u . \square

An r -partite graph can be partitioned into r independent sets. The complete r -partite graph K_{n_1, \dots, n_r} has all possible edges between distinct partition classes, where n_1, \dots, n_r are the cardinalities of the partition classes.

Example 2.

$$I_2(K_{n_1, \dots, n_r}; x) = \sum_{i=1}^r (1+x)^{n_i} + \sum_{i=1}^{r-1} \sum_{j=0}^2 \left[\binom{\sum_{p=1}^i n_p + n_{i+1}}{j} - \binom{\sum_{p=1}^i n_p}{j} - \binom{n_{i+1}}{j} \right] x^j.$$

Proof. The proof is by induction on the number of partition classes r . When $r = 1$, the formula reduces to the correct value of $(1+x)^{n_1}$. Now let $r > 1$ and assume that the formula holds for all $(r-1)$ -partite graphs. We will show that it holds for the r -partite graph K_{n_1, \dots, n_r} . The induction hypothesis implies that

$$I_2(K_{n_1, \dots, n_{r-1}}; x) = \sum_{i=1}^{r-1} (1+x)^{n_i} + \sum_{i=1}^{r-2} \sum_{j=0}^2 \left[\binom{\sum_{p=1}^i n_p + n_{i+1}}{j} - \binom{\sum_{p=1}^i n_p}{j} - \binom{n_{i+1}}{j} \right] x^j.$$

Notice that K_{n_1, \dots, n_r} can be constructed by performing a graph join between $K_{n_1, \dots, n_{r-1}}$ and an independent set of cardinality n_r . Theorem 17 implies that

$$I_2(K_{n_1, \dots, n_r}; x) = \sum_{i=1}^r (1+x)^{n_i} + \sum_{i=1}^{r-2} \sum_{j=0}^2 \left[\binom{\sum_{p=1}^i n_p + n_{i+1}}{j} - \binom{\sum_{p=1}^i n_p}{j} - \binom{n_{i+1}}{j} \right] x^j +$$

$$\sum_{j=0}^2 \left[\binom{\sum_{p=1}^{r-1} n_p + n_r}{j} - \binom{\sum_{p=1}^{r-1} n_p}{j} - \binom{n_r}{j} \right].$$

Upon simplifying, we obtain the desired formula. □

Notice that if $n_i = n$ for all i , then we obtain

$$I_2(K_{n,\dots,n}; x) = r(1+x)^n + \sum_{i=1}^{r-1} \sum_{j=0}^k \left[\binom{in+n}{j} - \binom{in}{j} - \binom{n}{j} \right] x^j.$$

Our next example is the path. The path P^n has vertex set $\{v_1, \dots, v_n\}$ and edge set $\{v_i v_{i+1} \mid 1 \leq i \leq n-1\}$. It is easy to see that

$$I_2(P^0; x) = 1, \quad I_2(P^1; x) = 1 + x, \quad \text{and} \quad I_2(P^2; x) = (1+x)^2.$$

By convention, $I_2(P^n; x) = 0$ for all $n < 0$.

Example 3. For $n \geq 3$, $I_2(P^n; x)$ satisfies the following recursion

$$I_2(P^n; x) = \sum_{i=1}^3 x^{i-1} I_2(P^{n-i}; x).$$

Proof. Notice that $P^n - v_n = P^{n-1}$, $P^n - N[v_n] = P^n - \{v_n, v_{n-1}\} = P^{n-2}$, and $P^n - \{N[v_n] \cup N[v_{n-1}]\} = P^n - \{v_n, v_{n-1}, v_{n-2}\} = P^{n-3}$. Applying Corollary 1 using v_n gives the following

$$I_2(P^n; x) = I_2(P^{n-1}; x) + x \cdot I_2(P^{n-2}; x) + x^2 \cdot I_2(P^{n-3}; x).$$

□

The coefficients of $I_2(P^n; x)$ have some additional interpretations. For example, given an integer $j \geq 1$, define $K_j = \{j, j+1, j+2\}$, written *mod* n . The polytope $P = \{x \in R^n : \sum_{j=1}^{n-2} x(K_j) \leq 2, 0 \leq x \leq 1\}$ is the convex hull of incidence vectors for co-2-plexes in P^n . Therefore, the coefficient of x^i in $I_2(P^n; x)$ is the number of vertices of the polytope P indexed by vectors with i nonzero components. The coefficients of $I_2(P^n; x)$ have also been studied in the context of binary strings with no triplet of 1's.

Our next example is the chordless cycle. The cycle C^n , where $n \geq 3$, has vertex set $\{v_1, \dots, v_n\}$ and edge set $\{v_1v_n\} \cup \{v_iv_{i+1} \mid 1 \leq i \leq n-1\}$. By convention, $I_2(C^n; x) = 0$ for all $n < 0$.

Example 4. For $n \geq 3$, $I_2(C^n; x)$ satisfies the following recursion

$$I_2(C^n; x) = I_2(P^{n-1}; x) + xI_2(P^{n-3}; x) + 2x^2I_2(P^{n-4}; x).$$

Proof. Notice that $C^n - v_n = P^{n-1}$, $C^n - N[v_n] = P^{n-3}$, and $C^n - \{N[v_n] \cup N[v_{n-1}]\} = C^n - \{N[v_n] \cup N[v_1]\} = P^{n-4}$. Applying Corollary 1 using v_n gives the following

$$I_2(C^n; x) = I_2(P^{n-1}; x) + x \cdot I_2(P^{n-3}; x) + x^2 \cdot I_2(P^{n-4}; x) + x^2 \cdot I_2(P^{n-4}; x).$$

□

It has also been shown that the polytope $P' = \{x \in R^n : \sum_{j=1}^n x(K_j) \leq 2, 0 \leq x \leq 1\}$ is the convex hull of incidence vectors of co-2-plexes in C^n . Therefore, the coefficient of x^i in $I_2(C^n; x)$ is the number of vertices of P' indexed by vectors with i nonzero components.

A connected and acyclic graph defines a tree. A spider, S_v , is a tree with exactly one vertex v of degree greater than or equal to three.

Example 5. Let S_v be a spider such that v has degree d . The graph $S - v$ consists of disjoint paths P^{n_1}, \dots, P^{n_r} and $I_2(S_v; x)$ satisfies the following recursion

$$I_2(S_v; x) = \prod_{i=1}^r I_2(P^{n_i}; x) + x \cdot \left[1 + x \cdot \sum_{j=1}^d \frac{I_2(P^{n_j-2}; x)}{I_2(P^{n_j-1}; x)} \right] \cdot \prod_{i=1}^r I_2(P^{n_i-1}; x).$$

Proof. The first part of the claim follows from the fact that $\Delta[S - v] \leq 2$. To obtain the recursive formula, we apply Corollary 1. By Lemma 15,

$$I_2(S_v - v; x) = \prod_{i=1}^r I_2(P^{n_i}; x).$$

Lemma 15 also implies that

$$I_2(S_v - N[v]; x) = \prod_{i=1}^r I_2(P^{n_i-1}; x).$$

It remains to calculate $\sum_{w \in N(v)} I_2(S_v - \{N[v] \cup N[w]\})$. Each neighbor of v belongs

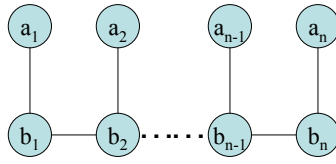


Figure 6.1: The centipede W_n .

to exactly one of the paths P^{n_1}, \dots, P^{n_r} . Therefore, Lemma 15 implies that

$$\sum_{w \in N(v)} I_2(S_v - \{N[v] \cup N[w]\}) = \sum_{j=1}^d \left[\frac{I_2(P^{n_j-2}; x)}{I_2(P^{n_j-1}; x)} \prod_{i=1}^r I_2(P^{n_i-1}; x) \right].$$

The desired formula is now obtained by plugging these values into the formula from Corollary 1. □

A centipede, W_n , is a tree with vertex set $A \cup B = \{a_1, \dots, a_n\} \cup \{b_1, \dots, b_n\}$ and edge set $\{a_i b_i : 1 \leq i \leq n\} \cup \{b_i b_{i+1} : 1 \leq i \leq n-1\}$. See Figure 6.1. It is easy to see that

$$I_2(W_0; x) = 1, \quad I_2(W_1; x) = (1+x)^2, \quad \text{and} \quad I_2(W_2; x) = 1 + 4x + 6x^2 + 2x^3.$$

By convention, $I_2(W_n; x) = 0$ for all $n < 0$.

Example 6. For $n \geq 3$, $I_2(W_n; x)$ satisfies the following recursion

$$I_2(W_n; x) = (1+x) \cdot [x^2 \cdot I_2(W_{n-3}; x) + (1+x)^2 \cdot I_2(W_{n-2}; x) + I_2(W_{n-1}; x) - (1+x) \cdot I_2(W_{n-2}; x)].$$

Proof. Consider the centipede shown in Figure 6.1. Let $W_n[a_n, b_n]$ denote the sub-

graph induced by $\{a_n, b_n\}$. Notice that $W_n = (W_n[a_n, b_n], b_n) \ominus (W_{n-1}, b_{n-1})$. Therefore, applying Theorem 18, first compute $I_2(W_n[a_n, b_n] - N_{W_n[a_n, b_n]}[b_n]; x) \cdot I_2(W_{n-1} - N_{W_{n-1}}[b_{n-1}]; x)$. Observe that $I_2(W_n[a_n, b_n] - N_{W_n[a_n, b_n]}[b_n]; x) = I_2(\emptyset; x) = 1$. Now since $W_{n-1} - N_{W_{n-1}}[b_{n-1}] = W_{n-2}[a_{n-2}] \cup W_{n-3}$, Lemma 15 implies

$$I_2(W_{n-1} - N_{W_{n-1}}[b_{n-1}]; x) = I_2(W_{n-2}[a_{n-2}]; x) \cdot I_2(W_{n-3}; x) = (1+x) \cdot I_2(W_{n-3}; x).$$

Now compute $I_2(W_n[a_n, b_n] - b_n; x)$ and $I_2(W_{n-1} - b_{n-1}; x)$. Clearly, $I_2(W_n[a_n, b_n] - b_n; x) = I_2(W_n[a_n]; x) = (1+x)$. Since $W_{n-1} - b_{n-1} = W_{n-1}[a_{n-1}] \cup W_{n-2}$, apply Lemma 15 to obtain $I_2(W_{n-1} - b_{n-1}; x) = (1+x) \cdot I_2(W_{n-2}; x)$. In addition, we know that $I_2(W_n[a_n, b_n]; x) = (1+x)^2$, so the formula from Theorem 18 gives

$$\begin{aligned} I_2(W_n; x) &= x^2 \cdot (1+x) \cdot I_2(W_{n-3}; x) + (1+x)^2 \cdot (1+x) \cdot I_2(W_{n-2}; x) + \\ &I_2(W_{n-1}; x) \cdot (1+x) - (1+x)^2 \cdot I_2(W_{n-2}; x). \end{aligned}$$

Upon simplifying, we obtain the desired formula. □

6.4 Conclusions

This chapter introduces a generalization of the independence polynomial. The resulting family of polynomials carries combinatorial information on co- k -plexes in a finite graph. The results in this chapter include theorems relating graph operations and co- k -plex polynomials and examples computing the co-2-plex polynomials for various structured graphs.

Chapter 7

Conclusions and Future Work

This thesis analyzes the polyhedral, algorithmic, and enumerative properties of co- k -plexes. Co- k -plexes are degree-bounded, vertex-induced subgraphs of a finite graph $G = (V, E)$, and they form a family of independence systems over V . Co- k -plexes arise naturally as stable set relaxations. Many results in this thesis are generalized theorems and algorithms from the stable set literature.

Chapter 3 focuses on composition of stable set polyhedra, or co-1-plex polyhedra, by generalizing a theorem of Barahona and Mahjoub concerning the composition of stable set polyhedra. Barahona and Mahjoub's theorem extends to the case where the separating set consists of a complete graph minus an edge. A further extension of Theorem 1 to more general cut-sets would be beneficial since composition can be applied recursively.

In other words, G can be decomposed into subgraphs G_1, \dots, G_m such that the defining system for each $P(G_i)$ is known. For example, decompose G into a set of perfect graphs. The defining systems for each $P(G_i)$ can then be composed to define $P(G)$. Another idea is to construct $P(G)$ starting from the leaves of a tree or

branch decomposition. These approaches have the potential to characterize the stable set polytope for graphs which admit a structured decomposition, but they require a more general form of Theorem 1.

Generalizing Theorem 1 might require techniques different from the lift and project method of Barahona and Mahjoub. Finding a \tilde{G}_k and F_k with the correct structure appears to be difficult. A subtle requirement is that $\tilde{G}_k[\tilde{C}]$ has to have exactly $|\tilde{C}|$ affinely independent maximum stable sets. Otherwise, the matrix A is not invertible and Lemma 4 fails. Without this restriction, Theorem 1 would have held for any cut-set which partitions into two cliques. While there exist many graphs $\tilde{G}_k[\tilde{C}]$ with exactly $|\tilde{C}|$ affinely independent maximum stable sets, the inequalities which define F_k must also involve the w_i vertices in a structured way. This structure would most likely involve extending the results of Section 3.2 to prevent the projection step from becoming too complicated.

Chapter 4 contains a polyhedral study of the co- k -plex polytope, including the derivation of five facet classes. The facets are related to 2-plexes, cycles, wheels, webs, and the claw. In addition, Chapter 4 presents a characterization of 2-plex clutter matrices A for which the polytope $\{x \in \mathbf{R}_+^n \mid Ax \leq 2, x \leq 1\}$ is integral. It turns out that 2-plex clutter matrices can be tested for this property in polynomial time. The final section of the chapter introduces co- k -plex coloring and attempts a combinatorial concept of k -plex perfection. It contains examples of k -plex perfect graphs and discusses some difficulties in generalizing certain properties of graph perfection.

Future work includes finding additional co- k -plex analogues for results on stable set polyhedra. For example, it seems likely that webs induce facets for general co- k -plex polyhedra. However, proving the validity of any such inequality can be difficult. In particular, generalizing Lemma 8 appears to be an interesting and challenging combinatorial problem. If the form and validity of general web inequalities can be shown, the matrix constructed in Theorem 5 would most likely verify the dimension of the corresponding faces.

Another avenue of research is a computational study on the strength and efficiency of the facets introduced in Section 4.3. It would especially be interesting to study the k -claw facets because the structure of k -claws is quite simple. Given a vertex v , finding a k -claw amounts to searching $N(v)$ for any co- k -plex on at least $\min\{3, k\}$ vertices. This structure might lead to straightforward separation algorithms.

A third possibility for future research is to explore alternative notions of k -plex perfection. Chapter 4 introduces two types of k -plex perfection: polyhedral and combinatorial. These definitions do not always coincide, and both characterizations fail to generalize many properties of graph perfection. It would be interesting to see if any k -plex perfection characterization has both nice polyhedral and combinatorial properties.

Chapter 5 describes combinatorial algorithms for finding maximum k -plexes in a graph. This problem is computationally equivalent to finding maximum co- k -plexes in the complement graph. Section 5.2 focuses on co- k -plex coloring heuristics. Co- k -

plex colorings provide an upper bound on the k -plex number. Section 5.3 discusses a heuristic for finding maximum k -plexes. This heuristic provides a lower bound on the k -plex number. Section 5.4 develops exact algorithms for finding maximum k -plexes.

The material in Chapter 5 suggests many avenues for future research. For example, the exact value for the co- k -plex chromatic number remains unknown for many of the DIMACS graphs, so future work includes designing an exact co- k -plex coloring algorithm. It would also be interesting to see how much the co- k -plex coloring heuristics could be improved. Another possibility is to design other heuristics for finding k -plexes in a graph.

Chapter 6 introduces a generalization of the independence polynomial. The resulting family of polynomials carries combinatorial information on co- k -plexes in a finite graph. The results in this chapter include theorems relating graph operations and co- k -plex polynomials and examples computing the co-2-plex polynomials for various structured graphs. Future research can involve further theorems and computations on the co- k -plex polynomial of structured graphs.

In addition, researchers (44; 61) study the first derivative of graph polynomials, e.g. the matching polynomial, independence polynomial, and characteristic polynomial. For example, it is well-known that $\frac{d}{dx}I_1(G; x) = \sum_{v \in V(G)} I_1(G - N[v]; x)$. An example of a result dealing with first derivatives of co- k -plex polynomials is the following. Given integers $k, n \geq 1$, recall from Section 6.3 that $I_{k+1}(K_n; x) = \sum_{j=0}^{k+1} \binom{n}{j} x^j$.

Therefore,

$$\frac{d}{dx}I_{k+1}(K_n; x) = \sum_{j=0}^{k+1} j \cdot \binom{n}{j} x^{j-1} = n \cdot \sum_{j=0}^k \binom{n-1}{j} x^j = n \cdot I_k(K_{n-1}; x),$$

and this simplifies to

$$\frac{d}{dx}I_{k+1}(K_n; x) = n \cdot I_k(K_{n-1}; x).$$

It would be interesting to obtain additional results relating the first derivatives of co- k -plex polynomials.

Overall, attempting to generalize stable set properties can both succeed and fail. For instance, the co- k -plex facets offer nice examples of successful analogues for stable set facets, and small changes to Östergård's algorithm produce a fast exact co- k -plex algorithm. On the other hand, the difficulties encountered concerning combinatorial perfection and the validity of the web inequalities for general k show that this approach can also fail.

On a higher level, this thesis demonstrates the benefit of unifying constructs such as independence systems. In the end, many results in the stable set literature follow from the axioms of an independence system. With this in mind, it is worth the effort to determine if any new results hold for a larger class of set systems. This approach can reduce the fragmentation of knowledge in the combinatorial optimization community, and researchers might then avoid the time-consuming demands of rediscovery each time a new constraint is added to a well-studied problem.

This view suggests the possibility of studying relaxations of other independence systems. In general, one could study the family of subsets containing a bounded number of circuits with bounded intersection. As in this thesis, these families of independence systems can be analyzed from polyhedral, algorithmic, and enumerative perspectives.

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