

Graph-dependent Covering Arrays and LYM Inequalities

ELIZABETH JANE MALTAIS

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Department of Mathematics and Statistics
Faculty of Science
University of Ottawa

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Abstract

The problems we study in this thesis are all related to covering arrays. Covering arrays are combinatorial designs, widely used as templates for efficient interaction-testing suites. They have connections to many areas including extremal set theory, design theory, and graph theory. We define and study several generalizations of covering arrays, and we develop a method which produces an infinite family of LYM inequalities for graph-intersecting collections. A common theme throughout is the dependence of these problems on graphs.

Our main contribution is an extremal method yielding LYM inequalities for H -intersecting collections, for every undirected graph H . Briefly, an H -intersecting collection is a collection of packings (or partitions) of an n -set in which the classes of every two distinct packings in the collection intersect according to the edges of H .

We define “ F -following” collections which, by definition, satisfy a LYM-like inequality that depends on the arcs of a “follow” digraph F and a permutation-counting technique. We fully characterize the correspondence between “ F -following” and “ H -intersecting” collections. This enables us to apply our inequalities to H -intersecting collections.

For each graph H , the corresponding inequality inherently bounds the maximum number of columns in a covering array with alphabet graph H . We use this feature to derive bounds for covering arrays with the alphabet graphs S_3 (the star on three vertices) and K_3^{loop} (K_3 with loops). The latter improves a known bound for classical covering arrays of strength two.

We define covering arrays on column graphs and alphabet graphs which generalize covering arrays on graphs. The column graph encodes which pairs of columns must be H -intersecting, where H is a given alphabet graph. Optimizing covering arrays on column graphs and alphabet graphs is equivalent to a graph-homomorphism problem to a suitable family of targets which generalize qualitative independence graphs. When H is the two-vertex tournament, we give constructions and bounds for covering arrays on directed column graphs.

FOR arrays are the broadest generalization of covering arrays that we consider. We define FOR arrays to encompass testing applications where constraints must be considered, leading to forbidden, optional, and required interactions of any strength. We model these testing problems using a hypergraph. We investigate the existence of FOR arrays, the compatibility of their required interactions, critical systems, and binary relational systems that model the problem using homomorphisms.

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Chapter 1

Introduction

Covering arrays are combinatorial designs, widely used as templates for efficient interaction-testing suites. They emerged as a generalization of orthogonal arrays, and they have connections to many interesting problems in several areas of mathematics including design theory, graph theory, extremal set theory, information theory, finite fields, coding theory, and geometry.

In this thesis, we consider several different problems, all of which are related to covering arrays.

The contributions of this thesis fall into three categories:

1. LYM inequalities for alphabet graphs
2. covering arrays on column and alphabet graphs
3. FOR arrays

We begin with a brief review, and then explain how these topics are related to covering arrays.

A (classical) **covering array**, denoted $CA(n; t, k, v)$, is an $n \times k$ array with symbols from the **alphabet** $\{1, \dots, v\}$. The parameter t denotes the **strength** of the array. In every t columns of a $CA(n; t, k, v)$, each t -tuple of symbols in $\{1, \dots, v\}^t$ must appear in at least one row. In other words, every set of t columns must **cover** every possible t -tuple of symbols. The **covering array number**, denoted $CAN(t, k, v)$, is the smallest integer n for which there exists a $CA(n; t, k, v)$. The **column number**, denoted $CAK(n; t, v)$, is the maximum k for which there exists a $CA(n; t, k, v)$.

The quantities CAK and CAN are related: $\text{CAN}(t, k, v) = \min\{n : k \leq \text{CAK}(n; t, v)\}$ and $\text{CAK}(n; t, v) = \max\{k : n \geq \text{CAN}(t, k, v)\}$. For fixed t and v , knowing $\text{CAN}(t, k, v)$ for all k is equivalent to knowing $\text{CAK}(n; t, v)$ for all n .

In terms of their applications to interaction-testing, covering arrays provide a template for the efficient design of test suites for objects comprised of several configurable components. Each column of a covering array corresponds to a component, and the symbols in each column represent v different options for that component. Each row corresponds to a test, that is, an assignment of one option to each factor. The strength of the covering array guarantees that all configurations of options, for every t components, are each tested at least once.

There are many situations where such test suites are desirable. Covering arrays are used extensively in software testing, hardware testing, drug-interaction testing, and material sciences; see [12, 28, 37] and the references therein for more on these applications. Adaptations have been made to covering arrays in order to suit the needs of more specialized testing applications; for some such examples, see [11, 19, 21, 22, 43, 46, 49].

In terms of testing applications, the covering array number $\text{CAN}(t, k, v)$ represents the optimal size of a test suite for a fixed number of factors k , a fixed number of configurations v , and a fixed strength t . In practice, however, efficient testing does not need to be optimal — reasonably small covering arrays suffice.

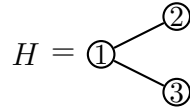
The question of knowing the exact values of covering array numbers is an interesting question in extremal set theory. For fixed t and v , we only know the answer (for all k) for one family of covering array numbers: the binary covering array numbers of strength 2 [32, 34, 50] (see Theorem 2.3.3). For all n , we have $\text{CAK}(n; 2, 2) = \binom{n-1}{\lfloor n/2 \rfloor - 1}$ and equivalently, for all k , we have $\text{CAN}(2, k, 2) = \min\{n : k \leq \binom{n-1}{\lfloor n/2 \rfloor - 1}\}$.

We extend the definition of covering arrays of strength 2 to include an alphabet graph. Alphabet graphs make it possible to customize the pairs of symbols that are covered between any two columns of a covering array.

An **alphabet graph** is an undirected graph H having no parallel edges, but may contain loops. A **covering array with alphabet graph** H , denoted $\text{CA}(n; 2, k, H)$, is an $n \times k$ array with symbols from the alphabet $V(H)$; for any column indices $i < j$, for each edge $ab \in E(H)$ there exist row indices $r, r' \in \{1, \dots, n\}$ such that $C_i(r) = a$ and $C_j(r) = b$ and $C_i(r') = b$ and $C_j(r') = a$.

The **covering array number**, denoted $\text{CAN}(2, k, H)$, is the minimum n for which there exists a $\text{CA}(n; 2, k, H)$. The **column number**, denoted $\text{CAK}(n; 2, H)$, is the maximum k for which there exists a $\text{CA}(n; 2, k, H)$.

Example 1 Consider the alphabet graph H , pictured below. The array beside H is a $\text{CA}(7; 2, 4, H)$. Since $\{1, 2\}$ and $\{1, 3\}$ are edges of H , in any pair of two distinct columns, we need to see each of the symbol pairs $(1, 2)$, $(1, 3)$, $(2, 1)$, and $(3, 1)$ in at least one row. Since $\{2, 3\} \notin E(H)$, we do not care whether the symbol pairs $(2, 3)$ or $(3, 2)$ appear in any rows.



1	1	2	2
1	2	3	3
1	3	1	2
2	1	1	3
3	2	1	1
2	3	2	1
3	1	3	1

Example 2 If H is the complete graph K_2 , then the columns of a $\text{CA}(n; 2, k, K_2)$ correspond to an antichain of subsets of $\{1, \dots, n\}$ as follows: From each column C_i , define a subset $A_i \subseteq \{1, \dots, n\}$ given by $A_i = \{r : C_i(r) = 1\}$. For any $i < j$, there exist row indices $r, r' \in [n]$ such that $C_i(r) = 0$ and $C_j(r) = 1$ and $C_i(r') = 1$ and $C_j(r') = 0$. It follows that the sets A_i and A_j satisfy $A_j \not\subseteq A_i$ and $A_i \not\subseteq A_j$, thus, the collection $\mathcal{A} = \{A_1, \dots, A_k\}$ is an antichain. Sperner's Theorem [54] gives the maximum size of an antichain which, rephrased in terms of covering arrays, says $\text{CAK}(n; 2, K_2) = \binom{n}{\lfloor n/2 \rfloor}$.

Example 3 If H is the complete graph K_2 with a loop on one of its vertices, then the columns of a $\text{CA}(n; 2, k, H)$ correspond to an intersecting antichain. The size of a maximum intersecting antichain is known [8, 52]. In terms of covering arrays, this result can be rephrased as $\text{CAK}(n; 2, H) = \binom{n}{\lfloor n/2 \rfloor + 1}$.

Example 4 If H is the complete graph K_2 with a loop on each of its vertices, then a $\text{CA}(n; 2, k, H)$ is simply a binary covering array of strength 2, and it is known that $\text{CAK}(n; 2, 2) = \binom{n-1}{\lfloor n/2 \rfloor - 1}$, as mentioned above.

Examples 2, 3, and 4 account for all possible connected alphabet graphs on two vertices, and, for these three alphabet graphs, the problem of determining CAN and

CAK is solved. In each case, there is an upper bound on CAK, based on some “LYM-like” inequality from extremal set theory, and a construction that meets the upper bound. In contrast, with alphabet size $v \geq 3$, no values of CAN or CAK are known for all k or for all n , respectively.

We now give the details of our main contributions.

LYM inequalities for alphabet graphs

There are ten pairwise non-isomorphic connected alphabet graphs to consider on three vertices. The natural first step to take, going from two to three vertices, is with a bipartite alphabet graph: the star on 3 vertices, which we denote by S_3 . We approached the alphabet graph S_3 by generalizing a known LYM inequality. We derived a LYM inequality specific to the columns of a covering array with alphabet graph S_3 . From this LYM inequality for S_3 , given in Corollary 7.1.2, we derived a new upper bound on $\text{CAK}(n; 2, S_3)$ involving the golden ratio; see Theorem 7.1.14.

Let K_3^{loop} denote the complete alphabet graph K_3 with a loop on each vertex. A covering array with alphabet graph K_3^{loop} corresponds to a ternary covering array of strength 2, thus, K_3^{loop} is another natural alphabet graph to consider on three vertices. We derived a new LYM inequality to capture the columns of a ternary covering array. From our LYM inequality for K_3^{loop} , given in Corollary 7.3.1, we derived a new upper bound on $\text{CAK}(n; 2, K_3^{\text{loop}})$. Using this upper bound, given in Theorem 7.3.20, we derived an upper bound on $\text{CAK}(n; 2, v)$ for any alphabet size $v \geq 3$. This upper bound is given in Corollary 7.4.1 and is an improvement on a known bound given in [48].

We extended our technique for obtaining the LYM inequalities for S_3 and K_3^{loop} to a general method in which, for any given alphabet graph H , we get a LYM-like inequality that captures the columns of a covering array with alphabet graph H . The infinite class of LYM inequalities which follow from our technique and the method we use to derive these inequalities is the main contribution of this thesis.

The technique we use to obtain LYM inequalities for any H involves counting permutations with certain “following” properties encoded by the arcs of a directed “follow digraph” F . The permutation-counting technique is inspired by proof techniques given in [33, 38, 59], but our technique, using follow digraphs, gives us the ability to

apply the method far more generally. We also introduce “ F -following collections” as a tool for obtaining LYM inequalities for alphabet graphs H . The key is to associate with each alphabet graph H the appropriate follow digraph F . We completely characterize the relationship between alphabet graphs and follow digraphs in Section 6.3.

For each alphabet graph H , our LYM inequality for H inherently bounds the column number of a covering array with alphabet graph H . We illustrate this fact by deriving bounds for the alphabet graphs S_3 and K_3^{loop} . To obtain these bounds, we used “balancing” lemmas. The idea of balancing lemmas is to make small changes to the parameters of a given LYM inequality, greedily increasing the formula, until a maximum is reached. The optimal balance of parameters of the maximum depends on the structure of H , so we need appropriate balancing lemmas.

If we assume that the proportion of symbols in the columns of optimal covering arrays with alphabet graph H tends to a limiting distribution, then, in Theorem 7.5.6, we prove that it suffices to consider a simplified version of our LYM inequalities: the “single-arc” terms. Using the single-arc terms, in Theorem 7.6.2, we derive an upper bound on the column number of v -ary covering arrays of strength 2, for all $v \geq 2$. If our assumptions about the limiting distribution of symbol proportions hold, then Theorem 7.6.2 is an even better bound on column numbers than the bound we gave in Corollary 7.4.1.

Covering arrays on column and alphabet graphs

We define covering arrays on column graphs and alphabet graphs as a generalization of covering arrays with alphabet graphs. The column graph simply encodes which pairs of columns must cover the pairs of symbols corresponding to the edges of the given alphabet graph. This generalization marries covering arrays with alphabet graphs with another variant called covering arrays on graphs, which have been previously studied in [42, 43].

Covering arrays on graphs have interesting connections to graph homomorphisms. In Section 3.2, we develop analogous homomorphism results which incorporate any given alphabet graph. We also consider covering arrays on directed column graphs and directed alphabet graphs. For these arrays, the pattern of symbols to be covered by two columns need not be symmetric.

Our main contributions for covering arrays on directed column and alphabet graphs include the determination of CAN for the simplest case in this context: where the column graph is T_k , a transitive tournament on k vertices, and the alphabet graph is T_2 ; in Theorem 4.4.3, we prove that $\text{CAN}(2, T_k, T_2) = \lceil \log_2 k \rceil$. We also define a special family of directed column graphs, called circular tournaments, denoted Ω_k . Optimizing covering arrays on circular tournament column graphs with T_2 as the alphabet graph can be viewed as a new Sperner-type problem. In Corollary 4.5.12, we give a recursive construction of $\text{CA}(n; 2, \Omega_k, T_2)$ that is optimal infinitely often.

In Section 4.4, we derive bounds on $\text{CAN}(2, O, T_2)$, where O is any k -tournament. In Corollary 4.4.7, we show that, for all k -tournaments, the lower and upper bounds we derived are asymptotically equal to $\log_2 k$, as k grows.

In Proposition 4.4.4, we give a new construction for binary covering arrays of strength 2; our construction is based on building blocks made from covering arrays on transitive tournament column graphs. Although this construction is not optimal, it gives us a new way to consider classical covering arrays as arrays built from smaller covering arrays on directed column graphs.

FOR arrays

The most general arrays we consider are “forbidden-optional-required” arrays, or FOR arrays for short. We define FOR arrays to model testing applications where prior knowledge leads to a combination of interaction strengths and types: forbidden, optional, and required. A forbidden interaction corresponds to a pattern of symbols in a given set of columns which should never appear in any row of the array. An optional interaction corresponds to a pattern of symbols in a given set of columns which does not need to appear in a row of the array, but we do not care if it does appear. A required interaction corresponds to a pattern of symbols in a given set of columns which must be covered by at least one row. Given a list of forbidden, optional, and required interactions, a FOR array is, informally, an array whose rows satisfy the constraints corresponding to each type of interaction.

We model the list of interactions using a FOR system, which is an accessory hypergraph with its edge set partitioned into three classes (one for each of the three types of interactions F, O, and R). Given a FOR system, it is not easy to decide whether there

exists a FOR array satisfying its prescribed constraints. In Section 8.2, we establish some properties that guarantee a FOR array’s existence and others that prevent it.

If a FOR array does exist, we prefer it to have as few rows as possible. This smallest number of rows is called the FOR array number, denoted FORN. In Proposition 8.3.1, we give bounds on FORN, and in Proposition 8.4.1, we establish that determining FORN is an NP-complete problem, even for relatively simple families of FOR systems.

In Sections 8.6 and 8.7, we study “critical” FOR systems. If we have an interaction that is either required or forbidden, when does switching it to an optional interaction guarantee a decrease in the size of an optimal FOR array? We give examples of critical systems and simple recursive constructions. We examine the relationship between certain classes of critical FOR systems and prove that these systems have vertex-critical “incompatibility” graphs.

In Section 8.8, we model a special case of the FOR array problem using binary relational systems. We define a target system that characterizes the problem of determining FORN in terms of finding homomorphisms to the smallest target system, and we determine that these target systems are cores for all $v \geq 2$.

Chapter 2

Preliminaries

In this chapter, we survey basic results and definitions from extremal set theory and graph theory. We include only those topics and results which have relevance to later parts of the thesis. We also include sections on qualitative independence, covering arrays, and the generalizations of covering arrays which are relevant to this thesis, namely classical covering arrays, mixed covering arrays, covering arrays on graphs, covering arrays avoiding forbidden edges (CAFES), and variable strength covering arrays (VCAs).

2.1 Extremal set theory

The principal reference for the results and definitions of this section is Anderson's text [3].

Let n be a positive integer. Denote by $[n]$ the set of integers $[n] = \{1, \dots, n\}$. If x is a real number, then $\lfloor x \rfloor$ denotes the **floor** of x , that is, the largest integer less than or equal to x . The **ceiling** of x , denoted $\lceil x \rceil$, is the smallest integer greater than or equal to x .

Let n and k be integers such that $n \geq k \geq 0$. Denote by $\binom{n}{k}$ the binomial coefficient

$$\binom{n}{k} = \frac{n!}{k!(n-k)!}.$$

Now let $k_1, \dots, k_t$ be integers such that $k_i \geq 0$ and $k_1 + k_2 + \dots + k_t = n$. Denote by $\binom{n}{k_1, k_2, \dots, k_t}$ the multinomial coefficient

$$\binom{n}{k_1, k_2, \dots, k_t} = \frac{n!}{k_1! k_2! \dots k_t!}.$$

A collection $\mathcal{A} = \{A_1, \dots, A_m\}$ of subsets of $[n]$ is an **antichain** if, for every two distinct sets $A_i, A_j \in \mathcal{A}$, we have $A_i \not\subseteq A_j$ and $A_j \not\subseteq A_i$.

The first extremal result we present is Sperner's Theorem [54], which provides the answer to the question: what is the maximum size of an antichain of subsets of $[n]$?

Theorem 2.1.1 (Sperner's Theorem [54]) If $\mathcal{A}$ is an antichain of subsets of $[n]$, then

$$|\mathcal{A}| \leq \binom{n}{\lfloor n/2 \rfloor}. \quad \blacksquare$$

A related result, stronger than Sperner's Theorem, is the so-called **LYM inequality**, named after Lubell [38], Yamamoto [60] and Mešalkin [45], who proved the following theorem:

Theorem 2.1.2 (LYM Inequality [38, 45, 60]) If $\mathcal{A} = \{A_1, \dots, A_m\}$ is an antichain of subsets of $[n]$, then

$$\sum_{i=1}^m \frac{1}{\binom{n}{|A_i|}} \leq 1.$$

Another related, and yet stronger result, is the following LYM-like inequality, given in Theorem 2.1.3. Note that the inequality of Theorem 2.1.3 has been proved independently many times, although it is sometimes referred to as **Bollobás's Inequality**.

Theorem 2.1.3 (Bollobás Inequality [4, 27, 30, 33, 59]) If $\mathcal{A} = \{A_1, \dots, A_m\}$ and $\mathcal{B} = \{B_1, \dots, B_m\}$ are two families of subsets of $[n]$ such that $A_i \cap B_j = \emptyset$ if and only if $i = j$, then

$$\sum_{i=1}^m \binom{|A_i| + |B_i|}{|A_i|}^{-1} \leq 1. \quad \blacksquare$$

We describe the inequality of Theorem 2.1.3 as “LYM-like,” or simply “a LYM inequality” because of its resemblance to the LYM Inequality: an upper bound for a

sum of some reciprocated binomial coefficients involving set cardinalities. In fact, Theorem 2.1.3 implies the LYM Inequality by using the complements of the sets in the antichain $\mathcal{A}$ as the second family $\mathcal{B}$. In turn, Theorem 2.1.2 implies Sperner's Theorem since, for all i , we have $\binom{n}{|A_i|} \leq \binom{n}{\lfloor n/2 \rfloor}$.

In Chapter 6, we develop a method that produces an infinite family of LYM inequalities including the inequality of Theorem 2.1.3. Our method uses a technique that is related to Lubell's proof of Theorem 2.1.2 and Katona's [33] proof of a special case of Theorem 2.1.3. It is also related to the technique used by Tarjan [59] for proving Theorem 2.1.3. For this reason, we provide complete proofs, as presented in [3], of Theorems 2.1.2 and 2.1.3 (see Theorem 1.2.1 and Theorem 1.3.1 in [3]). The particular proofs rely on a permutation-counting technique for which we need a few definitions.

Let π be a permutation of the symbols $[n]$, where $\pi(i) = \pi_i$ for each $i \in [n]$. We write π as an n -tuple: $\pi = (\pi_1, \dots, \pi_n)$.

Let A be a subset of $[n]$. A permutation $\pi = (\pi_1, \dots, \pi_n)$ of $[n]$ **begins with** A if $A = \{\pi_1, \dots, \pi_{|A|}\}$.

A permutation-counting proof of Theorem 2.1.2.

Let $\mathcal{A} = \{A_1, \dots, A_m\}$ be an antichain of subsets of $[n]$. We count the permutations of $[n]$ that begin with a set $A_i \in \mathcal{A}$. There are $|A_i|!(n - |A_i|)!$ permutations π that begin with A_i since there are $|A_i|!$ ways to arrange the elements of A_i in the first elements of π and there are $(n - |A_i|)!$ ways to arrange the remaining elements of $[n]$.

If a permutation $\pi = (\pi_1, \dots, \pi_n)$ began with two different sets $A_i, A_j \in \mathcal{A}$, then we would have $A_i \subseteq A_j$ or $A_j \subseteq A_i$, contradicting the fact that $\mathcal{A}$ is an antichain.

Therefore, each of the $n!$ permutations of $[n]$ is counted as a permutation that begins with A_i for at most one $A_i \in \mathcal{A}$. Consequently,

$$\sum_{A_i \in \mathcal{A}} |A_i|!(n - |A_i|)! \leq n! \quad (2.1.1)$$

If we divide both sides of (2.1.1) by $n!$ and notice that $\binom{n}{|A_i|}^{-1} = |A_i|!(n - |A_i|)!/n!$, then we obtain the LYM Inequality:

$$\sum_{i=1}^m \binom{n}{|A_i|}^{-1} \leq 1. \quad \blacksquare$$

Let A and B be disjoint nonempty subsets of $[n]$. A permutation $\pi = (\pi_1, \dots, \pi_n)$ of $[n]$ **contains A followed by B** if $i < j$ whenever $\pi_i \in A$ and $\pi_j \in B$. Equivalently, if we read π as an n -tuple from left to right, all the elements of A occur before all the elements of B .

A permutation-counting proof of Theorem 2.1.3.

Let $\mathcal{A} = \{A_1, \dots, A_m\}$ and $\mathcal{B} = \{B_1, \dots, B_m\}$ be two families of subsets of $[n]$ such that $A_i \cap B_j = \emptyset$ if and only if $i = j$. We count the permutations of $[n]$ that contain A_i followed by B_i for a fixed $i \in [m]$. There are $\binom{n}{|A_i| + |B_i|}$ ways to choose the positions of the elements of A_i and B_i in a permutation. There are $|A_i|!$ ways to arrange the elements of A_i in the first $|A_i|$ of these positions, and there are $|B_i|!$ ways to arrange the elements of B_i in the remaining positions. There are $(n - |A_i| - |B_i|)!$ ways to arrange the remaining elements of $[n]$. The number of permutations that contain A_i followed by B_i is thus

$$\binom{n}{|A_i| + |B_i|} |A_i|! |B_i|! (n - |A_i| - |B_i|)! = \frac{n!}{\binom{|A_i| + |B_i|}{|A_i|}}.$$

If, for some $i \neq j$, a permutation π contains A_i followed by B_i and π contains A_j followed by B_j , then either the last element of A_i occurs in π before the first element of B_j , or else the last element of A_i occurs in π at the same position or after the first element of B_j . In the first case, we would have $A_i \cap B_j = \emptyset$. In the second case, we would have $A_j \cap B_i = \emptyset$. Both cases contradict the intersection of the families $\mathcal{A}$ and $\mathcal{B}$.

It now follows that each permutation of $[n]$ is counted as a permutation that contains A_i followed by B_i for at most one $i \in [m]$, and we get the LYM-like inequality:

$$\sum_{i=1}^m \frac{n!}{\binom{|A_i| + |B_i|}{|A_i|}} \leq n! \quad \blacksquare$$

An **intersecting antichain** of subsets of $[n]$ is an antichain $\mathcal{A} = \{A_1, \dots, A_m\}$ such that $A_i \cap A_j \neq \emptyset$ for all $i, j \in [m]$.

Brace and Daykin [8], and Schönheim [52] gave the following extremal result for intersecting antichains.

Theorem 2.1.4 (Intersecting Antichain Bound [8, 52]) If $\mathcal{A}$ is an intersecting antichain of subsets of $[n]$, then

$$|\mathcal{A}| \leq \binom{n}{\lfloor n/2 \rfloor + 1}. \quad \blacksquare$$

A **partially ordered set** or **poset** is a pair $(S, \leq)$, where S is a set and $\leq$ is a partial order on S satisfying the following properties:

- reflexivity (for all $x \in S$, we have $x \leq x$),
- antisymmetry (for all $x, y \in S$, if $x \leq y$ and $y \leq x$, then $x = y$).
- transitivity (for all $x, y, z \in S$, if $x \leq y$ and $y \leq z$, then $x \leq z$).

The **poset of subsets** of $[n]$ is the poset $(\mathcal{P}([n]), \subseteq)$, where $\mathcal{P}([n])$ denotes the power set of $[n]$. The **rank** of a subset $A \subseteq [n]$ is the cardinality $|A|$. There are $\binom{n}{k}$ sets of rank k in the poset of subsets of $[n]$. If we have subsets $A_1, \dots, A_m \subseteq [n]$ such that $A_1 \subset A_2 \subset \dots \subset A_m$, then the sequence $A_1, \dots, A_m$ is a **chain**. If, further, we have $|A_{i+1}| = |A_i| + 1$, for $1 \leq i \leq m - 1$, and $|A_1| + |A_m| = n$, then the sequence $A_1, \dots, A_m$ is a **symmetric chain**. The following theorem of de Bruijn, van Ebbenhorst Tengbergen, and Kruyswijk [20] tells us that we can decompose the poset of subsets of $[n]$ into a disjoint union of symmetric chains.

Theorem 2.1.5 (Symmetric Chain Decomposition [20]) The poset of subsets of $[n]$ can be decomposed into a disjoint union of symmetric chains. $\blacksquare$

Example 2.1.6 Here is a symmetric chain decomposition of the poset of subsets of $[4]$ into six symmetric chains:

$$\begin{array}{ccccccc} \emptyset & \subset & \{1\} & \subset & \{1, 2\} & \subset & \{1, 2, 3\} & \subset & \{1, 2, 3, 4\} \\ & & \{2\} & \subset & \{2, 3\} & \subset & \{2, 3, 4\} \\ & & \{3\} & \subset & \{1, 3\} & \subset & \{1, 3, 4\} \\ & & \{4\} & \subset & \{1, 4\} & \subset & \{1, 2, 4\} \\ & & & & \{2, 4\} \\ & & & & \{3, 4\} \end{array}$$

Let $\mathcal{A}$ be a collection of k -subsets of $[n]$, for some $k \in \{2, \dots, n\}$. The **shadow** of $\mathcal{A}$, denoted $\Delta\mathcal{A}$, is the collection

$$\Delta\mathcal{A} = \{B \subseteq [n] : |B| = k - 1 \text{ and } B \subset A \text{ for some } A \in \mathcal{A}\}.$$

Given positive integers x and k , the k -**binomial representation** of x is the unique representation

$$x = \binom{a_k}{k} + \binom{a_{k-1}}{k-1} + \cdots + \binom{a_t}{t},$$

where $a_k > a_{k-1} > \cdots > a_t \geq t \geq 1$. For every x and k , the numbers $t, a_i, i \in [t]$ exist and are unique; see Theorem 7.2.1 in [3].

Kruskal [36] and Katona [31] determined the following lower bound on the cardinality of the shadow of a collection of k -subsets of $[n]$.

Theorem 2.1.7 (Kruskal–Katona Theorem [31, 36]) Let $\mathcal{A}$ be a collection of k -subsets of $[n]$. If the k -binomial representation of $|\mathcal{A}|$ is

$$|\mathcal{A}| = \binom{a_k}{k} + \binom{a_{k-1}}{k-1} + \cdots + \binom{a_t}{t},$$

where $a_k > a_{k-1} > \cdots > a_t \geq t \geq 1$, then

$$|\Delta\mathcal{A}| \geq \binom{a_k}{k-1} + \binom{a_{k-1}}{k-2} + \cdots + \binom{a_t}{t-1}. \quad \blacksquare$$

If A is a subset of $[n]$, then the **complement** of A , denoted $\bar{A}$, is the set $\bar{A} = [n] - A$. If A and B are subsets of $[n]$, then the **symmetric difference** of A and B , denoted $A \oplus B$, is the set $A \oplus B = (A \cap \bar{B}) \cup (\bar{A} \cap B)$. If A and B are k -sets, then, in **squashed order**, we have $A <_s B$ if the largest element of the symmetric difference $A \oplus B$ is in B . For fixed k , squashed order is a total order on the set of k -subsets. Indeed, the collection of k -sets for which the Kruskal–Katona Theorem holds with equality is the collection of k -sets that are smallest in squashed order. In other words, we have the following corollary (see Section 7.3 in [3]).

Corollary 2.1.8 The first m sets of rank k in squashed order have the smallest possible shadow among all collections of m sets of rank k . If $\mathcal{A}$ is a collection of the $|\mathcal{A}|$ smallest sets of rank k in squashed order, then $|\Delta\mathcal{A}|$ meets the bound given by the Kruskal–Katona Theorem with equality. Moreover, $\Delta\mathcal{A}$ consists of the smallest sets of rank $k-1$ in squashed order. $\blacksquare$

A v -**partition** of $[n]$ is a collection of v pairwise-disjoint subsets of $[n]$, say $P = \{P^1, \dots, P^v\}$, where $\bigcup_{a \in [v]} P^a = [n]$. The subsets $P^a \subseteq [n]$ are the **classes** of the partition P . Sometimes, the labelling of the classes P^a is important; in these cases, we write a partition P as an ordered collection $P = (P^1, \dots, P^v)$.

Let S be a finite set. An **abstract simplicial complex** or **downset** on S is a collection $\mathcal{D}$ of nonempty subsets of S such that $B \in \mathcal{D}$ whenever $B \subset A$ for some $A \in \mathcal{D}$ (and $B \neq \emptyset$). Each set A in $\mathcal{D}$ is a **face**. If a face A is not contained in any other face B in $\mathcal{D}$, then A is a **facet** of $\mathcal{D}$. Similarly, an **upset** on S is a collection $\mathcal{U}$ of nonempty subsets of S such that $B \in \mathcal{U}$ whenever $B \supset A$ for some $A \in \mathcal{U}$.

2.2 Graphs, hypergraphs, and relational systems

2.2.1 Basic graph notation

In this section, we establish some graph-theoretic notation and terminology used throughout the thesis. For more details, we refer the reader to the text of Bondy and Murty [7].

In this thesis, we do not consider graphs with parallel edges, although graphs may contain loops or be directed.

Given an undirected graph G , we refer to an edge of G by the unordered pair of (not necessarily distinct) vertices corresponding to its ends. Given a directed graph D , we refer to an arc of D by the ordered pair of (not necessarily distinct) vertices corresponding to its ends.

When it is clear that a given graph is undirected (or directed), for an edge (or arc) having ends u and v , we refer to the corresponding edge (or arc) simply as uv instead of the pair $\{u, v\}$ (or (u, v) , respectively).

Let D be a directed graph. If two vertices $a, b \in V(D)$ are joined by two oppositely directed arcs $ab, ba \in E(D)$, then we say that ab and ba are an **antiparallel** pair of arcs; we also say that a and b are **symmetrically adjacent**. Let $u \in V(D)$. If $\text{indeg}_D(u) = 0$, then u is called a **source**. If $\text{outdeg}_D(u) = 0$, then u is called a **sink**. If D does not contain any directed cycle as a subgraph, then D is called **acyclic**.

Let G be a graph (undirected or directed). The **symmetric digraph** of G , denoted G^* , is a directed graph such that $V(G^*) = V(G)$ and, for every pair of vertices $a, b \in V(G)$ such that at least one edge (or arc) joins a and b in G , there is an antiparallel pair of arcs $ab, ba \in E(G^*)$. That is, $E(G^*) = \bigcup_{ab \in E(G)} \{(a, b), (b, a)\}$.

Let G and H be two graphs. The **categorical product** of G and H , denoted $G \times H$,

is the graph with $V(G \times H) = V(G) \times V(H)$ and edges given by $(u_1, v_1)(u_2, v_2) \in E(G \times H)$ if and only if $u_1 u_2 \in E(G)$ and $v_1 v_2 \in E(H)$.

Let G be an undirected graph. We denote by $\omega(G)$ the clique number of G . A collection $\mathcal{C} = \{C_1, \dots, C_n\}$ of cliques of G is a **clique cover** of G , if every vertex of G belongs to at least one $C_i \in \mathcal{C}$. A collection $\mathcal{C} = \{C_1, \dots, C_n\}$ of cliques of G is an **edge clique cover** of G , if for every edge $uv \in E(G)$, there is a clique $C_i \in \mathcal{C}$ such that $u, v \in C_i$. The **clique cover number** of G , denoted $\theta(G)$, is the cardinality of a minimum clique cover of G . The **edge clique cover number** of G , denoted $\theta'(G)$, is the cardinality of a minimum edge clique cover of G .

Let G be a simple graph. A **matching** of G is a subset of edges $M \subseteq E(G)$ such that no two edges in M are incident with a common vertex. The **matching number** of G , denoted $\mu(G)$, is the cardinality of a maximum matching of G . Given a matching M of G , a vertex $u \in V(G)$ is called **M -covered** if u is an end of some edge in a M ; otherwise u is called **M -exposed**. If there exists a maximum matching M of G in which a vertex u is not M -covered, then u is called an **inessential vertex** of G . A matching M in which every vertex $u \in V(G)$ is M -covered is called a **perfect matching**. The **deficiency** of G , denoted $\text{def}(G)$, is $\text{def}(G) = |V(G)| - 2\mu(G)$.

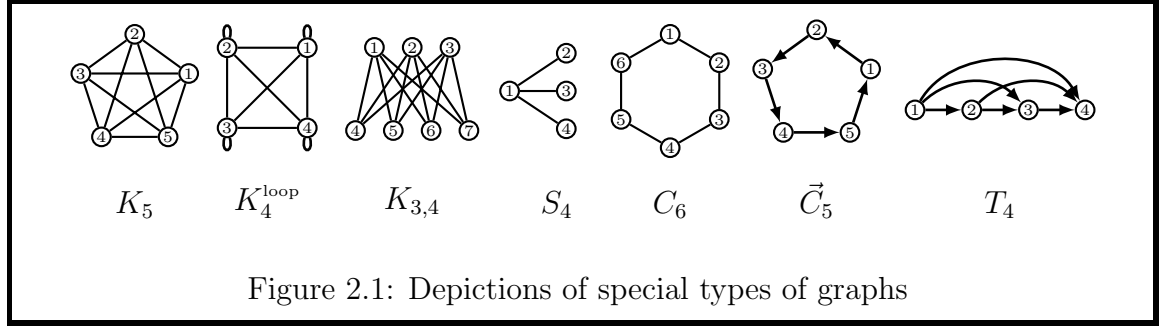
Let G be an undirected graph. A subset $I = \{u_1, \dots, u_k\}$ of k distinct vertices of G is an **independent set** of size k if $u_i u_j \notin E(G)$ for all $i, j \in [k]$. A proper **k -colouring** of G is partition of $V(G)$ into k classes $V_1, \dots, V_k$, where each V_i is an independent set. If there exists a proper k -colouring of G , then G is called **k -colourable** or **k -partite**. The classes V_i are the **colour classes** or the **parts** of G . The **chromatic number** of G , denoted $\chi(G)$, is the minimum integer k for which G is k -colourable. If G is 2-colourable, then G is called **bipartite**. It can be shown that G is bipartite if and only if G contains no odd cycles.

Let G be a graph. Let u be a vertex of G . Denote by $G - u$ the graph obtained from G by deleting the vertex u and all edges incident with u . Let e be an edge of G . Denote by $G - e$ the graph obtained from G by deleting the edge e .

An undirected graph G is **colour-critical**, or simply **critical**, if for every proper subgraph G' of G , we have $\chi(G') < \chi(G)$. A **critical element** of G is a vertex $u \in V(G)$ (or an edge $e \in E(G)$) such that $\chi(G - u) < \chi(G)$ (or $\chi(G - e) < \chi(G)$, respectively). If every vertex (or edge) of G is a critical element, then G is called **vertex-critical** (or **edge-critical**, respectively).

A **vertex cover** of an undirected graph G is a subset $V' \subseteq V(G)$ such that every edge of G is incident with some vertex in V' . A vertex cover V' is a **minimal vertex cover** if, for any vertex $u \in V'$, the set $V' - \{u\}$ is not a vertex cover of G .

The following special families of graphs appear throughout this thesis and are denoted as follows. Figure 2.1 gives one example from each family.



The **complete graph** on k vertices, denoted K_k , is a simple graph such that every two distinct vertices $u, v \in V(K_k)$ are adjacent.

The **complete graph with loops** on v vertices, denoted K_v^{loop} , is the complete graph K_v with a loop on each of its vertices.

The **complete bipartite graph** with parts of sizes p and q , denoted $K_{p,q}$, is a simple graph with $p + q$ vertices, where $V(K_{p,q})$ is partitioned into two parts X and Y such that $|X| = p$, $|Y| = q$, and $uv \in E(G)$ if and only if $u \in X$ and $v \in Y$.

For $v \geq 3$, the **star** on v vertices, denoted S_v , is the complete bipartite graph $K_{1,v-1}$. The vertex of degree $v - 1$ is called the **central vertex**; the vertices of degree 1 are called **leaves**.

The **k -cycle**, denoted C_k , is a simple graph with k vertices, say $v_1, \dots, v_k$, and k edges of the form $v_i v_{i+1}$, $1 \leq i \leq k$, where addition is done modulo k .

The **directed k -cycle**, denoted $\vec{C}_k$, is a directed graph with k vertices, say $v_1, \dots, v_k$, and k arcs of the form $v_i v_{i+1}$, $1 \leq i \leq k$, where addition is done modulo k .

The **transitive k -tournament**, denoted T_k , is a directed graph with $V(T_k) = [k]$ and $ij \in E(T_k)$ whenever $1 \leq i < j \leq k$.

2.2.2 Graph homomorphisms

In this section, we discuss graph homomorphisms. For further details, we refer the reader to the text of Hell and Nešetřil [29].

Let G and H be graphs which are both directed or both undirected. A map $f : V(G) \rightarrow V(H)$ is a **homomorphism** of G to H if $f(u)f(v) \in E(H)$ whenever $uv \in E(G)$. If there exists a homomorphism of G to H , then we say that G is **homomorphic to H** and we write $G \rightarrow H$. If there is no homomorphism of G to H , then we write $G \not\rightarrow H$. A homomorphism of G to H preserves edges, and when G and H are directed, a homomorphism of G to H must also preserve the direction of the edges. A homomorphism f of G to H is **vertex-injective** if the map $f : V(G) \rightarrow V(H)$ is injective. A bijection $f : V(G) \rightarrow V(H)$ is an **isomorphism** if $f(u)f(v) \in E(H)$ if and only if $uv \in E(G)$.

If there exists a homomorphism of G to H , then G is called **H -colourable**. This terminology is based on the following fact (see Proposition 1.7 in [29]).

Proposition 2.2.1 If G is a simple graph, then there exists a homomorphism of G to the complete graph K_k if and only if $\chi(G) \leq k$. In particular,

$$\chi(G) = \min\{k : G \rightarrow K_k\}.$$



Thus, a graph is k -colourable if and only if it is K_k -colourable. For a fixed graph H , the **H -colouring problem** is the problem of determining whether there exists a homomorphism of a given graph G to H . In the H -colouring problem, the graph H is the **target** of the homomorphism. Several covering array problems can be translated into graph-colouring problems for an appropriate choice of target.

An **endomorphism** of a graph G is a homomorphism of G to itself. An **automorphism** of G is an isomorphism of G to itself. If, for every two vertices u and v of G , there exists an automorphism $f : V(G) \rightarrow V(G)$ such that $f(u) = v$, then G is called **vertex-transitive**.

A **retraction** of G to a subgraph G' of G is an endomorphism $r : G \rightarrow G'$ such that $r(u) = u$ for all vertices $u \in V(G')$. If there exists a retraction of G to a subgraph G' , then we say that G **retracts to G'** .

A **core** is a graph which does not retract to any proper subgraph of itself. A subgraph G' of a graph G is a **core** of G , if G retracts to G' and G' is itself a core.

If, for two graphs G and H , we have $G \rightarrow H$ and $H \rightarrow G$, then G and H are called **homomorphically equivalent**. In particular, if G' is a core of G , then we have homomorphisms $G' \rightarrow G$, by inclusion, and $G \rightarrow G'$, since G retracts to G' . Thus, every graph G is homomorphically equivalent to its core. In fact, every graph G has a unique core, up to isomorphism, as follows (see Corollary 1.32 in [29]).

Proposition 2.2.2 If G is a graph, then G is homomorphically equivalent to a unique core, up to isomorphism. ■

In terms of the H -colouring problem, **the core** of H , denoted $H^\bullet$, is of particular interest since $H^\bullet$ is homomorphically equivalent to H , but might be a proper subgraph of H . Since homomorphisms compose (see Section 1.7 in [29]), there exists a homomorphism of G to H if and only if there exists a homomorphism of G to the core of H .

2.2.3 Hypergraphs and relational systems

A **hypergraph** H is a pair $(V(H), E(H))$, where $V(H)$ is a set of vertices and $E(H) \subset \mathcal{P}(V(H))$ is a collection of nonempty subsets of $V(H)$. Each subset of vertices in $E(H)$ is called an **edge** of H . If $e \in E(H)$, where $|e| = s$, then we say that e is an edge of **rank** s . An edge e of H is **incident with** each of the vertices $u \in e$.

A **vertex cover** of a hypergraph H is a subset $V' \subseteq V(H)$ such that every edge $e \in E(H)$ is incident with at least one vertex $u \in V'$. A **minimal vertex cover** of H is a vertex cover V' of H such that, for any vertex $u \in V'$, the set $V' - \{u\}$ is not a vertex cover of H .

A hypergraph H is **k -partite** if $V(H)$ can be partitioned into k classes $V_1, \dots, V_k$ such that no edge of H is incident with more than one vertex from each class.

The **underlying graph** of a hypergraph H is the simple graph G with $V(G) = V(H)$ and $E(G) = \{e \in E(H) : |e| = 2\}$.

In this thesis, a **matching of a hypergraph** refers to a matching of the given hypergraph's underlying graph. For hypergraphs, we use the notation and terminology of matching theory, as given for graphs, where it is understood that all definitions and concepts are applied to the underlying graph of H .

A **general relational system** S is a pair $(V(S), \mathcal{R}(S))$, where $V(S)$ is a nonempty finite set of vertices, and $\mathcal{R}(S)$ is a finite family of relations on $V(S)$, defined as follows. We have a finite set I called the **index set** of S and a set $\{k_i : i \in I\}$ of positive integers called the **pattern** of S . For each $i \in I$, we have a k_i -ary relation $R_i(S)$ on $V(S)$. The set $\mathcal{R}(S)$ is defined to be the family of relations $\mathcal{R}(S) = \{R_i(S) \subseteq V(S)^{k_i} : i \in I\}$. If $k_i = 2$ for all $i \in I$, then S is called a **binary relational system**, abbreviated **BRS**. For general relational systems, we write **GRS** for short.

A BRS restricted to any one of its relations is simply a directed graph. We can imagine a BRS as a directed graph with several colours of arcs, where, for each $i \in I$, the colour i corresponds to the relation R_i . Some pairs of vertices may be joined by arcs of more than one colour.

Within this thesis, we deal mainly with BRS and only mention GRS as potential avenues for future work. The following definitions hold, with slight adjustments, for GRS; however, we give them in terms of BRS to cater to the scope of the thesis.

Let S and T be two BRS, where the families of relations $\mathcal{R}(S) = \{R_i(S) : i \in I\}$ and $\mathcal{R}(T) = \{R_i(T) : i \in I\}$ have the same index set I . A map $f : V(S) \rightarrow V(T)$ is a **homomorphism** of S to T if, for all $i \in I$, we have $(f(u), f(v)) \in R_i(T)$ whenever $(u, v) \in R_i(S)$.

A BRS S' is a **subsystem** of a BRS S if $V(S') \subseteq V(S)$, the family $\mathcal{R}(S')$ of relations on S' are indexed by the same set I as the family $\mathcal{R}(S)$, and for each $i \in I$, we have $R_i(S') \subseteq R_i(S)$.

A BRS S is a **core** if S is not homomorphic to a proper subsystem of itself. As with graphs, every BRS is homomorphically equivalent to a unique core, up to isomorphism.

2.3 Classical covering arrays

In this section, we review “mixed” covering arrays, and we outline the terminology we use to describe covering arrays in terms of testing applications. For more details on mixed covering arrays, see [46].

Definition 2.3.1 A (mixed) **covering array**, denoted $\text{CA}(n; t, k, (v_1, \dots, v_k))$, is an $n \times k$ array A with the following properties:

- For each $i \in [k]$, column i has symbols from the **alphabet** $[v_i]$.
- A has **strength** t : in every subarray of A consisting of t distinct columns, say columns $i_1, \dots, i_t$, every t -tuple $(a_1, \dots, a_t) \in [v_{i_1}] \times [v_{i_2}] \times \dots \times [v_{i_t}]$ must appear at least once as a row in this subarray.

The minimum integer n for which there exists a $\text{CA}(n; t, k, (v_1, \dots, v_k))$ is the **covering array number** and it is denoted $\text{CAN}(t, k, (v_1, \dots, v_k))$.

A covering array with **homogeneous alphabet size** v , or a v -**ary** covering array, denoted $\text{CA}(n; t, k, v)$, is a $\text{CA}(n; t, k, (v_1, \dots, v_k))$ in which all columns have the same alphabet size $v_i = v$. The covering array number for a v -ary covering array is denoted $\text{CAN}(t, k, v)$.

A **binary covering array** is a $\text{CA}(n; t, k, 2)$.

Remark 2.3.2 In a v -ary covering array, we use symbols from the alphabet $[v] = \{1, \dots, v\}$; however, when $v = 2$, for binary covering arrays, we opt to use symbols from the alphabet $\{0, 1\}$ instead.

1	2	3	4	5	6	7	8	9	10	11	12
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	1	0	0	0	1	1	1	1	1
0	0	1	0	0	1	1	0	0	1	1	1
0	0	1	1	1	0	1	0	1	0	0	1
0	1	0	0	1	0	1	1	0	0	1	1
0	1	0	1	0	1	1	0	1	0	1	0
0	1	1	0	0	1	0	1	1	0	0	1
0	1	1	1	0	0	1	1	0	1	0	0
1	0	0	0	1	1	0	0	1	0	1	1
1	0	0	1	0	1	1	1	0	0	0	1
1	0	1	0	0	0	1	1	1	0	1	0
1	0	1	1	0	1	0	0	1	1	0	0
1	1	0	0	0	0	1	0	1	1	0	1
1	1	0	1	1	0	0	1	1	0	0	0
1	1	1	1	0	0	0	0	0	0	1	1
1	1	1	0	1	1	1	0	0	0	0	0
0	0	0	0	1	1	1	1	1	1	0	0
0	0	1	1	1	1	0	1	0	0	1	0
0	1	0	1	1	1	0	0	0	1	0	1
0	1	1	0	1	0	0	0	1	1	1	0
1	0	0	1	1	0	1	0	0	1	1	0
1	0	1	0	1	0	0	1	0	1	0	1
1	1	0	0	0	1	0	1	0	1	1	0
1	1	1	1	1	1	1	1	1	1	1	1

Table 2.1: A $\text{CA}(24; 4, 12, 2)$

In Table 2.1, we give an example of a binary covering array of strength $t = 4$ with $n = 24$ rows and $k = 12$ columns. This $\text{CA}(24; 4, 12, 2)$ is extracted from [37]. A construction for such an array is given in [14].

2.3.1 A testing application of covering arrays

An important application of covering arrays is the design of test suites. Suppose we have an object made of several components wherein each component can assume one of several states. We would like to test the object under its different settings to see if some combinations of states result in faulty interactions.

To be more concrete, suppose we have a *testing problem* where the object or system to be tested has k components, called *factors*, which we label $1, \dots, k$, and for each $i \in [k]$, factor i can be set to one of v_i possible states called *values*. A *test* is an assignment of one value to each factor, represented by a k -tuple $T = (t_1, \dots, t_k) \in [v_1] \times \dots \times [v_k]$. A *test suite* is a list of tests, represented as an array where each row is a k -tuple corresponding to one test. An *exhaustive* test suite consists of $\prod_{i \in [k]} v_i$ tests corresponding to the full enumeration of all k -tuples in $[v_1] \times \dots \times [v_k]$.

In practice, exhaustive testing is too expensive or too time-consuming. As an alternative to exhaustive testing, we would like a smaller test suite, but we would like to design our test suite to capture as many faulty interactions as possible.

The rows of a covering array $\text{CA}(n; t, k, (v_1, \dots, v_k))$ correspond to a test suite of n tests for k factors, where factor i has v_i values. The strength of the covering array guarantees that every possible t -tuple of values among any t factors is tested. If our testing problem has faulty interactions resulting from a combination of up to t factors, then at least one of our tests will “fail.”

Fix a testing problem with k factors, labelled $1, \dots, k$, where each factor $j \in [k]$ can be assigned one of $[v_j]$ possible values. A *factor-value pair* is a pair (j, a) , where j is one factor in $[k]$ and a is one of the values in $[v_j]$. An *interaction* is a set of factor-value pairs, say $I = \{(j_1, a_1), \dots, (j_t, a_t)\}$, where the factors j_i are pairwise distinct, and $a_i \in [v_{j_i}]$ for each $i \in [t]$. In particular, I is a *t -way* interaction since $|I| = t$. A test $T = (T_1, \dots, T_k) \in [v_1] \times \dots \times [v_k]$ *covers* the interaction I if $T_{j_l} = a_l$ for all $l \in [t]$. A set of columns of a test suite, indexed by $\{j_1, \dots, j_s\} \subseteq [k]$, *covers* I if $\{i_1, \dots, i_t\} \subseteq \{j_1, \dots, j_s\}$ and for some row index $r \in [n]$, row r covers I .

2.3.2 Qualitatively independent partitions

In this section, we discuss qualitative independence as it relates to covering arrays of strength two.

The columns of a $\text{CA}(n; t, k, v)$ are v -ary n -tuples. There is a bijection between v -ary n -tuples and v -partitions of $[n]$. If $\vec{x} = (x_1, \dots, x_n) \in [v]^n$ is a v -ary n -tuple, then the v -partition corresponding to $\vec{x}$ is the partition $P = (P^1, \dots, P^v)$, where $P^a = \{i \in [n] : x_i = a\}$ for each $a \in [v]$. Conversely, if $P = (P^1, \dots, P^v)$ is a v -partition of $[n]$, then the v -ary n -tuple corresponding to P is $\vec{x} = (x_1, \dots, x_n)$, where $x_i = a$ whenever $i \in P^a$.

Based on this correspondence, we think of the columns of a v -ary covering array $\text{CA}(n; t, k, v)$ interchangeably as v -ary n -tuples or as v -partitions of $[n]$.

Two v -partitions of $[n]$, $P_1 = (P_1^1, \dots, P_1^v)$ and $P_2 = (P_2^1, \dots, P_2^v)$, are **qualitatively independent** if $P_1^a \cap P_2^b \neq \emptyset$ for all $a, b \in [v]$. In terms of the corresponding v -ary n -tuples, $\vec{x} = (x_1, \dots, x_n)$ and $\vec{y} = (y_1, \dots, y_n)$, corresponding to P_1 and P_2 , respectively, the condition $P_1^a \cap P_2^b \neq \emptyset$ implies the existence of an index $r \in [n]$ such that $x_r = a$ and $y_r = b$. A collection $\mathcal{P} = \{P_1, \dots, P_k\}$ of v -partitions of $[n]$, where $P_i = (P_i^1, \dots, P_i^v)$ for each $i \in [k]$, is a **qualitatively independent collection** if P_i and P_j are qualitatively independent for every two distinct partitions $P_i, P_j \in \mathcal{P}$.

The columns of a v -ary covering array of strength 2 correspond to a qualitatively independent collection of v -partitions.

Rényi [50] raised the following question: what is the maximum number of qualitatively independent v -partitions of $[n]$? In covering array language, what is the column number $\text{CAK}(n; 2, v)$?

The only case where an exact answer is known is when $v = 2$, that is, for binary covering arrays of strength 2. For even values of n , Rényi [50] solved this problem. In a paper dedicated to the memory of Rényi, Katona [32] solved the problem for odd values of n . The result was also obtained independently by Bollobás [5], Brace and Daykin [8], and Kleitman and Spencer [34]. According to a survey on binary covering arrays [37], Schönheim [51] proved a result that implies Theorem 2.3.3 when n is odd. Another result, equivalent to Theorem 2.3.3, was proved by Gregory and Pullman [26]: they determined the edge clique cover number of the cocktail party graph on $2k$ vertices.

Here, we state the theorem in terms of binary covering arrays of strength 2.

Theorem 2.3.3 (Binary Covering Array Number [32, 34, 50]) For all $k \geq 1$, we have

$$\text{CAN}(2, k, 2) = \min \left\{ n : k \leq \binom{n-1}{\lfloor n/2 \rfloor - 1} \right\}. \quad \blacksquare$$

Poljak and Tuza [48] were also interested in answering Rényi's question: what is the maximum number of qualitatively independent v -partitions of $[n]$?

Let $m(n, v)$ denote the maximum number of v -partitions of $[n]$ in a qualitatively independent collection.

Poljak and Tuza [48] obtained the following upper bound on $m(n, v)$ for all $v \geq 2$.

Theorem 2.3.4 (Poljak and Tuza Bound on $m(n, v)$ [48]) For all integers $v \geq 2$ and $n \geq v$, the maximum number of v -partitions of $[n]$ in a qualitatively independent collection satisfies

$$m(n, v) \leq \frac{1}{2} \binom{\lfloor 2n/v \rfloor}{\lfloor n/v \rfloor}.$$

In terms of covering arrays, Theorem 2.3.4 says that $\text{CAK}(n; 2, v) \leq \frac{1}{2} \binom{\lfloor 2n/v \rfloor}{\lfloor n/v \rfloor}$. In Corollary 7.4.1, we improve the bound of Poljak and Tuza for all $v \geq 3$ using a new method which produces LYM-like inequalities for qualitatively independent collections of v -partitions of $[n]$, and for other “graph-intersecting collections” to be discussed later.

Gargano, Körner and Vaccaro [24, 25] completely solved an asymptotic problem closely related to Rényi's question.

Theorem 2.3.5 [24, 25] If $v \geq 2$ is fixed, then

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log_2 m(n, v) = \frac{2}{v}. \quad \blacksquare$$

The proof of Theorem 2.3.5 uses information theory and is based on a probabilistic construction using Markov chains. In Chapter 5, we discuss Theorem 2.3.5 and other results of Gargano, Körner and Vaccaro. We also give some slight extensions to their work.

In terms of covering arrays, Theorem 2.3.5 says that

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log_2 \text{CAK}(n; 2, v) = \frac{2}{v}.$$

2.3.3 Bounds on covering array numbers

Here we outline some bounds on $\text{CAN}(t, k, (v_1, \dots, v_k))$. More details can be found in [12]. We assume without loss of generality that $v_1 \geq v_2 \geq \dots \geq v_k$. The following bounds hold for $\text{CAN}(t, k, (v_1, \dots, v_k))$:

$$\prod_{i=1}^t v_i \leq \text{CAN}(t, k, (v_1, \dots, v_k)) \leq \sum_{1 \leq i_1 < \dots < i_t \leq k} v_{i_1} v_{i_2} \dots v_{i_t}.$$

Given an optimal $\text{CA}(N; t, k, (v_1, \dots, v_k))$ (where $v_1 \geq 2$), we can replace the symbol v_1 from the first column with any symbol from $[v_1 - 1]$ to obtain a $\text{CA}(N; t, k, (v_1 - 1, v_2, \dots, v_k))$. Thus

$$\text{CAN}(t, k, (v_1, v_2, \dots, v_k)) \leq \text{CAN}(t, k, (v_1 + 1, v_2, \dots, v_k)).$$

For v -ary covering arrays, the “fusion” operation given in [11] improves the above bound:

$$\text{CAN}(t, k, v) \leq \text{CAN}(t, k, v + 1) - 2.$$

We can always drop a column of a $\text{CA}(n; t, k, (v_1, v_2, \dots, v_k))$ to obtain a $\text{CA}(n; t, k - 1, (v_2, \dots, v_k))$. Thus,

$$\text{CAN}(t, k - 1, (v_2, \dots, v_k)) \leq \text{CAN}(t, k, (v_1, v_2, \dots, v_k)).$$

Suppose X is an optimal $\text{CA}(N; t, k, (v_1, v_2, \dots, v_k))$. Consider the first column which has symbols from $[v_1]$ and let n_a denote the number of times symbol a appears in this column for each $a \in [v_1]$. Assume without loss of generality that $n_1 \leq n_2 \leq \dots \leq n_{v_1}$. Remove all rows of X for which the symbol 1 does not appear in the first column and delete the first column of X . We are left with an $n_1 \times (k - 1)$ array Y which is a $\text{CA}(n_1; t - 1, k - 1, (v_2, \dots, v_k))$, and $v_1 n_1 = \sum_{a \in [v_1]} n_1 \leq \sum_{a \in [v_1]} n_a = N = \text{CAN}(t, k, (v_1, \dots, v_k))$. Thus,

$$\text{CAN}(t - 1, k - 1, (v_2, \dots, v_k)) \leq \frac{1}{v_1} \text{CAN}(t, k, (v_1, v_2, \dots, v_k)).$$

Using Theorem 2.3.5, Stevens, Moura and Mendelsohn [57] gave the lower bound

$$\text{CAN}(2, k, v) \geq \left\lceil \frac{v \log_2 k}{2} \right\rceil + 1.$$

Other lower bounds can be found in [57].

2.3.4 Constructions for strength-2 covering arrays

We briefly outline some known constructions for covering arrays of strength two.

An optimal construction for binary covering arrays of strength two is known. If $k \leq \binom{n-1}{\lceil n/2 \rceil}$, then a $\text{CA}(n; 2, k, 2)$ exists: the columns are simply k distinct binary n -tuples, each with $\lceil n/2 \rceil$ ones and a zero as the first entry.

Using finite fields, for each prime power q and integer k such that $2 \leq k \leq q$, we can build an optimal $\text{CA}(q^2; 2, k, q)$. (see Theorem 6.39 in [58]). Using this construction, we can also build a $\text{CA}(q^2; 2, q+1, q)$ (see Theorem 6.40 in [58]). For every prime power q and integer t such that $1 \leq t \leq q$, there exists a $\text{CA}(q^2-t; 2, q+1+t, q-t)$ [13].

Algebraic methods provide other direct constructions. For all positive integers n such that $n \equiv 10 \pmod{12}$ there exists an optimal $\text{CA}(n^2; 2, 4, n)$ (see Theorem 6.41 in [58]).

Given integers g and l , and a vector $\vec{v} = (v_0, \dots, v_{l-1}) \in (\mathbb{Z}_{g-1} \cup \{\infty\})^l$ such that $v_0 = \infty$ and $v_i \in \mathbb{Z}_{g-1}$ for $1 \leq i \leq l-1$, the ***s-apart differences*** of $\vec{v}$ are given by $D_s = \{(v_j - v_i) \pmod{g-1} : j-i \equiv s \pmod{l}, v_i \neq \infty, v_j \neq \infty\}$. When $D_s = \mathbb{Z}_{g-1}$ for $1 \leq s < l$, the vector $\vec{v}$ is a ***(g, l)-cover starter***. Meagher and Stevens [44] show that the existence of a (g, l) -cover starter implies the existence of a $\text{CA}(l(g-1)+1; 2, l, g)$.

There are many recursive constructions for covering arrays in which a larger covering array is built using smaller covering arrays as the ingredients, the simplest being the ***product construction*** of two strength-2 covering arrays (see Theorem 4.1 in Colbourn's survey [12]), which we now outline. Given a $\text{CA}(n; 2, k, v)$ and a $\text{CA}(m; 2, l, v)$, we build the product of these arrays, a $\text{CA}(n+m; 2, kl, v)$ as follows: Place l copies of the $\text{CA}(n; 2, k, v)$ side by side obtaining a $n \times kl$ array. Denote by C_i the i^{th} copy. Below each copy C_i place, side by side, k copies of the i^{th} column of the $\text{CA}(m; 2, l, g)$, yielding an $(n+m) \times kl$ array A . It is easy to verify that A forms a $\text{CA}(n+m; 2, kl, g)$.

Early papers on constructions for v -ary covering arrays of strength 2 were given by Stevens and Mendelsohn [55, 56]. Constructions for mixed alphabet covering arrays of strength 2 were given by Moura, Stardom, Stevens and Williams [46] and Colbourn, Martirosyan, Mullen, Shasha, Sherwood, and Yucas [15].

A survey on covering arrays of general strength, including many constructions, is given by Colbourn [12]. More recent constructions and classification results can be found in the paper by Colbourn, Kéri, Rivas Soriano, and Schlage-Puchta [11].

2.4 Covering arrays on graphs

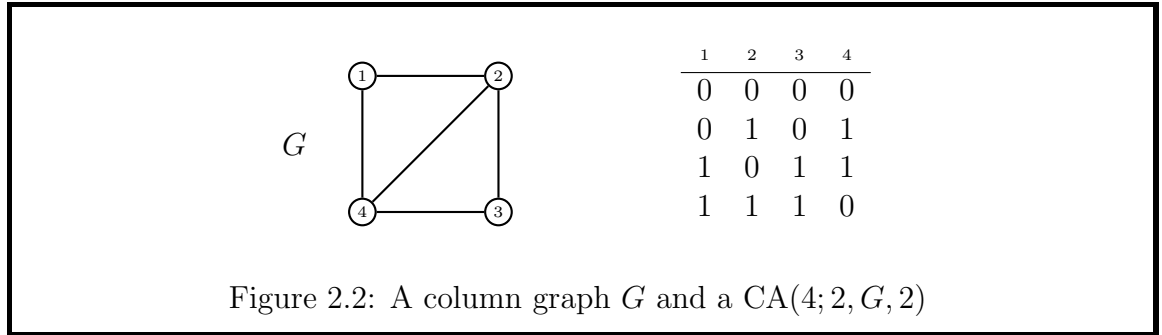
In this section, we outline basic definitions and results regarding covering arrays on graphs. For more details, see the following references of Meagher and Stevens [42, 43].

Covering arrays on graphs are covering arrays of strength $t = 2$ except for the fact that not every pair of columns is required to be qualitatively independent. They have an associated graph structure to encode which pairs of columns should be qualitatively independent.

Remark 2.4.1 In Chapter 3, we define a generalization of covering arrays on graphs in which we use two different graphs as accessories to the array. To avoid confusion, we refer to the graph of a covering array on a graph as a *column graph*.

A *column graph* is a simple graph G on k vertices labelled $1, \dots, k$. A *v -ary covering array on a column graph* G with $|V(G)| = k$, denoted $\text{CA}(n; 2, G, v)$, is an $n \times k$ array with symbols from the alphabet $[v]$ such that pairs of columns corresponding to adjacent vertices of G are qualitatively independent v -ary n -tuples.

The smallest n for which a $\text{CA}(n; 2, G, v)$ exists, denoted $\text{CAN}(2, G, v)$, is the *v -ary covering array number of the column graph G* .



It is easy to see that a $\text{CA}(n; 2, K_k, v)$ on the complete column graph K_k is simply a $\text{CA}(n; 2, k, v)$. Moreover, for a graph G with $|V(G)| = k$, we always have $\text{CAN}(2, G, v) \leq \text{CAN}(2, k, v)$; not all pairs of distinct columns in a $\text{CA}(n; 2, G, v)$ need to be qualitatively independent. In other words, the bound follows from the inclusion $G \subseteq K_k$.

In Figure 2.2 we give an example of a column graph G and an optimal $\text{CA}(4; 2, G, 2)$, taken from [43]. Since 1 and 3 are nonadjacent vertices of G , the first and third

columns of the $\text{CA}(4; 2, G, 2)$ need not be qualitatively independent. Indeed, we see that they are not qualitatively independent: neither $\{(1, 0), (3, 1)\}$ nor $\{(1, 1), (3, 0)\}$ are covered by those two columns. The other pairs of columns all correspond to adjacent pairs of vertices of G and hence are qualitatively independent.

Covering arrays on graphs are related to graph homomorphisms. If, for column graphs G and H , we have a homomorphism $G \rightarrow H$, then $\text{CAN}(2, G, v) \leq \text{CAN}(2, H, v)$ (see Lemma 1 in [43]). Since there are homomorphisms $K_{\omega(G)} \rightarrow G \rightarrow K_{\chi(G)}$, for any column graph G , we have

$$\text{CAN}(2, K_{\omega(G)}, v) \leq \text{CAN}(2, G, v) \leq \text{CAN}(2, K_{\chi(G)}, v).$$

In fact, finding the v -ary covering array number of a column graph G is equivalent to the $\text{QI}(n, v)$ -colouring problem for a special target graph, $\text{QI}(n, v)$, defined by Meagher and Stevens [42, 43]. For two positive integers v and n such that $n \geq v^2$, the **qualitative independence graph**, denoted $\text{QI}(n, v)$, has as its vertices all v -ary n -tuples in which each symbol from $[v]$ occurs at least v times; additionally, the first appearance of each symbol $a \in [v]$ of a v -ary n -tuple in $V(\text{QI}(n, v))$ occurs in alphabetic order. Two vertices are adjacent in $\text{QI}(n, v)$ if and only if they are a qualitatively independent pair of v -ary n -tuples.

For a column graph G and nonnegative integers v and n such that $n \geq v^2$, there exists a $\text{CA}(n; 2, G, v)$ if and only if there is a homomorphism $G \rightarrow \text{QI}(n, v)$. Moreover, if there exists a $\text{CA}(n; 2, G, v)$, then $\chi(G) \leq \chi(\text{QI}(n, v))$ and similarly, $\omega(G) \leq \omega(\text{QI}(n, v))$.

The clique number and chromatic number for the qualitative independence graph $\text{QI}(n, 2)$ are determined in [42, 43].

Meagher and Stevens [43] showed that the binary covering array number of a column graph G lies within the following range of at most two values:

$$\text{CAN}(2, K_{\chi(G)}, 2) - 1 \leq \text{CAN}(2, G, 2) \leq \text{CAN}(2, K_{\chi(G)}, 2).$$

Moreover, if $\text{CAN}(2, K_{\chi(G)}, 2)$ is odd, then $\text{CAN}(2, G, 2) = \text{CAN}(2, K_{\chi(G)}, 2)$.

Meagher and Stevens [42, 43] determined the core of $\text{QI}(n, 2)$: for n even, the core is $K_{\frac{1}{2}\binom{n}{n/2}}$; for n odd, the core of $\text{QI}(n, 2)$ is the induced subgraph of $\text{QI}(n, 2)$ containing the vertices of weight $\lfloor n/2 \rfloor$. Newman [47] proved that $\text{QI}(9, 3)$ is a core. Beyond these cases, we do not know the cores of qualitative independence graphs.

2.5 CAFES

We briefly summarize some basic definitions and results regarding covering arrays avoiding forbidden edges. All definitions and results in this section are given in the paper by Danziger, Mendelsohn, Moura and Stevens [19], except when explicitly referenced otherwise.

Covering arrays avoiding forbidden edges, CAFEs for short, are a generalization of covering arrays of strength 2 in which specified pairwise interactions are forbidden from appearing within any row of the array. CAFEs are defined using an accessory graph that encodes forbidden pairwise interactions of a given testing problem.

Let k and v_i , $i \in [k]$ be positive integers. A **forbidden edges graph** is a k -partite graph with vertices labelled by factor-value pairs (i, a_i) such that $i \in [k]$ and $a_i \in [v_i]$. For each $i \in [k]$, the part $P_i = \{(i, a) : a \in [v_i]\}$ corresponds to the values in factor i . The **family of forbidden edges graphs**, denoted $\mathcal{G}_{(v_1, \dots, v_k)}$, is the family of k -partite forbidden edges graphs with k parts of sizes $v_1, \dots, v_k$, respectively. If, for all $i \in [k]$, we have $v_i = v$, then we use $\mathcal{G}_{k,v}$ to denote $\mathcal{G}_{(v, \dots, v)}$. The edges of a graph $G \in \mathcal{G}_{(v_1, \dots, v_k)}$ are called **forbidden edges**; forbidden edges correspond to forbidden pairwise interactions of a testing problem. Each pairwise interaction $\{(i, a_i), (j, a_j)\}$, where $i \neq j$ and $\{(i, a_i), (j, a_j)\} \notin E(G)$, is called a **required interaction**.

A k -tuple $T = (a_1, \dots, a_k) \in [v_1] \times \dots \times [v_k]$ is said to be a **k -tuple avoiding** $G \in \mathcal{G}_{(v_1, \dots, v_k)}$ if, for all $i, j \in [k]$, we have $\{(i, a_i), (j, a_j)\} \notin E(G)$.

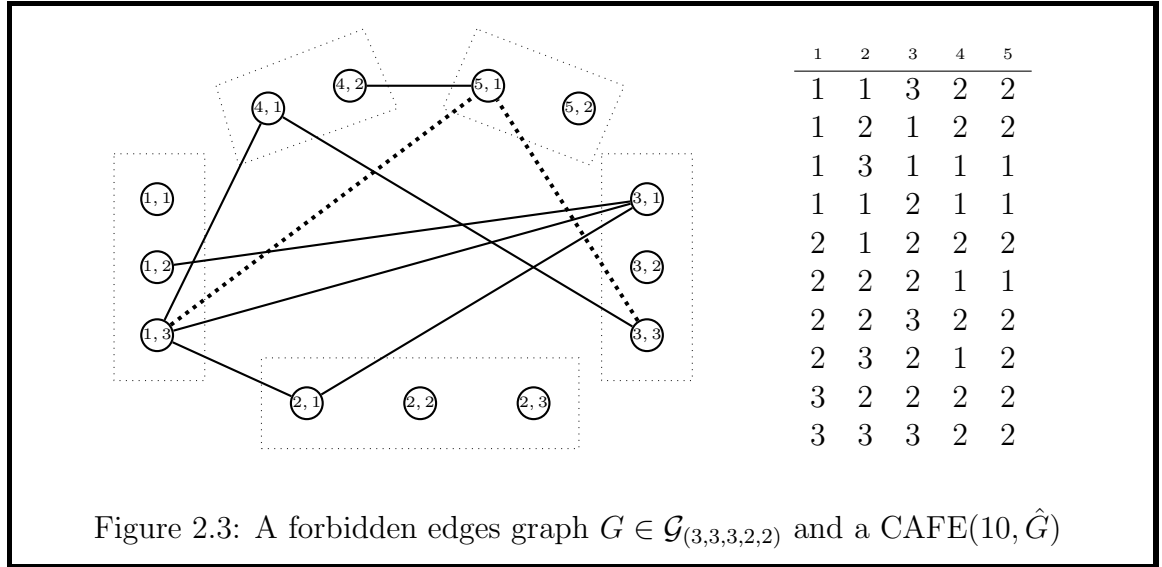
A **CAFE** for a forbidden edges graph $G \in \mathcal{G}_{(v_1, \dots, v_k)}$, denoted $\text{CAFE}(n, G)$, is an $n \times k$ array with columns labelled $1, \dots, k$. For each $i \in [k]$, column i has symbols from the alphabet $[v_i]$. Each row forms a k -tuple avoiding G . Moreover, for all pairs of vertices $(i, a_i), (j, a_j) \in V(G)$ with $i \neq j$, if $\{(i, a_i), (j, a_j)\} \notin E(G)$, then there exists a row that covers the required interaction $\{(i, a_i), (j, a_j)\}$.

The **CAFE number** for a forbidden edges graph $G \in \mathcal{G}_{(v_1, \dots, v_k)}$, denoted $\text{CAFEN}(G)$, is the minimum integer n for which a $\text{CAFE}(n, G)$ exists, if a CAFE for G exists; if a CAFE for G does not exist, then we write $\text{CAFEN}(G) = +\infty$.

A **k -uniform edge clique cover** of a graph G is an edge clique cover of G consisting entirely of k -cliques. If $G \in \mathcal{G}_{(v_1, \dots, v_k)}$, then determining $\text{CAFEN}(G)$ is equivalent to determining the k -uniform edge clique cover number of a specific subgraph of the complement of G (see Proposition 5 in [19]).

Not every forbidden edges graph $G \in \mathcal{G}_{(v_1, \dots, v_k)}$ admits a CAFE. A required interaction $I = \{(i, a_i), (j, a_j)\}$ is **consistent with** G if there exists a k -tuple $(r_1, \dots, r_k) \in [v_1] \times \dots \times [v_k]$ that covers I and avoids G . The graph G is **consistent** if all required interactions of G are consistent with G . Indeed, there exists a $\text{CAFE}(n, G)$ if and only if G is consistent.

If a forbidden edges graph $G \in \mathcal{G}_{(v_1, \dots, v_k)}$ is not consistent, then the minimal super-graph of G that is consistent, denoted $\hat{G}$, is the **avoidance closure** of G . The avoidance closure of G always exists and it is unique. Each required interaction of G that is inconsistent becomes a forbidden edge in $\hat{G}$. The most extreme situation occurs when the avoidance closure of G is a complete k -partite graph (all pairwise interactions are forbidden).



In Figure 2.3, we give an example, extracted from [19], of a forbidden edges graph $G \in \mathcal{G}_{(3,3,3,2,2)}$ (with solid black edges). The graph G is not consistent since the required interactions $\{(1, 3), (5, 1)\}$ and $\{(3, 3), (5, 1)\}$ are not consistent with G ; this can be seen as follows: Since $\{(1, 3), (4, 1)\}$ is forbidden, any consistent 5-tuple that covers the factor-value pair $(1, 3)$ necessarily covers the factor-value pair $(4, 2)$. Likewise, since $\{(4, 2), (5, 1)\}$ is forbidden, any consistent 5-tuple that covers $(5, 1)$ necessarily covers $(4, 1)$. Together, these two properties make it impossible to cover the factor-value pairs $(1, 3)$ and $(5, 1)$ in one consistent 5-tuple. For similar reasons, $\{(3, 3), (5, 1)\}$ is not consistent with G . By adding these two edges (dashed edges), we obtain the avoidance closure $\hat{G}$. A CAFE for $\hat{G}$ is also given.

A characterization of consistent forbidden edges graphs G in the family $\mathcal{G}_{k,2}$ is given in [19]. In Proposition 8.2.3, we explicitly state this characterization and show how it applies to a slightly more general setting.

Obvious lower and upper bounds on the CAFE number for a consistent forbidden edges graph $G \in \mathcal{G}_{(v_1, \dots, v_k)}$ are given by

$$\max_{1 \leq i < j \leq k} \{v_i v_j - |E^{i,j}(G)|\} \leq \text{CAFEN}(G) \leq \sum_{1 \leq i < j \leq k} (v_i v_j - |E^{i,j}(G)|),$$

where $E^{i,j}(G)$ denotes the set of edges with one end in part i and the other end in part j . These bounds are attained for forbidden edges graphs with $k = 2$ parts, but for $k \geq 3$ the upper bound can be tightened [40, 41]. If $G \in \mathcal{G}_{(v_1, \dots, v_k)}$ is consistent, then

$$\text{CAFEN}(G) \leq \sum_{1 \leq i < j \leq k} v_i v_j - |E(G)| - \binom{k}{2} + 1.$$

Constructions of CAFES and asymptotic results on CAFE numbers are given in [19]. Computational complexity results for optimization and existence of CAFES are also given. In [40, 41], it is shown that determining whether $\text{CAFEN}(G) \leq n$ for an arbitrary forbidden edges graph $G \in \mathcal{G}_{k,2}$ and a given integer n is an NP-complete problem.

Variable strength covering arrays

Variable strength covering arrays, VCAs for short, are another generalization of covering arrays, which we briefly mention here; we refer the reader to Raaphorst's thesis [49] for more details.

Let Δ be an abstract simplicial complex (downset) with vertex set $V(\Delta) = [k]$, and let Λ denote the set of facets of Δ . A **variable strength covering array** of Λ , denoted $\text{VCA}(n; \Lambda, v)$, is an $n \times k$ array with symbols from the alphabet $[v]$ and columns labelled $1, \dots, k$ such that, for all $A \in \Lambda$, the columns indexed by the elements of A cover each of the ordered $|A|$ -tuples of symbols in $[v]^{|A|}$ in at least one row. The **VCA number** of Λ , denoted $\text{VCAN}(\Lambda, v)$, is the smallest integer n such that a $\text{VCA}(n; \Lambda, v)$ exists.

Chapter 3

Covering arrays on column graphs and alphabet graphs

In this chapter, we define a generalization of covering arrays on graphs: we add an alphabet graph to encode the pairs of symbols to be covered. In Section 3.1, we introduce these arrays. In Section 3.2, we define H -dependence graphs, a generalization of qualitative independence graphs where the alphabet graph H is incorporated. Many homomorphism results for covering arrays on graphs extend to include the alphabet graph. In Section 3.3, we discuss covering arrays with alphabet graphs. In Section 3.4, we define covering arrays on directed column graphs.

These concepts provide the setup for Chapter 4, wherein we study a particular alphabet graph and directed column graphs.

3.1 Column graphs and alphabet graphs

A **column graph** is an undirected graph with no loops and no parallel edges. An **alphabet graph** is an undirected graph that contains no parallel edges, but may contain loops.

Definition 3.1.1 Let G be a column graph with $V(G) = [k]$ and let H be an alphabet graph with $V(H) = [v]$. A **covering array on column graph G and alphabet graph H** , denoted $\text{CA}(n; 2, G, H)$, is an $n \times k$ array with symbols from the alphabet $[v]$ such that

- for every edge $ij \in E(G)$ and for every edge $ab \in E(H)$, there exist rows $r_l = (r_{l1}, \dots, r_{lk})$ and $r_m = (r_{m1}, \dots, r_{mk})$ such that $(r_{li}, r_{lj}) = (a, b)$ and $(r_{mi}, r_{mj}) = (b, a)$.

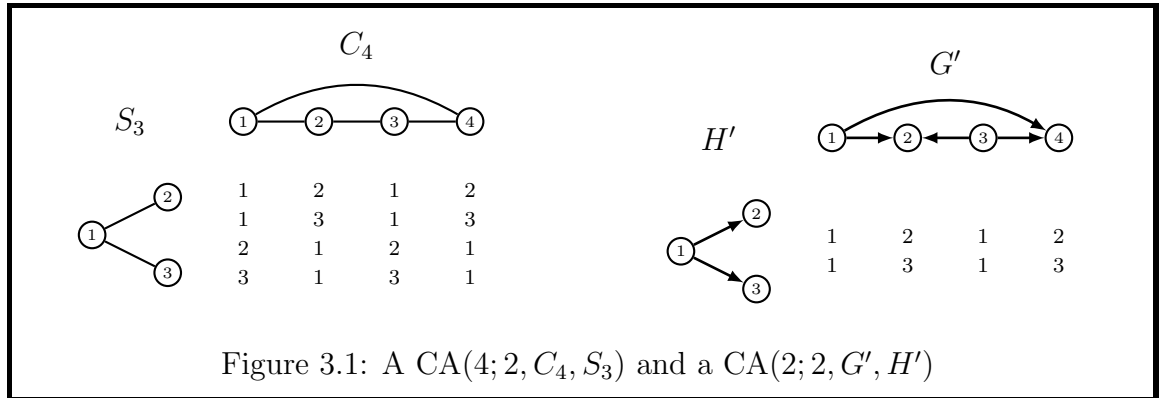
The **covering array number**, denoted $\text{CAN}(2, G, H)$, is the smallest integer n for which a $\text{CA}(n; 2, G, H)$ exists.

Remark 3.1.2 Our notation for covering arrays on column graphs and alphabet graphs includes a strength parameter “2”. Our definition for these arrays is only applicable for strength 2, making the “2” superfluous in our notation $\text{CA}(n; 2, G, H)$. We opted to record the strength nevertheless as covering array notation may then consistently be read as follows:

$\text{CA}(\text{ number rows } ; \text{ strength } , \text{ column information } , \text{ alphabet information })$.

Similarly, notation for the covering array number is consistently in the following form:

$\text{CAN}(\text{ strength } , \text{ column information } , \text{ alphabet information })$.



Example 3.1.3 Take the column graph $G = C_4$ (the undirected 4-cycle) and alphabet graph $H = S_3$ (the star on 3 vertices). The left side of Figure 3.1 shows an optimal $\text{CA}(4; 2, C_4, S_3)$. The right side of Figure 3.1 will be explained in Section 3.4.

Notice that a $\text{CA}(n; 2, G, K_v^{\text{loop}})$ is simply a covering array on G , that is, a $\text{CA}(n; 2, G, v)$. A $\text{CA}(n; 2, K_k, K_v^{\text{loop}})$ is simply a classical covering array of strength 2, that is, a $\text{CA}(n; 2, k, v)$.

Let G be a column graph and let H be an alphabet graph. If $ij \in E(G)$ and $ab \in E(H)$, then the pairwise interaction $I = \{(i, a), (j, b)\}$ is called a **required interaction** with respect to G and H . If an interaction $I \subseteq V(G) \times V(H)$ is not required with respect to G and H , then we say that I is **optional** with respect to G and H .

3.2 H-dependence graphs

In this section, we show that the problem of determining $\text{CAN}(2, G, H)$ is equivalent to a graph-colouring problem for the appropriate target corresponding to the alphabet graph H . We define these targets, called H -dependence graphs, and we some properties held by their cores. Dependence graphs are the natural extension of qualitative independence graphs. The terminology “ H -dependent” was introduced by Gargano, Körner, and Vaccaro [25].

Definition 3.2.1 Let H be an alphabet graph with $V(H) = [v]$, and let $\vec{x} = (x_1, \dots, x_n)$ and $\vec{y} = (y_1, \dots, y_n)$ be two v -ary n -tuples, that is, $\vec{x}, \vec{y} \in [v]^n$. If, for every edge $ab \in E(H)$, there exist indices $i, j \in [n]$ such that $(x_i, y_i) = (a, b)$ and $(x_j, y_j) = (b, a)$, then $\vec{x}$ and $\vec{y}$ are **H -dependent**.

Let $v \geq 2$ and consider the complete graph with loops K_v^{loop} . It is easy to see that two v -partitions of $[n]$ are qualitatively independent if and only if they are K_v^{loop} -dependent. In a covering array on a column graph G , every two distinct columns corresponding to an edge of G must be K_v^{loop} -dependent. Analogously, every two distinct columns of a $\text{CA}(n; 2, G, H)$ must be H -dependent whenever the corresponding vertices of the column graph G are adjacent.

Meagher and Stevens [42, 43] defined qualitative independence graphs to characterize covering arrays on graphs. We define analogous target graphs using the notion of H -dependence; these new targets characterize the problem of covering arrays on column and alphabet graphs in terms of graph homomorphisms.

Definition 3.2.2 Let H be an alphabet graph with $V(H) = [v]$. The **H -dependence graph**, denoted $\text{QI}(n, H)$, is the graph with vertex set $V(\text{QI}(n, H)) = [v]^n$ and $\vec{x}\vec{y} \in E(\text{QI}(n, H))$ if and only if $\vec{x}$ and $\vec{y}$ are H -dependent.

The problem of determining $\text{CAN}(2, G, H)$ for a given column graph and alphabet graph is now equivalent to a graph-colouring problem. The next two results are straightforward extensions of the analogous results given by Meagher and Stevens [43] (see Theorem 1, Lemma 1 and Corollary 1 in [43]).

Proposition 3.2.3 Let G be a column graph and let H be an alphabet graph. There exists a $\text{CA}(n; 2, G, H)$ if and only if there is a homomorphism $G \rightarrow \text{QI}(n, H)$. Thus,

$$\text{CAN}(2, G, H) = \min\{n : G \rightarrow \text{QI}(n, H)\}.$$

[proof] Let $V(G) = [k]$ and $V(H) = [v]$. If there exists a $\text{CA}(n; 2, G, H)$, then its columns are vertices of $\text{QI}(n, H)$. Define a map $f : G \rightarrow \text{QI}(n, H)$ given by $f(i) = C_i$ for each $i \in [k] = V(G)$, where C_i denotes the i th column of the $\text{CA}(n; 2, G, H)$ and $C_i = (c_{1i}, \dots, c_{ni}) \in [v]^n$ for each $i \in [k]$. If $ij \in E(G)$, then, for all $ab \in E(H)$, there are indices $l, l' \in [n]$ such that $c_{li} = a$ and $c_{lj} = b$ and $c_{l'i} = b$ and $c_{l'j} = a$. By definition of the H -dependence graph $\text{QI}(n, H)$, the vertices C_i and C_j are adjacent in $\text{QI}(n, H)$. Thus, f is a homomorphism.

If there exists a homomorphism $f : G \rightarrow \text{QI}(n, H)$, then we can build an $n \times k$ array with columns $C_1, \dots, C_k$ given by $C_i = f(i)$ for each $i \in [k]$. It is easy to see this array is a $\text{CA}(n; 2, G, H)$. ■

Proposition 3.2.4 Let H be an alphabet graph and let G_1, G_2 and G be column graphs. If there is a homomorphism $G_1 \rightarrow G_2$, then

$$\text{CAN}(2, G_1, H) \leq \text{CAN}(2, G_2, H).$$

In particular, we have

$$\text{CAN}(2, K_{\omega(G)}, H) \leq \text{CAN}(2, G, H) \leq \text{CAN}(2, K_{\chi(G)}, H),$$

where $\omega(G)$ and $\chi(G)$ denote the clique number and chromatic number of G , respectively.

[proof] Suppose we have an optimal $\text{CA}(n; 2, G_2, H)$ with columns $C_1, \dots, C_{|V(G_2)|}$. Let $f : G_1 \rightarrow G_2$ be a homomorphism and define an $n \times |V(G_1)|$ array where the i th column is the column $C_{f(i)}$. If $ij \in E(G_1)$, then $f(i)f(j) \in E(G_2)$. This means that column $C_{f(i)}$ is H -dependent with column $C_{f(j)}$ as required. ■

Considering Proposition 3.2.3, we ask the following question:

Question 3.2.5 For a given alphabet graph H , what is the core of $\text{QI}(n, H)$?

Let $\text{QI}(n, H)^\bullet$ denote the core of $\text{QI}(n, H)$.

Isolated vertices of $\text{QI}(n, H)$ are superfluous with respect to the core $\text{QI}(n, H)^\bullet$. Notice that every non-isolated vertex $\vec{x} \in V(\text{QI}(n, H))$ must have each symbol $a \in [v]$ occurring at least $|N_H(a)|$ times; here, we use $N_H(a)$ to denote the neighbourhood of a in H , which includes a if H has a loop $aa \in E(H)$. In order for $\text{QI}(n, H)$ to have at least one non-isolated vertex, n has to be large enough:

$$n \geq \sum_{a \in V(H)} |N_H(a)|.$$

In other words, if $n < \sum_{a \in V(H)} |N_H(a)|$, then all vertices of $\text{QI}(n, H)$ are isolated; in this case, the core is the trivial graph, that is, $\text{QI}(n, H)^\bullet = K_1$.

Lemma 3.2.6 Let H be an alphabet graph with $V(H) = [v]$. If $n \geq \sum_{a \in V(H)} |N_H(a)|$, then the core $\text{QI}(n, H)^\bullet$ is a subgraph of the graph $Q' \subset \text{QI}(n, H)$ such that every vertex $\vec{x} \in V(Q')$ has the following property: for all $a \in [v]$, the symbol a occurs at least $|N_H(a)|$ times as an entry of $\vec{x}$. ■

Consider $H = K_2$. For all n , we show that the core of $\text{QI}(n, K_2)$ is $K_{\binom{n}{\lfloor n/2 \rfloor}}$. The proof is similar to that given by Meagher and Stevens [43] in order to prove that the core of $\text{QI}(n, 2)$ is $K_{\binom{n}{n/2}/2}$ when n is even.

Proposition 3.2.7 Let $n \geq 2$. The core of $\text{QI}(n, K_2)$ is $K_{\binom{n}{\lfloor n/2 \rfloor}}$.

[proof] Let $M_n = \binom{n}{\lfloor n/2 \rfloor}$. Consider the vertices of $\text{QI}(n, K_2)$ as subsets of $[n]$ by letting $\vec{x} = (x_1, \dots, x_n) \in (V(K_2))^n$ represent the set $A \subset [n]$ given by $A = \{i \in [n] : x_i = 1\}$. The $\binom{n}{\lfloor n/2 \rfloor}$ vertices corresponding to sets of cardinality $\lfloor n/2 \rfloor$ clearly form a clique of $\text{QI}(n, K_2)$. Thus, $K_{M_n} \subseteq \text{QI}(n, K_2)$.

Using Theorem 2.1.5, we decompose the poset of subsets of $[n]$ into symmetric chains. Define a map $f : V(\text{QI}(n, K_2)) \rightarrow V(\text{QI}(n, K_2))$ as follows. For each subset $A \in V(\text{QI}(n, K_2))$ let $f(A)$ be the $\lfloor n/2 \rfloor$ -set in the chain containing A . We claim that f is a retraction of $\text{QI}(n, K_2)$ to $K_{\binom{n}{\lfloor n/2 \rfloor}}$. If $\{A, B\} \in E(\text{QI}(n, K_2))$, then $A \not\subseteq B$ and $B \not\subseteq A$ since A and B must be K_2 -dependent. Consequently, A and B must

belong to different chains and $f(A)$ and $f(B)$ must be two distinct $\lfloor n/2 \rfloor$ -sets. Thus, $\{f(A), f(B)\} \in E(\text{QI}(n, K_2))$.

It follows that $\text{QI}(n, K_2)$ retracts to K_{M_n} , and since K_{M_n} is a core, it follows that K_{M_n} must be the core of $\text{QI}(n, K_2)$. ■

Corollary 3.2.8 If G is an undirected column graph, then

$$\text{CAN}(2, G, K_2) = \min \left\{ n : \chi(G) \leq \binom{n}{\lfloor n/2 \rfloor} \right\}.$$

[proof] By Proposition 3.2.3, $\text{CAN}(2, G, K_2) = \min\{n : G \rightarrow \text{QI}(n, K_2)\}$. It remains to show that $G \rightarrow \text{QI}(n, K_2)$ if and only if $\chi(G) \leq \binom{n}{\lfloor n/2 \rfloor}$.

Let $M_n = \binom{n}{\lfloor n/2 \rfloor}$. By Proposition 2.2.2, $\text{QI}(n, K_2)$ is homomorphically equivalent to its core, which, by Proposition 3.2.7, is the complete graph K_{M_n} . Thus, there exists a homomorphism of G to $\text{QI}(n, K_2)$ if and only if there exists a homomorphism of G to K_{M_n} . By Proposition 2.2.1, there exists a homomorphism of G to K_{M_n} if and only if $\chi(G) \leq M_n$. ■

3.3 Covering arrays with alphabet graphs

Here we define covering arrays with alphabet graphs which require all pairs of columns to cover all pairs of adjacent vertices of an alphabet graph H .

Definition 3.3.1 Let H be an alphabet graph. A *covering array with alphabet graph* H , denoted $\text{CA}(n; 2, k, H)$, is a $\text{CA}(n; 2, K_k, H)$. The minimum integer n for which there exists a $\text{CA}(n; 2, k, H)$, denoted $\text{CAN}(2, k, H)$, is the *covering array number*. The maximum integer k for which there exists a $\text{CA}(n; 2, k, H)$, denoted $\text{CAK}(n; 2, H)$, is the *column number*.

Corollary 3.3.2 Let H be an alphabet graph. There exists a $\text{CA}(n; 2, k, H)$ if and only if $\omega(\text{QI}(n, H)) \geq k$.

[proof] Recall that a $\text{CA}(n; 2, k, H)$ is simply a $\text{CA}(n; 2, K_k, H)$. By Proposition 3.2.3, there is a $\text{CA}(n; 2, k, H)$ if and only if there is a homomorphism $K_k \rightarrow \text{QI}(n, H)$. There is a homomorphism $K_k \rightarrow \text{QI}(n, H)$ if and only if the clique number satisfies $\omega(\text{QI}(n, H)) \geq k$. ■

In light of Corollary 3.3.2, we ask the following question:

Question 3.3.3 Let H be an alphabet graph. What is the clique number of the H -dependence graph $\text{QI}(n, H)$?

For alphabet graphs without loops, we get the following bounds on column numbers.

Proposition 3.3.4 If H is an alphabet graph with $|V(H)| = v$ such that H has no loops, then $\text{CAK}(n; 2, K_v) \leq \text{CAK}(n; 2, H) \leq \text{CAK}(n; 2, K_{\chi(H)})$.

[proof] Since $H \subseteq K_v$, any collection of v -ary n -tuples that is K_v -dependent is clearly H -dependent. Thus, $\text{CAK}(n; 2, H) \geq \text{CAK}(n; 2, K_v)$.

Let $\vec{x}_1, \dots, \vec{x}_k$ be the columns of a $\text{CA}(n; 2, k, H)$, where $k = \text{CAK}(n; 2, H)$ and $\vec{x}_i = (x_{1i}, \dots, x_{ni})$ for each $i \in [k]$. Let $V_1, \dots, V_{\chi(H)}$ be the colour classes of a $\chi(H)$ -colouring of H . For each $a \in V(H)$, denote by $c(a)$ the colour class to which a belongs. For each $\vec{x}_i$, define a new n -tuple $\vec{x}_i'$ by $\vec{x}_i' = (c(x_{1i}), \dots, c(x_{ni}))$.

We claim that $\vec{x}_i' \neq \vec{x}_j'$ whenever $\vec{x}_i \neq \vec{x}_j$, and the collection $\vec{x}_1', \dots, \vec{x}_k'$ is $K_{\chi(H)}$ -dependent.

First, if $\vec{x}_i \neq \vec{x}_j$, then, for every edge $ab \in E(H)$, we have an index $r \in [n]$ such that $x_{ri} = a$ and $x_{rj} = b$. The colour classes of a and b must be distinct since $ab \in E(H)$, thus $c(x_{ri}) \neq c(x_{rj})$, so $\vec{x}_i' \neq \vec{x}_j'$ as required.

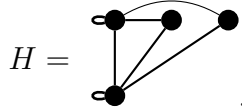
To see that $\vec{x}_i'$ and $\vec{x}_j'$ are $K_{\chi(H)}$ -dependent, take any two distinct colour classes V_p and V_q . Since the colouring $V_1, \dots, V_{\chi(H)}$ is optimal, there must be an edge of H with one end in V_p and its other end in V_q . If $ab \in E(H)$ is such an edge and $a \in V_p$, $b \in V_q$, then, for some indices $r, s \in [n]$, we have $x_{ri} = a$ and $x_{rj} = b$ while $x_{si} = b$ and $x_{sj} = a$. Consequently, $c(x_{ri}) = p$ and $c(x_{rj}) = q$ and $c(x_{si}) = q$ and $c(x_{sj}) = p$. It now follows that $\vec{x}_i'$ and $\vec{x}_j'$ are $K_{\chi(H)}$ -dependent. ■

In Chapters 6 and 7, we develop a method for deriving upper bounds on the maximum number of columns in a covering array with alphabet graph H and a fixed number of rows.

3.3.1 Expanding alphabets

Here we describe one potential testing application for covering arrays with alphabet graphs. Suppose we have a testing problem on k factors with v values each. We run a test suite based on a covering array $\text{CA}(n; 2, k, v)$. Later, each of the factors of our testing problem has expanded to include w new values as well as the v “old” values. We would like a covering array which tests all the new values together as well as all the pairwise interactions between old values and new values. This can be accomplished with a $\text{CA}(n'; 2, k, v + w)$; however, we do not require pairwise interactions corresponding to two old values to be retested.

In this situation, using a $\text{CA}(m; 2, k, H)$ is preferable, where H is the complete graph K_w^{loop} joined to v isolated vertices. For example, if we want to expand the alphabet of a binary $\text{CA}(n; 2, k, 2)$ with as few rows as possible in order to obtain a 4-ary $\text{CA}(n'; 2, k, 4)$, then $\text{CAN}(2, k, H)$ represents the fewest rows that have to be appended to the rows of a $\text{CA}(n; 2, k, 2)$ in order to obtain a $\text{CA}(n + \text{CAN}(2, k, H); 2, k, 4)$, where



Alphabet graphs of the above form, a complete graph with loops joined to several otherwise isolated vertices, fall into the category of “strong” graphs. In Section 6.4, we define strong graphs and show that they play a pivotal role in our method for deriving LYM inequalities.

3.4 Directed column and alphabet graphs

In this section, we make the observation that the definition of covering arrays on column graphs and alphabet graphs can easily be extended to directed graphs. We get analogous homomorphism results for directed H -dependence graphs as well. This section provides the general setup for Chapter 4, wherein we concentrate on one particular directed alphabet graph.

A **directed column graph** is a directed graph G such that G has no loops and no parallel arcs. A **directed alphabet graph** is a directed graph H such that H does not contain parallel arcs, but H may contain loops.

Definition 3.4.1 Let G be a directed column graph with $V(G) = [k]$ and let H be a directed alphabet graph with $V(H) = [v]$. A **covering array on directed column graph G and directed alphabet graph H** , denoted $\text{CA}(n; 2, G, H)$, is an $n \times k$ array with symbols from the alphabet $[v]$ such that

- for every arc $ij \in E(G)$ and for every arc $ab \in E(H)$, there exists a row $r_i = (r_{i1}, \dots, r_{ik})$ such that $(r_{li}, r_{lj}) = (a, b)$.

The **covering array number**, denoted $\text{CAN}(2, G, H)$, is the smallest integer n for which a $\text{CA}(n; 2, G, H)$ exists.

Example 3.4.2 The right side of Figure 3.1 shows an example of a directed column graph G' (where G' is an orientation of C_4) and a directed alphabet graph H' (where H' is an orientation of the star S_3) as well as an optimal $\text{CA}(2; 2, G', H')$.

Definition 3.4.3 Let H be a directed alphabet graph with $V(H) = [v]$. Let $\vec{x} = (x_1, \dots, x_n)$ and $\vec{y} = (y_1, \dots, y_n)$ be two v -ary n -tuples, that is, $\vec{x}, \vec{y} \in [v]^n$. If, for every arc $ab \in E(H)$, there exists an index $i \in [n]$ such that $x_i = a$ and $y_i = b$, then $\vec{x}$ is **H -dependent** with $\vec{y}$.

When H is a directed alphabet graph, the notion of two n -tuples being H -dependent also has a direction. Even if $\vec{x}$ is H -dependent with $\vec{y}$, it might still be the case that $\vec{y}$ is not H -dependent with $\vec{x}$. When H is undirected, being H -dependent is a symmetric relation; alternatively, we can imagine H is directed by replacing each edge $\{a, b\} \in E(H)$ by two oppositely directed arcs ab and ba .

Definition 3.4.4 Let H be a directed alphabet graph with $V(H) = [v]$. The (directed) **H -dependence graph**, denoted $\text{QI}(n, H)$, is the graph with vertex set $V(\text{QI}(n, H)) = [v]^n$ and arcs $\vec{x}\vec{y} \in E(\text{QI}(n, H))$ whenever $\vec{x}$ is H -dependent with $\vec{y}$.

For directed graphs, we get homomorphism results analogous to those we gave for the undirected version of the problem.

Proposition 3.4.5 Let G be a directed column graph and let H be a directed alphabet graph. There exists a $\text{CA}(n; 2, G, H)$ if and only if there is a homomorphism $G \rightarrow \text{QI}(n, H)$. Thus, $\text{CAN}(2, G, H) = \min\{n : G \rightarrow \text{QI}(n, H)\}$. ■

Proposition 3.4.6 Let H be a directed alphabet graph and let G_1 and G_2 be directed column graphs. If there is a homomorphism $G_1 \rightarrow G_2$, then

$$\text{CAN}(2, G_1, H) \leq \text{CAN}(2, G_2, H).$$



With respect to Question 3.2.5, we can also determine some properties that are held by the cores of H -dependence graphs, when H is a directed alphabet graph. The following lemma is the directed analogue of Lemma 3.2.6.

Lemma 3.4.7 Let H be a directed alphabet graph. If $\text{QI}(n, H)$ has a non-trivial core, then, for each $\vec{x} \in V(\text{QI}(n, H)^\bullet)$, we may assume that $\vec{x}$ satisfies at least one of the two following conditions:

1. each symbol $a \in [v]$ occurs at least $\text{outdeg}_H(a)$ times in $\vec{x}$, or
2. each symbol $a \in [v]$ occurs at least $\text{indeg}_H(a)$ times in $\vec{x}$.

In particular, we need $n \geq \max \left\{ \sum_{a \in V(H)} \text{outdeg}_H(a), \sum_{a \in V(H)} \text{indeg}_H(a) \right\}$.



Chapter 4

Binary covering arrays on directed column graphs

In this chapter, we consider covering arrays on directed column graphs with the directed binary alphabet graph T_2 (the transitive 2-tournament), where $V(T_2) = \{0, 1\}$ and $E(T_2) = \{(0, 1)\}$. We investigate the problem of finding $\text{CAN}(2, G, T_2)$ for directed column graphs G . In Section 4.1, we give bounds relating $\text{CAN}(2, G', T_2)$ to $\text{CAN}(2, G, 2)$, where G' is an orientation of G . In Section 4.2, we give properties of the T_2 -dependence graph $\text{QI}(n, T_2)$ and show that it is a core. In Section 4.3, we show that determining $\text{CAN}(2, G, T_2)$ is NP-complete for arbitrary directed column graphs G . In Section 4.4, we give bounds on $\text{CAN}(2, G, T_2)$ where the column graph G is a k -tournament. In Section 4.5, we consider a specific family of tournaments as column graphs: circular tournaments. We give constructions for covering arrays on circular tournament column graphs with the binary alphabet graph T_2 .

4.1 Bounds for binary covering arrays on directed column graphs

There is a natural correspondence between binary n -tuples and subsets of $[n]$. Let $\vec{x} = (x_1, \dots, x_n)$ and $\vec{y} = (y_1, \dots, y_n)$ be two binary n -tuples. We may consider $\vec{x}$ and $\vec{y}$ as subsets of $[n]$, namely $A = \{i \in [n] : x_i = 1\}$ and $B = \{i \in [n] : y_i = 1\}$. Notice that $\vec{x}$ is T_2 -dependent with $\vec{y}$ if and only if $B \not\subseteq A$.

The columns of a covering array $\text{CA}(n; 2, k, T_2)$ with alphabet graph T_2 correspond to an antichain of subsets of $[n]$. In fact, when a column graph G is undirected (or thought of as a symmetric digraph), the problem of finding a $\text{CA}(n; 2, G, T_2)$ is equivalent to the problem of finding a $\text{CA}(n; 2, G, K_2)$. By Corollary 3.2.8, determining $\text{CAN}(2, G, K_2)$ is equivalent to finding the minimum n such that $\chi(G) \leq \binom{n}{\lfloor n/2 \rfloor}$, and we consider this problem satisfactorily dealt with.

Since T_2 is a directed alphabet graph we are far more interested in covering arrays $\text{CA}(n; 2, G, T_2)$ where G is a directed column graph. We are especially interested in k -tournaments as column graphs with the alphabet graph T_2 . The latter half of this chapter will deal principally with this line of questioning.

We begin our investigation with the following bounds which compare a binary covering array on an undirected graph G to a covering array on column graph G' , an orientation of G , and alphabet graph T_2 .

If G is an undirected graph, then an **orientation** of G is a directed graph G' on $V(G') = V(G)$ such that G' has exactly one of the arcs ab or ba if and only if G contains the undirected edge $\{a, b\}$. If G is a directed graph, then the **reversal** of G is the directed graph G'' with $V(G'') = V(G)$ and arcs $ba \in E(G'')$ if and only if $ab \in E(G)$.

Proposition 4.1.1 Let G be an undirected column graph with $V(G) = [k]$. If G' is an orientation of G , then

$$\frac{1}{2} \text{CAN}(2, G, 2) - 1 \leq \text{CAN}(2, G', T_2) \leq \text{CAN}(2, G, 2) - 1.$$

[proof] Let A be an optimal $\text{CA}(n; 2, G', T_2)$ and let A' denote the array obtained from A by interchanging all zeros and ones. Let G'' denote the reversal of G' . Clearly A' is a $\text{CA}(n; 2, G'', T_2)$. Thus $\text{CAN}(2, G'', T_2) \leq \text{CAN}(2, G', T_2)$. Similarly, $\text{CAN}(2, G', T_2) \leq \text{CAN}(2, G'', T_2)$ so that $\text{CAN}(2, G'', T_2) = \text{CAN}(2, G', T_2)$. The $2n \times k$ array obtained by appending the rows of A to the rows of A' yields a $\text{CA}(2n; 2, G, K_2)$. Adding the constant row of all zeros and the constant row of all ones yields a $\text{CA}(2n+2; 2, G, 2)$. Consequently, $\text{CAN}(2, G, 2) \leq 2 \cdot \text{CAN}(2, G', T_2) + 2$, which gives the lower bound.

Now, take a $\text{CA}(n; 2, G, 2)$. We can assume without loss of generality that the first row is all zeros. Delete this row and we are left with an $\text{CA}(n-1; 2, G', T_2)$, for

any subgraph $G' \subseteq G^*$ of the symmetric digraph G^* . Thus, $\text{CAN}(2, G', T_2) \leq \text{CAN}(2, G, 2) - 1$. ■

We now provide infinite classes of graphs achieving the bounds given in Proposition 4.1.1.

Let G be a nonempty bipartite graph with bipartition (X, Y) . If G' is an orientation of G such that all arcs in G' are oriented from X to Y , then we call G' a **consistent orientation** of G .

Claim 4.1.2 If G' is a consistent orientation of a bipartite graph G , then G' achieves the lower bound of Proposition 4.1.1.

[proof] For any consistent orientation G' of a bipartite graph G , there is a homomorphism $G' \rightarrow T_2$ (map all vertices in X to the vertex $0 \in V(T_2)$ and map all vertices in Y to the vertex $1 \in V(T_2)$). It is easy to see that T_2 -dependence graph $\text{QI}(1, T_2)$ is isomorphic to T_2 , thus $G' \rightarrow \text{QI}(1, T_2)$. By Proposition 3.2.3, it follows that $\text{CAN}(2, G', T_2) \leq 1$. In contrast, a $\text{CA}(n; 2, G, 2)$ requires $n \geq 4$ rows (there are four pairs $(a, b) \in \{0, 1\}^2$ to cover). Thus, for any bipartite column graph G and consistent orientation G' of G , the lower bound of Proposition 4.1.1 is achieved:

$$1 = \frac{1}{2}(4) - 1 \leq \frac{1}{2}\text{CAN}(2, G, 2) - 1 \leq \text{CAN}(2, G', T_2) \leq 1. \quad \blacksquare$$

Claim 4.1.3 If G' is an orientation of a 3-chromatic graph G such that G' is not homomorphic to one of the graphs shown in Figure 4.1, then G' achieves the upper bound of Proposition 4.1.1.

[proof] Let G be a graph such that $\chi(G) = 3$, and let G' be an orientation of G such that G' is not homomorphic to one of the graphs shown in Figure 4.1. Since $G \rightarrow K_3$, there exist homomorphisms $G' \rightarrow G^* \rightarrow K_3^*$, where G^* and K_3^* denote the symmetric digraphs of G and K_3 , respectively. The vertices of $\text{QI}(3, T_2)$ corresponding to subsets of rank one induce a copy of K_3^* , thus, there exists a homomorphism $K_3^* \rightarrow \text{QI}(3, T_2)$. Consequently, $G' \rightarrow \text{QI}(3, T_2)$. By Proposition 3.2.3, it follows that $\text{CAN}(2, G', T_2) \leq 3$.

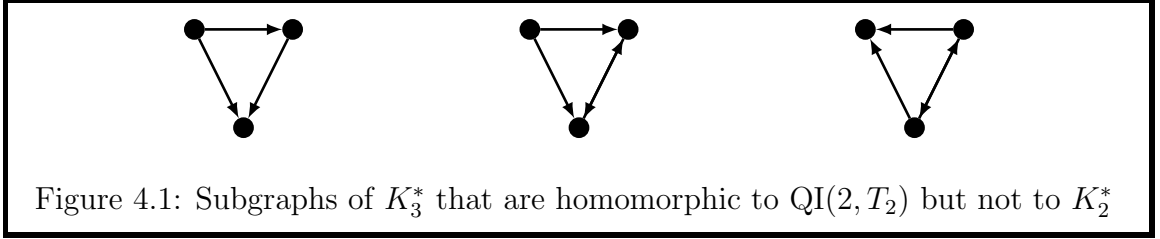
Since $G' \rightarrow K_3^*$, the graph G' must be homomorphic to some subgraph of K_3^* . Since $\chi(G) = 3$, it follows that G' cannot be homomorphic to K_2^* (if it were, then G would

be 2-colourable). The three acyclic subgraphs of K_3^* shown in Figure 4.1 are the only subgraphs of K_3^* which are homomorphic to $\text{QI}(2, T_2)$ but not homomorphic to K_2^* . By assumption, G' is not homomorphic to one of the subgraphs in Figure 4.1; thus, G is not homomorphic to $\text{QI}(2, T_2)$, hence $\text{CAN}(2, G', T_2) \geq 3$.

It now follows that $\text{CAN}(2, G', T_2) = 3$, which achieves the upper bound of Proposition 4.1.1 as follows:

$$3 = \text{CAN}(2, G', T_2) = 4 - 1 = \text{CAN}(2, G, 2) - 1. \quad \blacksquare$$

For example, if G is an odd cycle, and if G' is the orientation of G that is a directed odd cycle, then G' is not homomorphic to any of the three subgraphs shown in Figure 4.1, but G' is homomorphic to $\text{QI}(3, T_2)$.



Using the following graph-homomorphism result, we get a bound on acyclic column graphs; for a proof of Proposition 4.1.4, see Proposition 1.13 in [29].

Proposition 4.1.4 A digraph G with k vertices is acyclic if and only if $G \rightarrow T_k$. $\blacksquare$

Proposition 4.1.5 Let G be a directed column graph on k vertices. If G is acyclic, then $\text{CAN}(2, G, T_2) \leq \lceil \log_2 k \rceil$.

[proof] By Proposition 4.1.4, G is acyclic if and only if G is homomorphic to the transitive tournament T_k . It is easy to see that T_k is a subgraph of $\text{QI}(\lceil \log_2 k \rceil, T_2)$. Thus, $\text{CAN}(2, G, T_2) \leq \lceil \log_2 k \rceil$. $\blacksquare$

Let G be a directed column graph with $V(G) = [k]$. Let $i, j \in [k]$. The interaction $\{(i, 0), (j, 1)\}$ is a **distance- d interaction** if $d \in [k-1]$ and $j - i \equiv d \pmod{k}$. The next result reveals why, in some cases, we can expect a covering array $\text{CA}(2, G, T_2)$ to cover a substantial number of optional interactions with respect to G and T_2 .

Lemma 4.1.6 Let G be a directed column graph with $V(G) = [k]$. In each row, R_i , of a $\text{CA}(n; 2, G, T_2)$, the number of distance- d interactions covered in R_i is equal to the number of distance- $(k - d)$ interactions covered in R_i , for each d such that $1 \leq d \leq k - 1$.

[proof] Fix a distance d such that $1 \leq d \leq k - 1$ and let $f = \gcd(d, k)$. We partition $V(G)$ into f disjoint cyclic sequences, namely:

$$\begin{aligned} C_1 &= 1, 1 + d, 1 + 2d, \dots, 1 + \left(\frac{k}{f} - 1\right)d \\ C_2 &= 2, 2 + d, 2 + 2d, \dots, 2 + \left(\frac{k}{f} - 1\right)d \\ &\vdots \\ C_f &= f, f + d, f + 2d, \dots, f + \left(\frac{k}{f} - 1\right)d \end{aligned}$$

where addition is done modulo k .

Within each cyclic sequence C_j consecutive vertices are distance d apart.

For each row R_i of a $\text{CA}(2, G, T_2)$, taking the entries of R_i in the order induced by the above cyclic sequences yields f cyclic sequences of zeros and ones, which we denote by $C_j(R_i)$ for $j = 1, \dots, f$. That is, $C_j(R_i) = R_i(j), R_i(j + d), \dots, R_i(j + (\frac{k}{f} - 1)d)$. Since consecutive entries of these cyclic sequences correspond to vertices that are distance d apart, each time a sequence has a 0 entry followed by a 1 entry corresponds to one of the distance- d interactions covered by R_i . Summing over all $C_j(R_i)$, the number of times a 0 is followed by a 1, gives the total number of distance- d interactions covered by R_i .

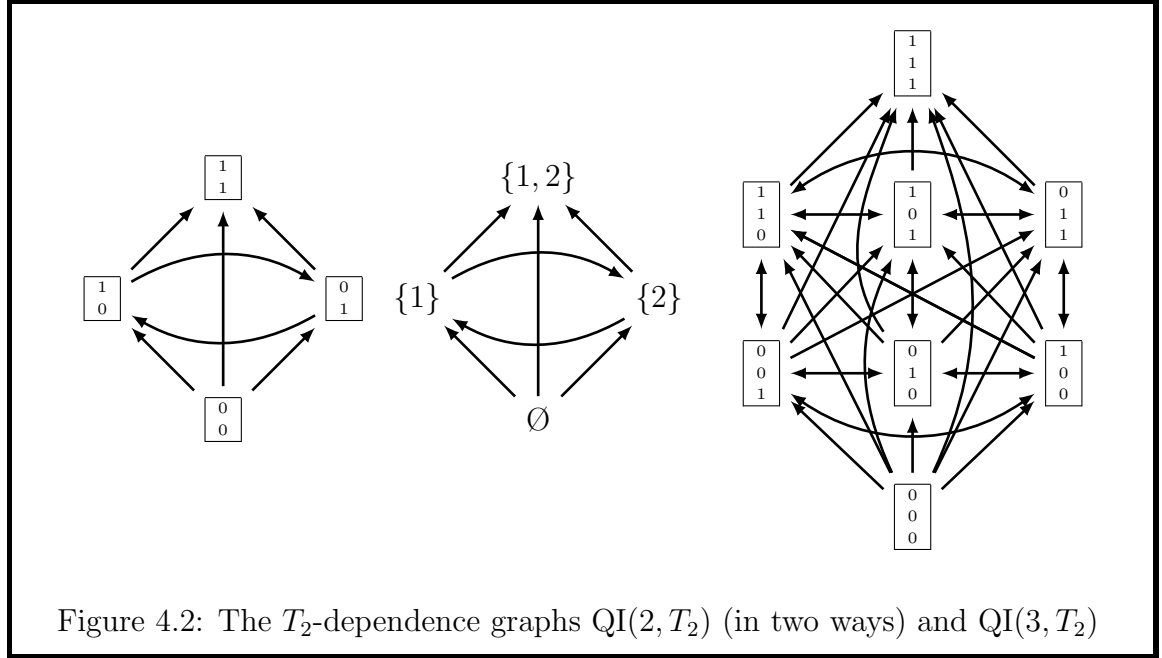
Now, it is easy to see that the number of times a binary cyclic sequence switches from 0 to 1 must be equal to the number of times that sequence switches from 1 to 0. It remains to observe that a 1 entry followed by a 0 entry in one of the cyclic sequences $C_j(R_i)$ corresponds to a distance- $(k - d)$ interaction that is covered by R_i . ■

Although, for each $d \in [k - 1]$, Lemma 4.1.6 tells us that each row of a $\text{CA}(n; 2, G, T_2)$ covers the same number of distance- d interactions as distance- $(k - d)$ interactions, this property does not hold more globally. The total number of distinct distance- d interactions covered by an entire array can be different from the total number of distance- $(k - d)$ interactions covered by the array.

4.2 Properties of $\text{QI}(n, T_2)$

Recall from the proof Proposition 3.2.3 that finding covering arrays with column graph G and alphabet graph T_2 is equivalent to finding homomorphisms of G to $\text{QI}(n, T_2)$. In this section, we give some properties of the T_2 -dependence graph.

For $n \geq 1$, the vertices of $\text{QI}(n, T_2)$ are all binary n -tuples, hence $|V(\text{QI}(n, T_2))| = 2^n$. These n -tuples correspond to the subsets of $[n]$, so we think of the vertices interchangeably as n -tuples or subsets. Figure 4.2 shows $\text{QI}(2, T_2)$ in two ways: with vertices as binary 2-tuples (on the left) and with vertices as subsets of $\{1, 2\}$ (in the centre). Figure 4.2 also shows the T_2 -dependence graph $\text{QI}(3, T_2)$ (on the right).



For $A, B \subseteq [n]$, we have an arc $AB \in E(\text{QI}(n, T_2))$ if and only if $B \not\subseteq A$. Every pair of distinct vertices $A, B \in V(\text{QI}(n, T_2))$ has $A \not\subseteq B$ or $B \not\subseteq A$ (or both), thus the underlying graph of $\text{QI}(n, T_2)$ is K_{2^n} . In fact, most pairs of vertices in $\text{QI}(n, T_2)$ are symmetrically adjacent (both AB and BA are arcs of $\text{QI}(n, T_2)$). Observe that $AB \notin E(\text{QI}(n, T_2))$ if and only if $B \subseteq A$. Moreover, if A and B are distinct vertices, then $AB \notin E(\text{QI}(n, T_2))$ if and only if B is a proper subset of A . Using this fact, we can count the pairs of vertices of $\text{QI}(n, T_2)$ that are not symmetrically adjacent, as follows.

Lemma 4.2.1 The number of pairs of distinct vertices $A, B \in V(\text{QI}(n, T_2))$ such that exactly one of AB and BA is an arc of $\text{QI}(n, T_2)$ is $3^n - 2^n$.

[proof] Consider the vertices of $\text{QI}(n, T_2)$ as subsets of $[n]$. Each k -set is a proper subset of $\binom{n-k}{i}$ sets of rank $k+i$. For each fixed k -set A , the number of subsets in which A is properly contained is thus equal to

$$\sum_{i=1}^{n-k} \binom{n-k}{i} = 2^{n-k} - 1.$$

Summing over all sets of rank k and summing over all ranks $k \in \{0, 1, \dots, n\}$, we have

$$\sum_{k=0}^n \binom{n}{k} (2^{n-k} - 1) = \sum_{k=0}^n \binom{n}{k} 2^{n-k} - \sum_{k=0}^n \binom{n}{k} = 2^n \sum_{k=0}^n \binom{n}{k} \left(\frac{1}{2}\right)^k - 2^n = 3^n - 2^n$$

pairs of distinct vertices $A, B \in V(\text{QI}(n, T_2))$ such that $A \subset B$. These are the only pairs of vertices for which $BA \in E(\text{QI}(n, T_2))$ and $AB \notin E(\text{QI}(n, T_2))$. Thus, there are $3^n - 2^n$ pairs of distinct vertices in $V(\text{QI}(n, T_2))$ such that exactly one of AB and BA is an arc of $\text{QI}(n, T_2)$. ■

Corollary 4.2.2 The graph $\text{QI}(n, T_2)$ has $2^{2n-1} + 2^{n-1} - 3^n$ pairs of distinct vertices A and B such that both AB and BA are arcs of $\text{QI}(n, T_2)$. In particular, as $n \rightarrow \infty$, the proportion $(2^{2n-1} + 2^{n-1} - 3^n) / \binom{2^n}{2} \rightarrow 1$, where $\binom{2^n}{2}$ is the total number of pairs of vertices in $\text{QI}(n, T_2)$.

[proof] There are $\binom{2^n}{2}$ pairs of distinct vertices in $\text{QI}(n, T_2)$. By Lemma 4.2.1, $3^n - 2^n$ pairs are not symmetrically adjacent. Thus, the number of symmetrically adjacent pairs is $\binom{2^n}{2} - [3^n - 2^n] = 2^{n-1}(2^n - 1) - 3^n + 2^n = 2^{2n-1} + 2^{n-1} - 3^n$. Asymptotically, we have

$$\lim_{n \rightarrow \infty} \frac{2^{2n-1} + 2^{n-1} - 3^n}{\binom{2^n}{2}} = \lim_{n \rightarrow \infty} \frac{4^n + 2^n - 2 \cdot 3^n}{4^n - 2^n} = 1. \quad \blacksquare$$

Corollary 4.2.2 is another reason for us to expect covering arrays $\text{CA}(n; 2, G, T_2)$ on non-symmetric column digraphs G to cover a substantial number of optional interactions. Consider a homomorphism $f : G \rightarrow \text{QI}(n, T_2)$ and an arc $ij \in E(G)$. Given Corollary 4.2.2, there is a good chance that both $f(i)f(j)$ and $f(j)f(i)$ are arcs of $\text{QI}(n, T_2)$ whether or not $ji \in E(G)$.

Proposition 4.2.3 The graph $\text{QI}(n, T_2)$ is a core.

[proof] No two vertices of $\text{QI}(n, T_2)$ can be identified by an endomorphism since $\text{QI}(n, T_2)$ has no loops, and, for all $A, B \in V(\text{QI}(n, T_2))$, we have $AB \in E(\text{QI}(n, T_2))$ or $BA \in E(\text{QI}(n, T_2))$. Thus, there does not exist a retraction of $\text{QI}(n, T_2)$ to any proper subgraph, so $\text{QI}(n, T_2)$ is a core. ■

In a directed graph X , a *symmetric clique* is a subset of vertices $C \subseteq V(X)$ such that, for all distinct $u, v \in C$, we have $uv \in E(X)$ and $vu \in E(X)$. In $\text{QI}(n, T_2)$, a symmetric clique corresponds to an antichain of subsets of $[n]$. From Sperner's Theorem (see Theorem 2.1.1), we get the following result.

Lemma 4.2.4 The largest symmetric clique in $\text{QI}(n, T_2)$ has size $\binom{n}{\lfloor n/2 \rfloor}$. If n is even, the unique largest symmetric clique consists of the vertices of rank $n/2$. If n is odd, there are two largest symmetric cliques: the set of vertices of rank $\lfloor n/2 \rfloor$, and the set of vertices of rank $\lceil n/2 \rceil$. ■

4.3 Complexity of determining $\text{CAN}(2, G, T_2)$

In this section, we discuss computational complexity results related to covering arrays on directed column graphs with alphabet graph T_2 . For background related to complexity theory, see Chapter 34 in [17].

Let T_2 -CAN denote the following decision problem for covering arrays on column graphs with alphabet graph T_2 , namely

$$T_2\text{-CAN} = \{(G, n) : \text{CAN}(2, G, T_2) \leq n\}$$

where G is a directed column graph and n is a positive integer.

For undirected graphs G , let 3-COL denote the 3-colouring decision problem

$$3\text{-COL} = \{G : \chi(G) \leq 3\}.$$

Let 2-CANG denote the decision problem for binary covering arrays on (undirected column) graphs

$$2\text{-CANG} = \{(G, n) : \text{CAN}(2, G, 2) \leq n\}.$$

Seroussi and Bshouty [53] proved that 2-CANG is NP-complete, which implies T_2 -CAN is NP-hard, as follows. Given an instance (G, n) for the problem 2-CANG, it is clear that (G^*, n) is an instance for T_2 -CAN, where G^* is the symmetric digraph of G . Indeed, $(G, n) \in 2\text{-CANG}$ if and only if $(G^*, n) \in T_2\text{-CAN}$. If $T_2\text{-CAN}$ could be solved in polynomial time, then we could solve 2-CANG in polynomial time which is possible only if $P = NP$.

Corollary 4.3.1 The decision problem $T_2\text{-CAN}$ is NP-hard. ■

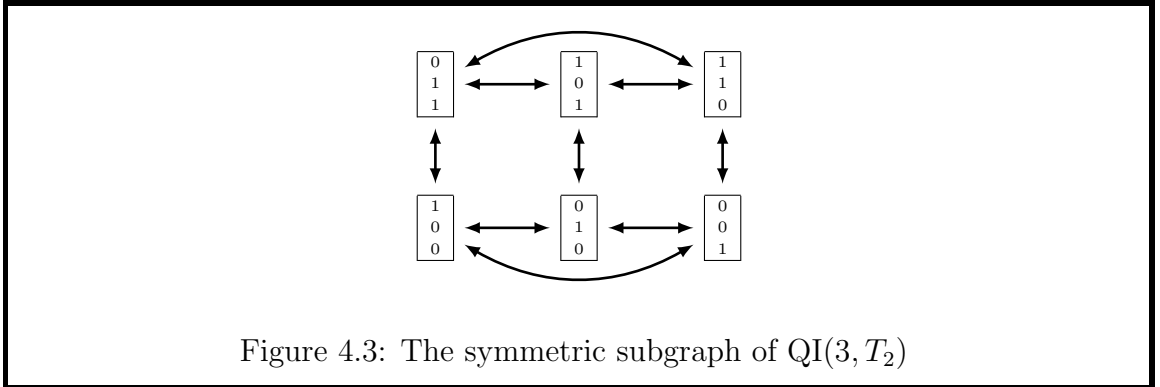
In their proof, Seroussi and Bshouty [53] showed the reduction $3\text{-COL} \leq_P 2\text{-CANG}$. Here, we give a proof that $3\text{-COL} \leq_P T_2\text{-CAN}$ directly, using properties of the graph $\text{QI}(3, T_2)$.

Proposition 4.3.2 The decision problems 3-COL and $T_2\text{-CAN}$ satisfy $3\text{-COL} \leq_P T_2\text{-CAN}$. Thus, $T_2\text{-CAN}$ is NP-hard.

[proof] Let G be an instance for 3-COL and label the vertices of G as $1, \dots, k$. Let G^* be the symmetric digraph of G . We claim that $G \in 3\text{-COL}$ if and only if $(G^*, 3) \in T_2\text{-CAN}$.

If $G \in 3\text{-COL}$, then $G^* \rightarrow K_3^* \rightarrow \text{QI}(3, T_2)$. Thus, $(G^*, 3) \in T_2\text{-CAN}$.

Conversely, if $(G^*, 3) \in T_2\text{-CAN}$, then $G^* \rightarrow \text{QI}(3, T_2)$; moreover, (symmetrically) adjacent vertices in G^* can only be mapped to vertices in the symmetric subgraph of $\text{QI}(3, T_2)$ shown in Figure 4.3 (these are the only pairs of vertices of $\text{QI}(3, T_2)$ which are symmetrically adjacent).



It is easy to see that the subgraph of $\text{QI}(3, T_2)$, shown in Figure 4.3, is homomorphic to K_3^* . Consequently, $G \rightarrow K_3$ and so $G \in 3\text{-COL}$.

Thus, $3\text{-COL} \leq_P T_2\text{-CAN}$ and $T_2\text{-CAN}$ is NP-hard ■

4.4 Binary covering arrays on tournament column graphs

A ***k-tournament*** is an orientation of the complete graph on K_k . Our convention for *k-tournaments* is to label the vertices as $1, 2, \dots, k$ (except when $k = 2$ in which case we use 0 and 1).

We are interested in *k-tournaments* as column graphs with T_2 as the alphabet graph. Among all *k-tournaments*, which families of tournaments are extremal with respect to covering array numbers? Do binary covering arrays on *k-tournaments* generally require as many rows as binary covering arrays?

Recall from Proposition 4.1.1 that the following bounds hold, where G' is an orientation of a graph G :

$$\frac{1}{2}\text{CAN}(2, G, 2) - 1 \leq \text{CAN}(2, G', T_2) \leq \text{CAN}(2, G, 2) - 1. \quad (4.4.1)$$

A binary covering array of strength 2, $\text{CA}(n; 2, k, 2)$, is equivalent to a covering array on the complete column graph K_k , that is, a $\text{CA}(n; 2, K_k, 2)$. We thus have the following bound:

Corollary 4.4.1 If O is a *k-tournament*, then

$$\frac{1}{2}\text{CAN}(2, k, 2) - 1 \leq \text{CAN}(2, O, T_2) \leq \text{CAN}(2, k, 2) - 1. \quad \blacksquare$$

We now prove that the upper and lower bounds of Corollary 4.4.1 can be tightened for *k-tournaments*.

Lemma 4.4.2 If O is a *k-tournament*, then $\lceil \log_2 k \rceil \leq \text{CAN}(2, O, T_2)$.

[proof] Suppose $\text{CAN}(2, O, T_2) = n$. Then there is a homomorphism $f : O \rightarrow \text{QI}(n, T_2)$, and f must be vertex-injective since $\text{QI}(n, T_2)$ does not contain any loops and each pair of distinct vertices in O is joined by an arc. It now follows that $k \leq 2^n$ since $|V(\text{QI}(n, T_2))| = 2^n$. Therefore, $\log_2 k \leq n$. ■

We now show that the lower bound of Lemma 4.4.2 is tight by considering transitive tournaments.

Theorem 4.4.3 If $k \geq 2$, then $\text{CAN}(2, T_k, T_2) = \lceil \log_2(k) \rceil$.

[proof] Notice that $AB \in E(\text{QI}(n, T_2))$ if and only if $A \neq B$ and $B \not\subseteq A$. We can thus order the vertices of $\text{QI}(n, T_2)$ in non-descending rank, arbitrarily ordering the vertices of any fixed rank, and this ordering will have the property that $AB \in E(\text{QI}(n, T_2))$ whenever A precedes B . With this ordering in place, it is clear that $\text{QI}(n, T_2)$ contains T_{2^n} as an induced subgraph.

It now follows that for all $k \leq 2^n$ there exist homomorphisms $T_k \rightarrow T_{2^n} \rightarrow \text{QI}(n, T_2)$. By Proposition 3.4.5, we have $\text{CAN}(2, T_k, T_2) \leq \lceil \log_2 k \rceil$.

By Lemma 4.4.2, we have $\text{CAN}(2, T_k, T_2) \geq \lceil \log_2 k \rceil$, which completes the proof. $\blacksquare$

Note that the proof of Theorem 4.4.3 says even more than $\text{CAN}(2, T_k, T_2) = \lceil \log_2(k) \rceil$; it says that we can construct a $\text{CA}(n; 2, T_k, T_2)$ for any $n \geq \log_2 k$ by arranging k distinct binary n -tuples, corresponding to k distinct subsets of $[n]$ in non-descending order of cardinality.

Indeed, the lower bound of Lemma 4.4.2 is achieved by many k -tournaments. Any k -tournament that is a subgraph of $\text{QI}(\lceil \log_2 k \rceil, T_2)$ achieves the bound (remember that $\text{QI}(n, T_2)$ has many pairs of symmetrically adjacent vertices, so there are many non-transitive tournaments contained in $\text{QI}(n, T_2)$).

Using transitive tournaments, we provide a new construction for binary covering arrays. Said construction, given in Proposition 4.4.4, is not optimal in general, and arguably, it is useless for building binary covering arrays; recall that the exact value of $\text{CAN}(2, k, 2)$ and an optimal construction for binary covering arrays are already known (see Theorem 2.3.3). Nevertheless, we believe the idea behind the construction of Proposition 4.4.4 may be useful, if it could be generalized to higher alphabet sizes $v \geq 3$.

Proposition 4.4.4 If $k \geq 2$, then there exists a positive integer $m \leq \lceil \log_2 k \rceil + 1$ such that

$$\text{CAN}(2, k, 2) \leq \text{CAN}(2, T_k, T_2) + \text{CAN}(2, T_m, T_2) + 2.$$

Consequently,

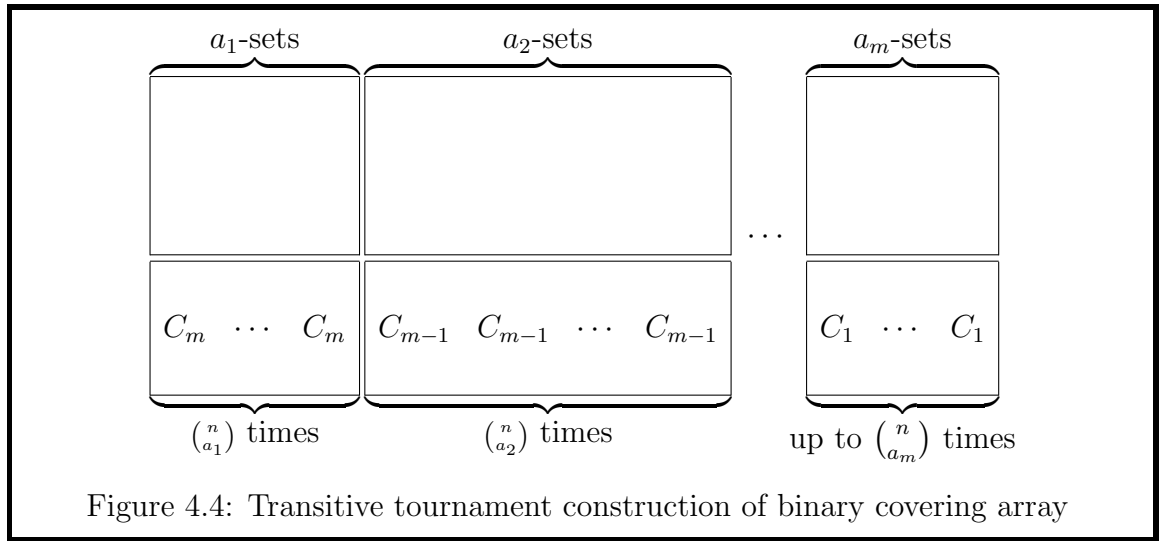
$$\text{CAN}(2, k, 2) \leq \lceil \log_2 k \rceil + \lceil \log_2 (\lceil \log_2 k \rceil + 1) \rceil + 2.$$

[proof] Let $n = \lceil \log_2 k \rceil$. Since $n = \lceil \log_2 k \rceil$, it follows that $k \leq 2^n = \sum_{i=0}^n \binom{n}{i}$. Let m be the minimum number of binomial coefficients needed to write

$$k \leq \binom{n}{a_1} + \binom{n}{a_2} + \cdots + \binom{n}{a_m},$$

where $0 \leq a_1 < a_2 < \cdots < a_m \leq n$. Clearly, $m \leq n + 1 = \lceil \log_2 k \rceil + 1$. We will construct a $\text{CA}(n + \lceil \log_2 m \rceil + 2; 2, k, 2)$ by appending a blown-up $\text{CA}(\lceil \log_2 m \rceil; 2, T_m, T_2)$ to a $\text{CA}(n; 2, T_k, T_2)$, and adding two constant rows.

By Theorem 4.4.3, there exists a $\text{CA}(n; 2, T_k, T_2)$. By the proof of Theorem 4.4.3, we may assume that the k columns of a $\text{CA}(n; 2, T_k, T_2)$ are the subsets of $[n]$ of cardinalities $a_1, a_2, \dots, a_{m-1}$ and (as many as needed of) the a_m -subsets of $[n]$, sorted in non-descending order of cardinality.



The $\text{CA}(n; 2, T_k, T_2)$ covers all interactions of the form $\{(i, 0), (j, 1)\}$, whenever $1 \leq i < j \leq k$. Moreover, it covers all interactions of the form $\{(i, 0), (j, 1)\}$ for all i, j such that $\binom{n}{a_1} + \cdots + \binom{n}{a_{l-1}} + 1 \leq j < i \leq \binom{n}{a_1} + \cdots + \binom{n}{a_l}$, for each $2 \leq l \leq m$. The array also covers all interactions of the form $\{(i, 0), (j, 1)\}$ for all i, j such that $1 \leq j < i \leq \binom{n}{a_1}$. In other words, a collection of a_l -subsets of an n -set forms an antichain, thus the corresponding n -tuples are K_2 -dependent (that is, T_2^* -dependent). Thus, the $\text{CA}(n; 2, T_k, T_2)$ is “almost” a $\text{CA}(n; 2, k, K_2)$. In fact, the only interactions that may not be covered are of the form $\{(i, 0), (j, 1)\}$ where, for some l with $l < m$, we have $1 \leq j \leq \binom{n}{a_1} + \cdots + \binom{n}{a_l} < i$.

Now, take an optimal $\text{CA}(\lceil \log_2 m \rceil; 2, T_m, T_2)$, denoted B , with columns $C_1, \dots, C_m$. Build a new array A from B as follows. The first $\binom{n}{a_1}$ columns of A are copies of C_m ; for the next $\binom{n}{a_2}$ columns, we repeat C_{m-1} ; then, we repeat C_{m-2} $\binom{n}{a_3}$ times, etc. so that C_{m-l+1} is repeated $\binom{n}{a_l}$ times for $1 \leq l \leq m-1$. Lastly, we repeat C_1 as many times as required to obtain a total of k columns for the array A . Clearly, A covers all interactions of the form $\{(i, 0), (j, 1)\}$, where, for some l with $l < m$, we have $1 \leq j \leq \binom{n}{a_1} + \dots + \binom{n}{a_l} < i$.

Append A to the $\text{CA}(n; 2, T_k, T_2)$, as shown in Figure 4.4, and add a row of all zeros and a row of all ones. We now have a $\text{CA}(n + \lceil \log_2 m \rceil + 2; 2, k, 2)$. Thus,

$$\text{CAN}(2, k, 2) \leq n + \lceil \log_2 m \rceil + 2 \leq \lceil \log_2 k \rceil + \lceil \log_2(\lceil \log_2 k \rceil + 1) \rceil + 2. \quad \blacksquare$$

We now illustrate the construction of Proposition 4.4.4 with an example.

Example 4.4.5 Take $k = 6$. We have $\lceil \log_2 6 \rceil = 3$ and the smallest integer m such that we can write $6 = \binom{3}{a_1} + \dots + \binom{3}{a_m}$, where $0 \leq a_1 < \dots < a_m \leq 3$, is $m = 2$: $6 = \binom{3}{1} + \binom{3}{2}$. By Proposition 4.4.4, we have $\text{CAN}(2, 6, 2) \leq \lceil \log_2 6 \rceil + \lceil \log_2 2 \rceil + 2 = 6$, which is actually optimal. Here is the array constructed.

1	2	3	4	5	6
0	0	1	0	1	1
0	1	0	1	0	1
1	0	0	1	1	0
1	1	1	0	0	0
0	0	0	0	0	0
1	1	1	1	1	1

For k -tournaments, we can now show that the lower bound of Lemma 4.4.2 is better than the lower bound given in Corollary 4.4.1 for all $k \geq 5$.

Corollary 4.4.6 For $k \geq 5$, we have $\lceil \frac{1}{2} \text{CAN}(2, k, 2) \rceil - 1 < \lceil \log_2 k \rceil$.

[proof] By Theorem 2.3.3, we have $\text{CAN}(2, k, 2) = \min\{n : k \leq \binom{n-1}{\lfloor n/2 \rfloor - 1}\}$. For $5 \leq k \leq 31$, we can verify that $\lceil \frac{1}{2} \text{CAN}(2, k, 2) \rceil - 1 < \lceil \log_2 k \rceil$, so the result holds for $5 \leq k \leq 31$.

By Proposition 4.4.4, we have

$$\frac{1}{2} \text{CAN}(2, k, 2) \leq \frac{\lceil \log_2 k \rceil + \lceil \log_2(\lceil \log_2 k \rceil + 1) \rceil + 2}{2}.$$

For $k \geq 32$, it is easy to see that $\lceil \log_2 k \rceil + 1 < \frac{k}{4}$. Thus,

$$\frac{\lceil \log_2 k \rceil + \lceil \log_2(\lceil \log_2 k \rceil + 1) \rceil + 2}{2} \leq \frac{\lceil \log_2 k \rceil + \lceil \log_2 \frac{k}{4} \rceil + 2}{2} = \lceil \log_2 k \rceil.$$

It now follows that $\lceil \frac{1}{2} \text{CAN}(2, k, 2) \rceil \leq \lceil \log_2 k \rceil$ and so $\lceil \frac{1}{2} \text{CAN}(2, k, 2) \rceil - 1 < \lceil \log_2 k \rceil$, as claimed. ■

Corollary 4.4.7 If $\{O_k\}_{k=1}^\infty$ is an infinite sequence of k -tournaments, then

$$\lim_{k \rightarrow \infty} \frac{\text{CAN}(2, O_k, T_2)}{\lceil \log_2 k \rceil} = 1.$$

[proof] By Proposition 4.1.1, we have $\text{CAN}(2, O_k, T_2) \leq \text{CAN}(2, K_k, 2) - 1$. Using the fact that $\text{CAN}(2, K_k, 2) = \text{CAN}(2, k, 2)$ and Proposition 4.4.4, we get the upper bound

$$\text{CAN}(2, O_k, T_2) \leq \lceil \log_2 k \rceil + \lceil \log_2(\lceil \log_2 k \rceil + 1) \rceil + 1.$$

By Lemma 4.4.2 we have $\lceil \log_2 k \rceil \leq \text{CAN}(2, O_k, T_2)$. Thus,

$$\lceil \log_2 k \rceil \leq \text{CAN}(2, O_k, T_2) \leq \lceil \log_2 k \rceil + \lceil \log_2(\lceil \log_2 k \rceil + 1) \rceil + 1.$$

It now follows that

$$1 = \lim_{n \rightarrow \infty} \frac{\lceil \log_2 k \rceil}{\lceil \log_2 k \rceil} \leq \lim_{n \rightarrow \infty} \frac{\text{CAN}(2, O_k, T_2)}{\lceil \log_2 k \rceil} \leq \lim_{n \rightarrow \infty} \frac{\lceil \log_2 k \rceil + \lceil \log_2(\lceil \log_2 k \rceil + 1) \rceil + 1}{\lceil \log_2 k \rceil} = 1. \quad \blacksquare$$

At this point, we have tightened the lower bound of Proposition 4.1.1 to $\lceil \log_2 k \rceil$, given a k -tournament column graph. Next, we will tighten the upper bound slightly, though not by more than one.

Lemma 4.4.8 Let $k \geq 2$. If O is a k -tournament, then

$$\text{CAN}(2, O, T_2) \leq \min \left\{ n : k \leq \binom{n}{\lfloor n/2 \rfloor} \right\}.$$

Moreover,

$$\text{CAN}(2, k, K_2) \leq \text{CAN}(2, k, 2) - 1 \leq \text{CAN}(2, k, K_2) + 1.$$

[**proof**] It is clear that every k -tournament O satisfies $O \rightarrow K_k^*$, where K_k^* denotes the symmetric digraph of K_k . By Proposition 3.4.6, we have

$$\text{CAN}(2, O, T_2) \leq \text{CAN}(2, K_k^*, T_2). \quad (4.4.2)$$

By Corollary 3.2.8, the upper bound of Equation (4.4.2) is

$$\text{CAN}(2, K_k^*, T_2) = \text{CAN}(2, k, K_2) = \min \left\{ n : k \leq \binom{n}{\lfloor n/2 \rfloor} \right\}.$$

Thus, $\text{CAN}(2, O, T_2) \leq \min \left\{ n : k \leq \binom{n}{\lfloor n/2 \rfloor} \right\}$, as claimed.

Now we prove that $\text{CAN}(2, k, K_2) \leq \text{CAN}(2, k, 2) - 1 \leq \text{CAN}(2, k, K_2) + 1$.

By Corollary 3.2.8, we have $\text{CAN}(2, k, K_2) = \min \left\{ n : k \leq \binom{n}{\lfloor n/2 \rfloor} \right\}$. If $n = \text{CAN}(2, k, K_2)$, then it follows that

$$\binom{n-1}{\lfloor (n-1)/2 \rfloor} < k \leq \binom{n}{\lfloor n/2 \rfloor}.$$

It is easy to check that $\binom{n-1}{\lfloor n/2 \rfloor - 1} \leq \binom{n-1}{\lfloor (n-1)/2 \rfloor}$ and $\binom{n}{\lfloor n/2 \rfloor} < \binom{n+1}{\lfloor n/2 \rfloor} = \binom{(n+2)-1}{\lfloor (n+2)/2 \rfloor - 1}$.

Thus,

$$\binom{n-1}{\lfloor n/2 \rfloor - 1} < k < \binom{(n+2)-1}{\lfloor (n+2)/2 \rfloor - 1}. \quad (4.4.3)$$

By Theorem 2.3.3, we have

$$\text{CAN}(2, k, 2) = \min \left\{ n : k \leq \binom{n-1}{\lfloor n/2 \rfloor - 1} \right\}. \quad (4.4.4)$$

Comparing the bounds in (4.4.3) with (4.4.4), we see that $\text{CAN}(2, k, 2)$ must be greater than n and no greater than $n + 2$. Thus,

$$n \leq \text{CAN}(2, k, 2) - 1 \leq n + 1. \quad \blacksquare$$

We now have a slightly better upper bound for $\text{CAN}(2, O, T_2)$ when O is a k -tournament; however, this bound is based on K_k^* , and compared with a k -tournament, K_k^* has twice as many arcs. Can our new upper bound, namely

$$\text{CAN}(2, O, T_2) \leq \text{CAN}(2, K_k^*, T_2) = \text{CAN}(2, k, K_2),$$

be met with equality? The answer is yes (as we will show in Lemma 4.4.13); however, the following construction sometimes gives a slightly better upper bound.

Proposition 4.4.9 Let $k \geq 2$. If O is a k -tournament, then

$$\text{CAN}(2, O, T_2) \leq \min \left\{ n : k \leq 2 \binom{n-1}{\lfloor (n-1)/2 \rfloor} \right\}.$$

[proof] If $k = 2$, then there is only one 2-tournament to consider, namely $O = T_2$. By Theorem 4.4.3, we have $\text{CAN}(2, T_2, T_2) = \lceil \log_2 2 \rceil = 1$, which satisfies this Proposition.

Now, we may assume $k \geq 3$. If $k \leq 2 \binom{n-1}{\lfloor (n-1)/2 \rfloor}$, then $n \geq 2$ and $\lfloor k/2 \rfloor \leq \lceil k/2 \rceil \leq \binom{n-1}{\lfloor (n-1)/2 \rfloor}$. We can partition $V(O)$ into two parts of sizes $\lceil k/2 \rceil$ and $\lfloor k/2 \rfloor$ so that a matching of size $\lfloor k/2 \rfloor$ between the two parts has all its arcs oriented from the first part to the second. Relabel the vertices of O so that the vertices of the first part of the partition are labelled $1, \dots, \lceil k/2 \rceil$ and the vertices of the second part of the partition are labelled $\lceil k/2 \rceil + 1, \dots, k$.

We build a $\text{CA}(n; 2, O, T_2)$ as follows. First, build an $(n-1) \times k$ array with columns $C_1, \dots, C_k$ corresponding to $\lfloor \frac{n-1}{2} \rfloor$ -subsets of $[n-1]$, as follows. Take $\lceil k/2 \rceil$ of the $\lfloor \frac{n-1}{2} \rfloor$ -sets in some order, followed by the same first $\lceil k/2 \rceil$ columns repeated in the same order, that is, $C_1, \dots, C_{\lceil k/2 \rceil}$ are distinct $\lfloor \frac{n-1}{2} \rfloor$ -sets and $C_{i+\lceil k/2 \rceil} = C_i$ for $1 \leq i \leq \lceil k/2 \rceil$. Add an n th row to cover the arcs of the matching of O : the row has zeros as its first $\lceil k/2 \rceil$ entries and ones as its last $\lfloor k/2 \rfloor$ entries.

Since every two distinct $\lfloor \frac{n-1}{2} \rfloor$ -sets are K_2 -dependent, any two distinct columns C_i and C_j (of length $n-1$) are K_2 -dependent except when $|j-i| = \lceil k/2 \rceil$. The extra row ensures that we cover the arcs of the matching.

Thus, we have constructed a $\text{CA}(n; 2, O, T_2)$, and it follows that $k \leq 2 \binom{n-1}{\lfloor (n-1)/2 \rfloor}$ implies $\text{CAN}(2, O, T_2) \leq n$. ■

When n is even, we have $2 \binom{n-1}{\lfloor (n-1)/2 \rfloor} = \binom{n}{\lfloor n/2 \rfloor}$; in this case, the bounds of Lemma 4.4.8 and Proposition 4.4.9 are equal. When n is odd, we have $\binom{n}{\lfloor n/2 \rfloor} < 2 \binom{n-1}{\lfloor (n-1)/2 \rfloor}$; in this case, the bound of Proposition 4.4.9 is a tighter bound than the bound of Lemma 4.4.8.

The following corollary gives the improved bounds for binary covering arrays on tournaments.

Corollary 4.4.10 If O is a k -tournament, then

$$\lceil \log_2 k \rceil \leq \text{CAN}(2, O, T_2) \leq \min \left\{ n : k \leq 2 \binom{n-1}{\lfloor (n-1)/2 \rfloor} \right\}. \quad \blacksquare$$

4.4.1 Analysis of small k -tournaments

For small values of k , we analyze which k -tournaments hit the upper bound of Corollary 4.4.10. This will give us a clue as to which k -tournaments are the “worst” in general, that is, which k -tournaments have the largest covering array number for the alphabet graph T_2 .

If $k = 2$, then there is only one 2-tournament: the transitive tournament T_2 . In this case, $\text{CAN}(2, T_2, T_2) = 1 = \log_2 2$, which is equal to the upper bound given by Corollary 4.4.10.

Up to isomorphism, there are two 3-tournaments, namely, T_3 (transitive) and $\vec{C}_3$ (directed 3-cycle). In this case, $\lceil \log_2 3 \rceil = \text{CAN}(2, T_3, T_2) < \min\{n : 3 \leq 2^{\lfloor \frac{n-1}{2} \rfloor}\} = 3$. For the directed cycle, $\vec{C}_3$, the following lemma proves that $\text{CAN}(2, \vec{C}_3, T_2) = 3$, and so the upper bound, given in Corollary 4.4.10, is tight when $k = 3$.

Lemma 4.4.11 For a directed k -cycle $\vec{C}_k$, we have $\text{CAN}(2, \vec{C}_k, T_2) = 2$ if k is even, and $\text{CAN}(2, \vec{C}_k, T_2) = 3$ if k is odd.

[proof] It is easy to see that each row of a $\text{CA}(n; 2, \vec{C}_k, T_2)$ can cover at most $\lfloor k/2 \rfloor$ arcs of $\vec{C}_k$. Thus, $\text{CAN}(2, \vec{C}_k, T_2) \geq 2$ when k is even, and $\text{CAN}(2, \vec{C}_k, T_2) \geq 3$ when k is odd.

If k is even, then we have homomorphisms $\vec{C}_k \rightarrow C_k^* \rightarrow K_2^*$. The subgraph of $\text{QI}(2, T_2)$ induced by the vertices of rank 1 is isomorphic to K_2^* so $\vec{C}_k \rightarrow \text{QI}(2, T_2)$. Thus, when k is even, $\text{CAN}(2, \vec{C}_k, T_2) = 2$.

If k is odd, then we have homomorphisms $\vec{C}_k \rightarrow C_k^* \rightarrow K_3^* \rightarrow \text{QI}(3, T_2)$. Consequently, $\text{CAN}(2, \vec{C}_k, T_2) \leq 3$. ■

If $k = 4$, then, by Corollary 4.4.10, we have $2 \leq \text{CAN}(2, O, T_2) \leq 3$. We consider two types of 4-tournaments: those that are acyclic and those that contain directed cycles. If O is an acyclic 4-tournament, then, by Proposition 4.1.4, we have homomorphisms $O \rightarrow T_4 \rightarrow \text{QI}(2, T_2)$; in this case, $\text{CAN}(2, O, T_2) = 2$.

Lemma 4.4.12 If O is a k -tournament containing a directed cycle, then O contains a directed 3-cycle.

[proof] We prove by induction that if O contains a directed l -cycle for some $3 \leq l \leq k$, then O contains a directed 3-cycle. Clearly, if $l = 3$, then the result

holds. Assume that O contains a directed 3-cycle whenever O contains a directed l -cycle for some l such that $3 \leq l < k$. Now suppose O contains a directed $(l+1)$ -cycle, say $v_1 v_2 \dots v_l v_{l+1} v_1$. Consider the vertices v_{l-1} and v_{l+1} . If $v_{l+1} v_{l-1} \in E(O)$, then $v_{l-1} v_l v_{l+1} v_{l-1}$ is a directed 3-cycle. Otherwise, $v_{l-1} v_{l+1} \in E(O)$. In this case, $v_1 v_2 \dots v_{l-1} v_{l+1} v_1$ is a directed l -cycle of O , and by the induction hypothesis, O must contain a directed 3-cycle. $\blacksquare$

Let O be a 4-tournament that contains a directed cycle. By Lemma 4.4.12, O must contain a directed 3-cycle. By Lemma 4.4.11, we have $\text{CAN}(2, O, T_2) \geq 3$. The upper bound given by Corollary 4.4.10 is $n = 3$, which is tight for all 4-tournaments containing directed cycles.

When $k = 5$, the lower bound of Corollary 4.4.10 is $n = 3$. With one exception, all 5-tournaments are homomorphic to $\text{QI}(3, T_2)$. The exception, which we denote by Ω_5 , is one of the graphs shown in Figure 4.5.

Lemma 4.4.13 The 5-tournament Ω_5 has $\text{CAN}(2, \Omega_5, T_2) = 4 = \text{CAN}(2, 5, K_2)$.

[proof] If $\text{CAN}(2, \Omega_5, T_2) = 3$, then, to cover the arcs of the directed 3-cycle $(1, 3, 4, 1)$ (see Ω_5 in Figure 4.5), we know that a $\text{CA}(3; 2, \Omega_5, T_2)$ must have the following entries (by permuting rows if necessary):

1	2	3	4	5
0		1		
		0	1	
1			0	

We now have three options to cover the arc $(5, 2)$, in row 1, row 2, or row 3. Suppose we cover $(5, 2)$ in row 1. Then $(2, 3)$ must be covered in row 3, thereby forcing $(3, 5)$ to be covered in row 2, which in turn forces $(4, 5)$ to be covered in row 3, which leaves nowhere for $(5, 1)$ to be covered.

1	2	3	4	5		1	2	3	4	5		1	2	3	4	5		1	2	3	4	5
0	1	1		0	$\Rightarrow$	0	1	1		0	$\Rightarrow$	0	1	1		0	$\Rightarrow$	0	1	1		0
		0	1					0	1					0	1	1				0	1	1
1			0			1	0	1	0			1	0	1	0			1	0	1	0	1

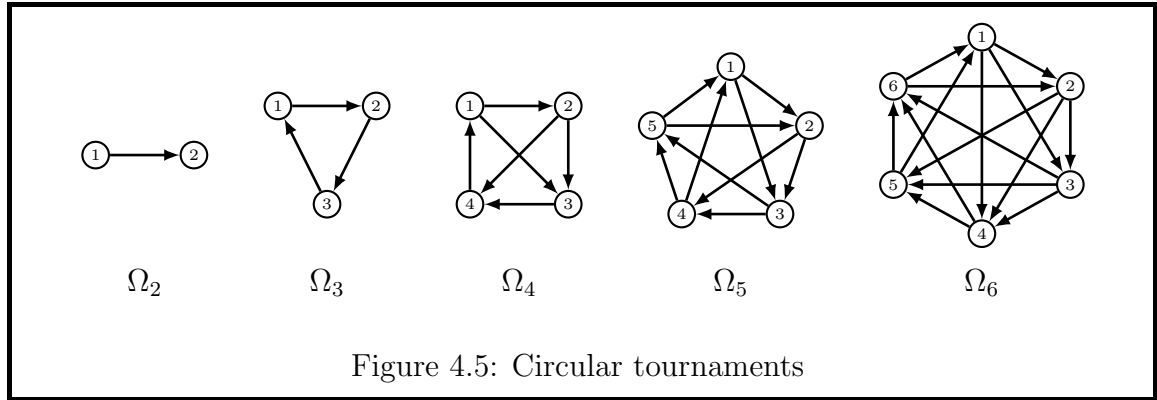
Similarly, if we cover $(5, 2)$ initially in row 2, or in row 3, we are forced to fill the array until we reach an arc of Ω_5 that cannot be covered within these three rows.

Thus, $\text{CAN}(2, \Omega_5, T_2) \geq 4$. Since $4 = \text{CAN}(2, 5, K_2)$ is the upper bound, we have $\text{CAN}(2, \Omega_5, T_2) = 4$. ■

Our analysis of k -tournaments for small values of k has shown that, for $2 \leq k \leq 5$, the upper bound of Corollary 4.4.10 is met with equality. For $k = 2$, there is only one 2-tournament, T_2 , and it hits the upper bound. For $k = 3$, the unique 3-tournament that hits the upper bound is $\vec{C}_3$. For $k = 4$, the upper bound is the same as the upper bound for $k = 3$, and the only 4-tournaments that meet the upper bound contain $\vec{C}_3$ as a subgraph. For $k = 5$ the unique 5-tournament that achieves the upper bound is Ω_5 . The tournaments T_2 , $\vec{C}_3$ and Ω_5 actually have a similar structure, which we define precisely in the following section.

4.5 Circular tournaments

The *circular k -tournament*, denoted Ω_k , has vertex set $V(\Omega_k) = [k]$ and arcs as follows. If k is odd, then $ij \in E(\Omega_k)$ whenever $1 \leq d \leq \lfloor k/2 \rfloor$, where $j - i \equiv d \pmod{k}$. If k is even, then $ij \in E(\Omega_k)$ whenever $1 \leq d < \lfloor k/2 \rfloor$, where $j - i \equiv d \pmod{k}$; furthermore, $(i, i + k/2 \pmod{k}) \in E(\Omega_k)$ for all i such that $1 \leq i \leq k/2$. Depictions of circular k -tournaments are given in Figure 4.5 for some small values of k .



For $k \leq 5$, we have $\text{CAN}(2, O, T_2) \leq \text{CAN}(2, \Omega_k, T_2)$ whenever O is a k -tournament. We are interested in knowing whether this is true in general. In other words, is Ω_k the “worst” k -tournament in terms of the number of rows required? We believe that circular tournaments are a likely candidate for “worst” tournament, so we venture to make the following conjecture.

Conjecture 4.5.1 If O is a k -tournament, then $\text{CAN}(2, O, T_2) \leq \text{CAN}(2, \Omega_k, T_2)$.

Consider Lemma 4.1.6 applied to column graph $G = \Omega_k$. Since Ω_k has required distance- d interactions for all $1 \leq d \leq \lfloor k/2 \rfloor$, each row necessarily covers some number of distance- $(k-d)$ interactions, which are not required by Ω_k . We can expect binary covering arrays on Ω_k to have coverage closer to the coverage required by binary covering arrays on K_k^* . This may be why circular tournaments tend to achieve the upper bound given in Corollary 4.4.10, at least for small values of k .

Regardless of the state of Conjecture 4.5.1, circular tournaments are tantalizing tournaments to study in terms of extremal combinatorics. Determining the exact value of $\text{CAN}(2, \Omega_k, T_2)$ as a function of k seems possible. Such a result would make a nice counterpart to Sperner's Theorem [54] for the size of a maximum antichain (see Theorem 2.1.1); in terms of covering arrays, Sperner's Theorem determines $\text{CAN}(2, K_k^*, T_2)$ as a function of k .

For the remainder of this section, we collect several properties of circular tournaments, including a construction that proves $\text{CAN}(2, \Omega_k, T_2)$ does not meet the upper bound given by Corollary 4.4.10 in general. We also provide the results of a computer search for determining $\text{CAN}(2, \Omega_k, T_2)$ for $k \leq 37$.

Lemma 4.5.2 If k is odd, then the circular tournament Ω_k is vertex-transitive.

[proof] The vertices of Ω_k are $1, \dots, k$. Choose vertices $i \neq j$. We can write $j = i + l \pmod{k}$ for a unique $l \in \{1, \dots, k-1\}$, and the map $f : \Omega_k \rightarrow \Omega_k$ given by $f(x) = x + l \pmod{k}$ is the required isomorphism such that $f(i) = j$. ■

Lemma 4.5.3 If k is even, then the circular tournament Ω_k has but one endomorphism: the identity.

[proof] Note that Ω_k is a loopless digraph in which every pair of vertices are adjacent. Consequently, endomorphisms of Ω_k must be vertex-injective, hence automorphisms.

Write $k = 2l$. The vertices of Ω_k are of two types: the vertices labelled $1, 2, \dots, l$ which have outdegree l and indegree $l-1$, and the vertices labelled $l+1, l+2, \dots, 2l$ which have outdegree $l-1$ and indegree l .

Suppose there is a homomorphism $f : \Omega_k \rightarrow \Omega_k$ such that $f(i) = j$ for some $j \neq i$. If $i \in \{1, 2, \dots, l\}$, then, in order for their in- and outdegrees to match, j must also

be from among those vertices. Suppose $j = i + x$ for some $x > 0$. Then j will have x more neighbours than i from among the vertices in the set $\{l + 1, l + 2, \dots, 2l\}$, which means that those neighbours of j will not have the correct degrees. Similarly, if $j = i - x$ for some $x > 0$, then j does not have the correct number of neighbours from $\{l + 1, l + 2, \dots, 2l\}$. Thus, it is impossible that $f(i) = j$ in this case. Similarly, if $i \in \{l + 1, l + 2, \dots, 2l\}$, then $j \in \{l + 1, l + 2, \dots, 2l\}$ also. In this case, $f(i) = j$ is also not possible for similar reasons. $\blacksquare$

Lemma 4.5.4 For all $k \geq 2$, there exists a homomorphism $\Omega_k \rightarrow \Omega_{k+1}$.

[proof] If k is even, then $k = 2l$, for some $l \geq 1$. We will show that $\Omega_{2l-1} \rightarrow \Omega_{2l}$. Define a map $f : \Omega_{2l-1} \rightarrow \Omega_{2l}$ by $f(i) = i$, if $1 \leq i \leq l - 1$ and $f(i) = i + 1$ if $l \leq i \leq 2l - 1$. We claim that f is a homomorphism.

If $ij \in E(\Omega_{2l-1})$, then there are four cases to consider:

1. If $1 \leq i < j \leq l - 1$ (and, by definition of Ω_{2l-1} , we have $j \leq i + l - 1$), then $f(i)f(j) = ij \in E(\Omega_{2l})$.
2. If $1 \leq i \leq l - 1$ and $l \leq j \leq 2l - 1$ (and, by definition of Ω_{2l-1} , we have $j \leq i + l - 1$), then $f(i)f(j) = i(j + 1)$. In this case $l + 1 \leq j + 1 \leq 2l$ and $j + 1 \leq i + l$. Thus, $i(j + 1) \in E(\Omega_{2l})$.
3. If $l \leq i < j \leq 2l - 1$ (and, by definition of Ω_{2l-1} , we have $j \leq i + l - 1$), then $f(i)f(j) = (i + 1)(j + 1)$. In this case, $l + 1 \leq i + 1 < j + 1 \leq 2l$ and $j + 1 \leq i + l$. Thus, $(i + 1)(j + 1) \in E(\Omega_{2l})$.
4. If $l \leq i \leq 2l - 1$ and $1 \leq j \leq l - 1$ (and, by definition of Ω_{2l-1} , we have $j + 2l - 1 \leq i + l - 1$), then $f(i)f(j) = (i + 1)j$. In this case, $l + 1 \leq i + 1 \leq 2l$ and $1 \leq j \leq l - 1$ and $2l + j \leq i + l$. Thus, $(i + 1)j \in E(\Omega_{2l})$.

Thus, $\Omega_{2l-1} \rightarrow \Omega_{2l}$, as claimed.

If k is odd, then $k = 2l + 1$, for some $l \geq 1$. We will show that $\Omega_{2l} \rightarrow \Omega_{2l+1}$. Define a map $f : \Omega_{2l-1} \rightarrow \Omega_{2l}$ by $f(i) = i$. We claim that f is a homomorphism.

If $ij \in E(\Omega_{2l})$, then there are three cases to consider:

1. If $1 \leq i \leq l$ and $i < j \leq 2l$ (and, by definition of Ω_{2l} , we have $j \leq i + l$), then $f(i)f(j) = ij \in E(\Omega_{2l+1})$.
2. If $l + 1 \leq i < j \leq 2l$ (and, by definition of Ω_{2l} , we have $j \leq i + l - 1$), then $f(i)f(j) = ij \in E(\Omega_{2l+1})$.

3. If $l + 1 \leq i \leq 2l$ and $1 \leq j \leq l - 1$ (and, by definition of Ω_{2l} , we have $j + 2l \leq i + l - 1$), then $j + 2l + 1 \leq i + l$ so $f(i)f(j) = ij \in E(\Omega_{2l+1})$.

Thus, $\Omega_{2l} \rightarrow \Omega_{2l+1}$, as claimed. ■

Corollary 4.5.5 For all $k \geq 1$, we have $\text{CAN}(2, \Omega_k, T_2) \leq \text{CAN}(2, \Omega_{k+1}, T_2)$ ■

In Lemma 4.4.13, we found $\text{CAN}(2, \Omega_5, T_2) = 4$. For $k = 6$, the upper bound for $\text{CAN}(2, \Omega_6, T_2)$ given by Corollary 4.4.10 is 4; thus, all 6-tournaments O that contain Ω_5 , including Ω_6 , have covering array number $\text{CAN}(2, O, T_2) = 4$. Once again, the upper bound given by Corollary 4.4.10 is tight.

Although the upper bound of Corollary 4.4.10 is achieved for $2 \leq k \leq 6$, the following construction shows that this is not to be expected of circular tournaments in general. If Conjecture 4.5.1 is true, then the construction that follows proves that the upper bound of Corollary 4.4.10 is not tight in general. If Conjecture 4.5.1 is false, then some k -tournament other than Ω_k might achieve the upper bound given by Corollary 4.4.10.

Our construction for circular tournaments is based on the Kruskal–Katona Theorem [31, 36] (see Theorem 2.1.7). The idea is to use sets from the two largest ranks in the poset of subsets, so long as the shadow of the larger sets is not too big. This construction is given in Proposition 4.5.6, following a review of some terminology.

Recall the following definitions. If $\mathcal{A}$ is a collection of k -subsets of $[n]$, then the **shadow** of $\mathcal{A}$, denoted $\Delta\mathcal{A}$, is the set

$$\Delta\mathcal{A} = \{B \subset [n] : |B| = k - 1, B \subset A \text{ for some } A \in \mathcal{A}\}.$$

Given positive integers x and k , recall that the **k -binomial representation of x** is the (unique) representation

$$x = \binom{a_k}{k} + \binom{a_{k-1}}{k-1} + \cdots + \binom{a_t}{t},$$

where $a_k > a_{k-1} > \cdots > a_t \geq t \geq 1$.

If A and B are k -sets, then, in **squashed order**, we have $A <_s B$ if the largest element of the symmetric difference $A \oplus B$ is in B . The collection of k -sets for which the Kruskal–Katona Theorem holds with equality is the collection of k -sets that are smallest in squashed order (see Corollary 2.1.8).

We now take advantage of the squashed order to construct binary covering arrays on circular tournaments.

Proposition 4.5.6 Let k and n be integers, where $\binom{n}{\lfloor n/2 \rfloor} < k \leq \binom{n}{\lfloor n/2 \rfloor} + \binom{n}{\lfloor n/2 \rfloor + 1}$. Write $k = \binom{n}{\lfloor n/2 \rfloor} + x$ and let

$$x = \binom{a_{\lfloor n/2 \rfloor + 1}}{\lfloor n/2 \rfloor + 1} + \binom{a_{\lfloor n/2 \rfloor}}{\lfloor n/2 \rfloor} + \cdots + \binom{a_t}{t},$$

where $a_{\lfloor n/2 \rfloor + 1} > a_{\lfloor n/2 \rfloor} > \cdots > a_t \geq t \geq 1$ (this is the $(\lfloor n/2 \rfloor + 1)$ -binomial representation of x). If

$$\binom{n}{\lfloor n/2 \rfloor} - \left[\binom{a_{\lfloor n/2 \rfloor + 1}}{\lfloor n/2 \rfloor} + \binom{a_{\lfloor n/2 \rfloor}}{\lfloor n/2 \rfloor - 1} + \cdots + \binom{a_t}{t - 1} \right] \geq \left\lfloor \frac{k}{2} \right\rfloor,$$

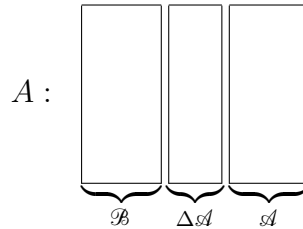
then $\text{CAN}(2, \Omega_k, T_2) \leq n$.

[proof] Let $\mathcal{A}$ be the collection of the first x $(\lfloor n/2 \rfloor + 1)$ -subsets of $[n]$ in squashed order. By the Kruskal–Katona Theorem (Theorem 2.1.7) and Corollary 2.1.8, the shadow $\Delta\mathcal{A}$ has cardinality

$$|\Delta\mathcal{A}| = \binom{a_{\lfloor n/2 \rfloor + 1}}{\lfloor n/2 \rfloor} + \cdots + \binom{a_t}{t - 1}.$$

By Corollary 2.1.8, $\Delta\mathcal{A}$ consists of the first $|\Delta\mathcal{A}|$ of the $\lfloor n/2 \rfloor$ -subsets of $[n]$ in squashed order. Let $\mathcal{B}$ denote the collection of $\lfloor n/2 \rfloor$ -sets that are not in $\Delta\mathcal{A}$.

Define an array A with columns, from right to left, corresponding to the collections $\mathcal{A}$, then $\Delta\mathcal{A}$, then $\mathcal{B}$, as shown below.



The array A covers all 0-1 interactions from any column in $\mathcal{B} \cup \Delta\mathcal{A}$ to any column in $\mathcal{A}$ as the sets in $\mathcal{A}$ have larger cardinality. Furthermore, $\mathcal{B} \cup \Delta\mathcal{A}$ is an antichain, so it covers all 0-1 interactions among its columns. In fact, $\mathcal{A} \cup \mathcal{B}$ is an antichain since $\mathcal{B}$ is itself an antichain, $\mathcal{A}$ is itself an antichain, and no set in $\mathcal{B}$ is contained in any set in $\mathcal{A}$ and vice versa. Thus, the only type of required interaction that A might fail to cover would be an interaction $\{(i, 0), (j, 1)\}$ for some column i corresponding to a

subset in $\mathcal{A}$ and a column j corresponding to a subset in $\Delta\mathcal{A}$. We show that this is not possible.

Consider column k . From k , we must cover interactions $\{(k, 0), (d, 0)\}$ for all d such that $1 \leq d \leq \lfloor k/2 \rfloor$. As long as the first $\lfloor k/2 \rfloor$ columns of A belong to $\mathcal{B}$, then A suffices to cover these required interactions as $\mathcal{A} \cup \mathcal{B}$ is an antichain. This is indeed the case as $\lfloor k/2 \rfloor \leq |\mathcal{B}| = \binom{n}{\lfloor n/2 \rfloor} - |\Delta\mathcal{A}|$, by assumption. Now it is clear that all required interactions beginning from a column in $\mathcal{A}$, either end in $\mathcal{A}$, or end in $\mathcal{B}$; in both cases they are covered.

Therefore, the array A is a $\text{CA}(n; 2, \Omega_k, T_2)$ so $\text{CAN}(2, \Omega_k, T_2) \leq n$. ■

Let us compute an example to clarify the construction in Proposition 4.5.6.

Example 4.5.7 Take $k = 22 = \binom{6}{3} + 2$. So $n = 6$ and $x = 2$. We write x in its 4-binomial representation: $2 = \binom{4}{4} + \binom{3}{3}$. Let $\mathcal{A}$ be the collection of the 2 smallest 4-subsets of $[6]$ in squashed order. By the Kruskal–Katona Theorem, we have $|\Delta\mathcal{A}| = \binom{4}{3} + \binom{3}{2} = 7$ and $\binom{6}{3} - |\Delta\mathcal{A}| = 20 - 7 = 13 > 11 = \lfloor \frac{k}{2} \rfloor$. By Proposition 4.5.6, we have $\text{CAN}(2, \Omega_{22}, T_2) \leq 6$. Here is the array constructed:

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
0	0	0	1	0	0	1	0	1	1	0	0	1	0	1	1	0	1	1	1	1	1
0	0	1	0	0	1	0	1	0	1	0	1	0	1	0	1	1	0	1	1	1	1
0	1	0	0	1	0	0	1	1	0	1	0	0	1	1	0	1	1	0	1	1	1
1	0	0	0	1	1	1	0	0	0	1	1	1	0	0	0	1	1	1	0	1	0
1	1	1	1	0	0	0	0	0	0	1	1	1	1	1	1	0	0	0	0	0	1
1	1	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0

Corollary 4.5.8 If $k \leq \binom{n}{\lfloor n/2 \rfloor} + \binom{n-2}{\lfloor n/2 \rfloor + 1}$, then $\text{CAN}(2, \Omega_k, T_2) \leq n$. In particular,

$$\text{CAN}(2, \Omega_k, T_2) \leq \min \left\{ n : k \leq \binom{n}{\lfloor n/2 \rfloor} + \binom{n-2}{\lfloor n/2 \rfloor + 1} \right\}.$$

[proof] First, if $k \leq \binom{n}{\lfloor n/2 \rfloor}$, then the result is clear: the subsets of $[n]$ of rank $\lfloor n/2 \rfloor$ form an antichain. Otherwise, write $k = \binom{n}{\lfloor n/2 \rfloor} + x$ where $0 < x \leq \binom{n-2}{\lfloor n/2 \rfloor + 1}$ and apply Proposition 4.5.6, as follows:

Let $\mathcal{A}$ be the collection of the first x $(\lfloor n/2 \rfloor + 1)$ -subsets of $[n]$ in squashed order. Let $\mathcal{D}$ be the collection of the first $\binom{n-2}{\lfloor n/2 \rfloor + 1}$ $(\lfloor n/2 \rfloor + 1)$ -subsets in squashed order. Since $x \leq \binom{n-2}{\lfloor n/2 \rfloor + 1}$, it follows that $\mathcal{A} \subseteq \mathcal{D}$. We also have $\Delta\mathcal{A} \subseteq \Delta\mathcal{D}$. By the Kruskal–Katona Theorem, we know that $|\Delta\mathcal{D}| = \binom{n-2}{\lfloor n/2 \rfloor}$. Thus $|\Delta\mathcal{A}| \leq |\Delta\mathcal{D}| = \binom{n-2}{\lfloor n/2 \rfloor}$.

We now prove that $\lfloor k/2 \rfloor \leq \binom{n}{\lfloor n/2 \rfloor} - |\Delta \mathcal{A}|$ so we may apply Proposition 4.5.6.

Since

$$\lfloor k/2 \rfloor \leq \frac{k}{2} = \frac{1}{2} \left(\binom{n}{\lfloor n/2 \rfloor} + x \right) \leq \frac{1}{2} \left(\binom{n}{\lfloor n/2 \rfloor} + \binom{n-2}{\lfloor n/2 \rfloor + 1} \right)$$

and

$$\binom{n}{\lfloor n/2 \rfloor} - \binom{n-2}{\lfloor n/2 \rfloor} = \binom{n}{\lfloor n/2 \rfloor} - |\Delta \mathcal{D}| \leq \binom{n}{\lfloor n/2 \rfloor} - |\Delta \mathcal{A}|,$$

it suffices to prove the following stronger inequality:

$$\frac{1}{2} \left(\binom{n}{\lfloor n/2 \rfloor} + \binom{n-2}{\lfloor n/2 \rfloor + 1} \right) \leq \binom{n}{\lfloor n/2 \rfloor} - \binom{n-2}{\lfloor n/2 \rfloor}.$$

Equivalently, we will prove

$$\binom{n-2}{\lfloor n/2 \rfloor + 1} + 2 \binom{n-2}{\lfloor n/2 \rfloor} \leq \binom{n}{\lfloor n/2 \rfloor}. \quad (4.5.1)$$

We have

$$\begin{aligned} \binom{n-2}{\lfloor n/2 \rfloor + 1} + 2 \binom{n-2}{\lfloor n/2 \rfloor} &= \binom{n-1}{\lfloor n/2 \rfloor + 1} + \binom{n-2}{\lfloor n/2 \rfloor} \\ &\quad \left(\text{since } \binom{x}{y+1} + \binom{x}{y} = \binom{x+1}{y+1} \right) \\ &< \binom{n-1}{\lfloor n/2 \rfloor + 1} + \binom{n-1}{\lfloor n/2 \rfloor} \\ &= \binom{n}{\lfloor n/2 \rfloor + 1} \\ &\leq \binom{n}{\lfloor n/2 \rfloor} \end{aligned}$$

Thus, the inequality in (4.5.1) holds. It now follows that $\lfloor k/2 \rfloor \leq \binom{n}{\lfloor n/2 \rfloor} - |\Delta \mathcal{A}|$. By Proposition 4.5.6, we have $\text{CAN}(2, \Omega_k, T_2) \leq n$. ■

Corollary 4.5.8 gives us infinitely many values of k for which $\text{CAN}(2, \Omega_k, T_2)$ is strictly smaller than the upper bound of Corollary 4.4.10; however, the bound from Corollary 4.5.8 is no better than one row less than the upper bound given in Corollary 4.4.10. In particular, if n is even or if $n \geq 9$, then

$$2 \binom{n-1}{\lfloor (n-1)/2 \rfloor} < \binom{n}{\lfloor n/2 \rfloor} + \binom{n-2}{\lfloor n/2 \rfloor + 1} < 2 \binom{n}{\lfloor n/2 \rfloor}.$$

To obtain more data, we used a simple backtracking algorithm to search for homomorphisms from Ω_k to $\text{QI}(n, T_2)$. Table 4.1 summarizes our findings and includes columns for the lower and upper bounds given in Corollary 4.4.10. The bounds are abbreviated as follows: L.B. = $\lceil \log_2 k \rceil$ and U.B. = $\min\{n : k \leq 2\binom{n-1}{\lfloor (n-1)/2 \rfloor}\}$.

k	L.B.	$\text{CAN}(2, \Omega_k, T_2)$	U.B.	k	L.B.	$\text{CAN}(2, \Omega_k, T_2)$	U.B.
2	1	1	1	20	5	5	6
3	2	3	3	21	5	6	7
4	2	3	3	22	5	6	7
5	3	4	4	23	5	6	7
6	3	4	4	24	5	6	7
7	3	4	5	25	5	6	7
8	3	4	5	26	5	6	7
9	4	4	5	27	5	6	7
10	4	5	5	28	5	6	7
11	4	5	5	29	5	6	7
12	4	5	5	30	5	6	7
13	4	5	6	31	5	6	7
14	4	5	6	32	5	6	7
15	4	5	6	33	6	6	7
16	4	5	6	34	6	6	7
17	5	5	6	35	6	6	7
18	5	5	6	36	6	6	7
19	5	5	6	37	6	6	7

Table 4.1: $\text{CAN}(2, \Omega_k, T_2)$ for $2 \leq k \leq 37$

Here are some observations regarding Table 4.1:

For $k \in \{2, 9, 17, 18, 19, 20, 33, 34, 35, 36\}$, we have $\lceil \log_2 k \rceil = \text{CAN}(2, \Omega_k, T_2)$. If Conjecture 4.5.1 is true, then for some values of k , all k -tournaments hit the lower bound given by Corollary 4.4.10.

Notice that $36 > \binom{6}{3} + \binom{6}{4}$ but $\text{CAN}(2, \Omega_{36}, T_2) = 6$. It is not possible for the 36 columns of a $\text{CA}(6; 2, \Omega_{36}, T_2)$ to consist only of subsets of $[6]$ of the two largest ranks 3 and 4. Therefore, it is not true that optimal binary covering arrays on circular tournaments can be assumed to have columns from among the two largest ranks only.

Up to $k = 9$, our computer search for homomorphisms of Ω_k to the T_2 -dependence graph was exhaustive, that is, we found all homomorphisms of Ω_k to $\text{QI}(n, T_2)$ for all $n \leq \text{CAN}(2, \Omega_k, T_2)$. For larger values of k , we made use of the following results to

cut down on search time, and we stopped searching once at least one homomorphism was found.

Lemma 4.5.9 If A is a $\text{CA}(n; 2, \Omega_k, T_2)$, then the columns of the complement of A , the array obtained from A by interchanging all zeros and ones, can be rearranged to give a $\text{CA}(n; 2, \Omega_k, T_2)$.

[proof] The columns of A are indexed by $1, \dots, k$. We take the complementary columns to build an array A' with columns indexed by $f(1), \dots, f(k)$, where $f(i) = k + 1 - i \pmod{k}$. That is, $A' = [C_{f(1)}, \dots, C_{f(k)}]$ where $C_{f(i)}$ is the complement of column i of A . We now prove that A' is a $\text{CA}(n; 2, \Omega_k, T_2)$. Let $\{(x, 0), (y, 1)\}$ be a required interaction with respect to Ω_k and T_2 . We want to show that this 0-1 interaction is covered by columns C_x and C_y of A' . Well, $x = f(i)$ and $y = f(j)$ for some $i, j \in \{1, \dots, k\}$. So $y - x = (k + 1 - j) - (k + 1 - i) = i - j$. This means that in A , columns j and i needed to cover the interaction $\{(j, 0), (i, 1)\}$. Therefore, the corresponding complemented columns C_y and C_x of A' must cover the interaction $\{(y = f(j), 1), (x = f(i), 0)\}$. Thus, A' is indeed a $\text{CA}(n; 2, \Omega_k, T_2)$. ■

Lemma 4.5.10 Let $k \geq 3$. If $\Omega_k \rightarrow \text{QI}(n, T_2)$, then $k \leq 2^n - 2$.

[proof] Consider, as subsets of $[n]$, the vertices $\emptyset$ and $[n]$ of $V(\text{QI}(n, T_2))$. Neither of these vertices have both in- and out-neighbours, so they cannot be the image of a vertex of Ω_k (all of which have nonzero indegree and outdegree, with the exception of Ω_2). Since homomorphisms of tournaments to $\text{QI}(n, T_2)$ must be vertex-injective, it follows that $\Omega_k \rightarrow \text{QI}(n, T_2)$ only if $k \leq 2^n - 2$. ■

Since 37 is the largest value of k for which our algorithm succeeded to find a homomorphism (within a reasonable amount of time), we provide an example of a $\text{CA}(6; 2, \Omega_{37}, T_2)$.

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37
1	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	0	0	1	0	0	0	1	1	1	0	1	0	1	0	0	
1	0	1	1	0	0	1	1	0	0	1	1	0	0	1	0	1	1	0	0	1	0	0	0	1	0	0	1	1	0	1	1	1	0	0	1	0
0	1	1	1	1	1	1	1	1	1	1	1	1	1	0	0	0	1	1	1	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	1	1	1	0	0	0	0	1	1	1	0	0	0	0	0	0	1	1	1	1	0	0	1	1	0	0	0	0	1	1	1	1	
1	0	0	0	0	0	0	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	1	1	1	1	1	1	1	
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1	1	0	1	1	0	1	1	0	0	1	

In Table 4.1, we see that circular tournaments hit the lower bound $\lceil \log_2 k \rceil$ several

times. In fact, the following construction proves that circular tournaments will hit the lower bound for infinitely many values of k .

For the construction, given in Proposition 4.5.11, we consider a supergraph of the circular tournament, denoted Ω_k^+ , defined for even values of k as follows. The vertex set of Ω_k^+ is $V(\Omega_k^+) = [k]$ and $ij \in E(\Omega_k^+)$ if and only if $1 \leq j - i \pmod{k} \leq k/2$. The only difference between Ω_k and Ω_k^+ is that Ω_k^+ has symmetric pairs of arcs joining the vertices at distance $k/2$.

Proposition 4.5.11 If k is even, then $\text{CAN}(2, \Omega_{2k}^+, T_2) \leq \text{CAN}(2, \Omega_k^+, T_2) + 1$.

[proof] Let $n = \text{CAN}(2, \Omega_k^+, T_2)$, and let $C_1, \dots, C_k$ denote the columns of a $\text{CA}(n; 2, \Omega_k^+, T_2)$. Take two copies of this array and interleave their columns as shown below. Add a row of alternating zeros and ones. Let us call the array we obtain A .

$$A \quad \begin{array}{|c|c|c|c|c|c|c|} \hline C_1 & C_1 & C_2 & C_2 & \cdots & C_k & C_k \\ \hline 0 & 1 & 0 & 1 & \cdots & 0 & 1 \\ \hline \end{array}$$

For each $j \in [2k]$, the j th column of A corresponds to column $C_{\lceil j/2 \rceil}$. Consider two distinct columns i and j of A such that $j - i \pmod{2k} \leq k$. We must show that A covers the interaction $\{(i, 0), (j, 1)\}$.

If $\lceil j/2 \rceil = \lceil i/2 \rceil$, then i and j correspond to the same column $C_{j/2}$; in this case, the extra row of alternating zeros and ones covers $\{(i, 0), (j, 1)\}$.

If $j > i$, then $1 \leq j - i \leq k$. In this case, we consider all possibilities for the parity of i and j : If i and j are both odd, or if i and j are both even, then $\lceil j/2 \rceil - \lceil i/2 \rceil = j/2 - i/2 \leq k/2$; in these cases, the i th column of A ($C_{\lceil i/2 \rceil}$) and the j th column of A ($C_{\lceil j/2 \rceil}$) cover $\{(i, 0), (j, 1)\}$ since $\{(\lceil i/2 \rceil, 0), (\lceil j/2 \rceil, 1)\}$ is a required interaction with respect to Ω_k^+ and T_2 . If i is odd and j is even, then the extra row of alternating zeros and ones covers $\{(i, 0), (j, 1)\}$. If i is even and j is odd, then $1 \leq j - i \leq k - 1$, since k is even. It now follows that $j/2 + 1/2 - i/2 = \lceil j/2 \rceil - \lceil i/2 \rceil \leq k/2$; in these cases, the i th column of A ($C_{\lceil i/2 \rceil}$) and the j th column of A ($C_{\lceil j/2 \rceil}$) cover $\{(i, 0), (j, 1)\}$ since $\{(\lceil i/2 \rceil, 0), (\lceil j/2 \rceil, 1)\}$ is a required interaction with respect to Ω_k^+ and T_2 .

If $j < i$, then $1 \leq 2k + j - i \leq k$, and the case-analysis is similar to show that the array A covers each required interaction of the form $\{(i, 0), (j, 1)\}$.

Thus, the array A is a $\text{CA}(n+1; 2, \Omega_{2k}^+, T_2)$, and it follows that $\text{CAN}(2, \Omega_{2k}^+, T_2) \leq \text{CAN}(2, \Omega_k^+, T_2) + 1$. ■

We now apply Proposition 4.5.11 to circular tournaments and we obtain infinitely many values of k for which $\text{CAN}(2, \Omega_k, T_2) = \lceil \log_2 k \rceil$.

Corollary 4.5.12 For infinitely many values of k , we have

$$\text{CAN}(2, \Omega_k, T_2) = \lceil \log_2 k \rceil.$$

[proof] For all $L \geq 0$, we prove that $\lceil \log_2 k \rceil = \text{CAN}(2, \Omega_k, T_2)$ whenever $16 \cdot 2^L < k \leq 20 \cdot 2^L$.

First, when $k = 20$, we have a $\text{CA}(5; 2, \Omega_{20}^+, T_2)$:

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	1	0	1	0	1	0	0	1	1	0	0	0	0	1	1	1	1	0	0
1	0	1	1	0	0	1	0	0	0	1	1	0	0	1	1	0	0	1	1
1	0	0	0	1	1	1	0	0	0	0	0	1	1	0	0	1	1	1	1
0	1	1	1	1	1	1	0	1	0	1	0	1	0	0	0	0	0	0	0
0	0	0	0	0	0	0	1	1	1	1	1	1	1	0	1	0	1	0	1

By Proposition 4.5.11, for all $L \geq 0$, we have

$$\text{CAN}(2, \Omega_{20 \cdot 2^L}^+, T_2) \leq \text{CAN}(2, \Omega_{20}^+, T_2) + L = L + 5 = \lceil \log_2(20 \cdot 2^L) \rceil. \quad (4.5.2)$$

Since, for all even values of k , we have $\Omega_{k-1} \subset \Omega_k \subset \Omega_k^+$, the above bound applies to all circular tournaments Ω_k for which $k \leq 20 \cdot 2^L$. In particular, if k lies in the range $16 \cdot 2^L < k \leq 20 \cdot 2^L$, for some integer $L \geq 0$, then $\lceil \log_2 k \rceil = L + 5$. By Lemma 4.4.2, we have the lower bound $\lceil \log_2 k \rceil \leq \text{CAN}(2, \Omega_k, T_2)$. This bound together with the bound given in (4.5.2) yields the following bounds:

$$L + 5 = \lceil \log_2 k \rceil \leq \text{CAN}(2, \Omega_k, T_2) \leq \text{CAN}(2, \Omega_{20 \cdot 2^L}^+, T_2) = L + 5.$$

Thus, for all k such that $16 \cdot 2^L < k \leq 20 \cdot 2^L$, we have $\text{CAN}(2, \Omega_k, T_2) = \lceil \log_2 k \rceil$. ■

Chapter 5

Sperner capacities

In this chapter, we give two slight extensions of the results of Gargano, Körner and Vaccaro [24, 25] regarding Sperner capacities. In Section 5.1, we discuss the results in [24, 25] related to covering arrays with alphabet graphs. In Section 5.2, we extend a result given in [24] from stars to arbitrary complete bipartite graphs. In Section 5.3, we define Sperner capacities of alphabet graphs with respect to transitive tournaments and we determine a formula for these new Sperner capacities for any directed alphabet graph H .

5.1 Definitions and background

In this section, we outline the relevant definitions and results of Gargano, Körner and Vaccaro given in [24] and [25]. The results in both these papers are similar in nature, but the setting in [25] is more general. We concentrate on those results related to covering arrays with alphabet graphs, but observe that the main theorem given in [25] (namely, Theorem 2 in [25]) is far more general than the results we discuss presently.

We begin with the statement of two theorems, translated to use the language of covering arrays.

Theorem 5.1.1 (see Theorem 1 in [24]) If $v \geq 2$, then

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log_2 \text{CAK}(n; 2, v) = \frac{2}{v}.$$



The **binary entropy function**, denoted h , is a map $h : [0, 1] \rightarrow [0, 1]$, where, for all $x \in (0, 1)$, we have

$$h(x) = -x \log_2(x) - (1 - x) \log_2(1 - x),$$

and $h(0) = h(1) = 0$.

Theorem 5.1.2 (see Corollary 1 in [25]) If H is an undirected alphabet graph, then

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log_2 \text{CAK}(n; 2, H) = \max_P \min_{ab \in E(H)} (P_a + P_b) \cdot h\left(\frac{P_a}{P_a + P_b}\right),$$

where the maximum is taken over all probability distributions P on $V(H)$ given by $P(a) = P_a$ for each $a \in V(H)$. ■

Theorem 5.1.1 is obtained as a special case of Theorem 5.1.2 by using $H = K_v^{\text{loop}}$ and determining that the maximizing probability distribution is uniform for K_v^{loop} .

The limits in Theorem 5.1.1 and Theorem 5.1.2 are specific instances of Sperner capacities, as we will explain below using covering array terminology wherever applicable.

Let $\mathcal{G}$ be a family of directed alphabet graphs, all on a common vertex set $V = [v]$. Let $\vec{x}$ and $\vec{y}$ be two v -ary n -tuples, where $\vec{x} = (x_1, \dots, x_n) \in V^n$ and $\vec{y} = (y_1, \dots, y_n) \in V^n$. We say that $\vec{x}$ **precedes** $\vec{y}$ **relative to** $\mathcal{G}$ if, for every $G \in \mathcal{G}$, there is an index $i \in [n]$ such that $(x_i, y_i) \in E(G)$. Notice that, for each $G \in \mathcal{G}$, we do not require $\vec{x}$ and $\vec{y}$ to cover all arcs of G ; we require $\vec{x}$ and $\vec{y}$ to cover *at least* one arc of each G .

A collection $C \subseteq V^n$ is **incomparable** for $\mathcal{G}$, if, for every ordered pair of distinct n -tuples $(\vec{x}, \vec{y}) \in C \times C$, it is the case that $\vec{x}$ precedes $\vec{y}$ relative to $\mathcal{G}$.

Let $I(\mathcal{G}, n)$ denote the largest cardinality of a collection $C \subseteq V^n$ that is incomparable for $\mathcal{G}$. The **Sperner capacity** of $\mathcal{G}$, denoted $\Sigma(\mathcal{G})$, is the limit

$$\Sigma(\mathcal{G}) = \limsup_{n \rightarrow \infty} \frac{1}{n} \log_2 I(\mathcal{G}, n).$$

In [25], it is observed that the limit superior in $\Sigma(\mathcal{G})$ may be replaced by a limit.

Example 5.1.3 If $\mathcal{G}$ is a family consisting of one member, the single-arc graph T_2 , then a collection $C \subseteq V^n$ is incomparable for $\mathcal{G}$ if and only if it corresponds to an antichain of subsets. In this special case, $I(\mathcal{G}, n) = \binom{n}{\lfloor n/2 \rfloor}$ as given by Sperner [54] (see Theorem 2.1.1), and we have $\Sigma(\mathcal{G}) = 1$.

Example 5.1.3 is the motivation behind the terminology “Sperner” capacity.

Example 5.1.4 Let H be an undirected alphabet graph with $V(H) = [v]$, and let H' denote an orientation of H . Let $\mathcal{E}(H)$ denote the family of one-arc graphs on vertex set $[v]$ such that the union of these arcs is $E(H')$. In this case, we have $I(\mathcal{E}(H), n) = \text{CAK}(n; 2, H)$, and the limit in Theorem 5.1.2 is but one special case of Sperner capacity. That is,

$$\Sigma(\mathcal{E}(H)) = \lim_{n \rightarrow \infty} \frac{1}{n} \log_2 \text{CAK}(n; 2, H).$$

In particular, if $H = K_v^{\text{loop}}$, then $I(\mathcal{E}(K_v^{\text{loop}}), n) = \text{CAK}(n; 2, v)$, and the limit in Theorem 5.1.1 is another special case of Sperner capacity. That is,

$$\Sigma(\mathcal{E}(K_v^{\text{loop}})) = \lim_{n \rightarrow \infty} \frac{1}{n} \log_2 \text{CAK}(n; 2, v).$$

In Example 5.1.4, the family $\mathcal{E}(H)$ depends on the particular orientation H' of H ; however, the Sperner capacity of $\mathcal{E}(H)$ is unaffected by the particular orientation that was chosen. Given an undirected alphabet graph H , we use $\mathcal{E}(H)$ to denote any such family of one-arc digraphs whose union corresponds to the edge set of some orientation of H . The particular orientation of H will not come into play.

Although Sperner capacities are defined in terms of arbitrary families of directed graphs, in the context of this chapter, we only consider Sperner capacities of families of one-arc graphs whose union is the edge set of an orientation of an undirected alphabet graph H , that is, $\mathcal{E}(H)$. For a given alphabet graph H , we sometimes refer to the limit in Theorem 5.1.2 as the **Sperner capacity** of H , where it is understood that we are talking about the Sperner capacity of the family of one-arc digraphs $\mathcal{E}(H)$.

5.2 Sperner capacity of complete bipartite graphs

As one application of Theorem 5.1.2, Gargano, Körner and Vaccaro determined the maximizing probability distribution in Theorem 5.1.2 whenever H is a star. In this section, we apply Theorem 5.1.2 to complete bipartite graphs and determine their maximizing probability distribution.

To begin, we outline the results for stars. Recall that S_v denotes the star on v vertices.

In [24], Gargano, Körner and Vaccaro prove that

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log_2 \text{CAK}(n; 2, S_v) = \max_{\alpha} (1 - (v-2)\alpha) \cdot h\left(\frac{\alpha}{1 - (v-2)\alpha}\right). \quad (5.2.1)$$

Comparing (5.2.1) to the limit in Theorem 5.1.2, we see that the maximizing probability distribution for stars gives equal probability to each of the leaves (the leaves each have probability α , while the central vertex has probability $1 - (v-1)\alpha$). To determine the Sperner capacity of the star S_v , we only need to find the maximizing value of α . In particular, Gargano, Körner and Vaccaro [24] show that $\Sigma(\mathcal{E}(S_v))$ is equal to the unique positive real root t of the equation

$$2^{-t} + 2^{-(v-1)t} = 1. \quad (5.2.2)$$

In Table 5.1, we give the approximate probabilities in the maximizing distributions for the Sperner capacities of stars, with respect to (5.2.1). These values obtained by computer.

v	central probability	leaf probability	Sperner capacity of S_v
2	0.5	0.5	1
3	0.4472135955	0.276393203	0.694241913631
4	0.417237987926	0.194254004	0.551463089746
5	0.39665063816	0.150837341	0.464958417216
6	0.381157147833	0.123768571	0.405685231376
7	0.368841155014	0.105193141	0.361991800696
8	0.358685190969	0.091616401	0.328173397042
9	0.350086482564	0.081239190	0.301066229039
10	0.342659672098	0.073037814	0.278757614255

Table 5.1: Probabilities in maximizing distribution for Sperner capacity of stars

Let $\mathcal{E}(K_{l,m})$ denote the family of one-arc graphs on $V(K_{l,m}) = [l + m]$, each graph corresponding to an orientation of one of the edges of the complete bipartite graph $K_{l,m}$. For the Sperner capacity of $K_{l,m}$, Theorem 5.1.2 says

$$\Sigma(\mathcal{E}(K_{l,m})) = \max_P \min_{ab \in E(K_{l,m})} (P_a + P_b) \cdot h\left(\frac{P_a}{P_a + P_b}\right). \quad (5.2.3)$$

The next lemma is of use for determining the maximizing probability distribution in (5.2.3).

For an edge $e = ab$ and a probability distribution P on $V(K_{l,m})$, we use $F(e, P)$ to denote

$$F(e, P) = (P_a + P_b) \cdot h\left(\frac{P_a}{P_a + P_b}\right).$$

For simplicity, if $e = ab$ has ends with probabilities $P_a = p$ and $P_b = q$, we write $F(p, q)$ interchangeably with $F(e, P)$.

Lemma 5.2.1 Let $q \in (0, 1)$ be fixed, and let $f : (0, 1 - q) \rightarrow \mathbb{R}$ be a function defined by

$$f(p) = F(p, q) = (p + q) \left[-\left(\frac{p}{p+q}\right) \log_2 \left(\frac{p}{p+q}\right) - \left(\frac{q}{p+q}\right) \log_2 \left(\frac{q}{p+q}\right) \right].$$

Then $f(p)$ is an increasing function on $(0, 1 - q)$.

[proof] We have $f(p) = -p \log_2 \left(\frac{p}{p+q}\right) - q \log_2 \left(\frac{q}{p+q}\right)$. Thus, the derivative of f with respect to p satisfies

$$\begin{aligned} f'(p) &= -\log_2 \left(\frac{p}{p+q}\right) - \frac{p}{\ln 2} \left(\frac{p+q}{p}\right) \left(\frac{p+q-p}{(p+q)^2}\right) - \frac{q}{\ln 2} \left(\frac{p+q}{q}\right) \left(\frac{-q}{(p+q)^2}\right) \\ &= -\log_2 \left(\frac{p}{p+q}\right) - \frac{1}{\ln 2} \left(\frac{q}{p+q}\right) + \frac{1}{\ln 2} \left(\frac{q}{p+q}\right) \\ &= -\log_2(p) + \log_2(p+q). \end{aligned}$$

Since $q \neq 0$, we see that $f(p)$ has no critical points since $0 = -\log_2(p) + \log_2(p+q)$ implies $q = 0$.

Clearly, $\frac{1}{2}(1 - q) \in (0, 1 - q)$. Notice that $1 - q < 1$ and $1 + q > 1$. Thus, $\frac{1-q}{1+q} < 1$. Consequently, $\log_2 \left(\frac{1-q}{1+q}\right) < 0$. Now, $f'(\frac{1}{2}(1 - q)) = -\log_2 \left(\frac{1-q}{1+q}\right) > 0$. Thus f is increasing on $(0, 1 - q)$. ■

Proposition 5.2.2 The Sperner capacity of the complete bipartite graph $K_{l,m}$ satisfies

$$\Sigma(\mathcal{C}(K_{l,m})) = \lim_{n \rightarrow \infty} \frac{1}{n} \log_2 \text{CAK}(n; 2, K_{l,m}) = \max_{\alpha \in (0,1)} F\left(\alpha, \frac{1-l\alpha}{m}\right).$$

[proof] Let $K_{l,m}$ have bipartition (X, Y) , where $|X| = l$ and $|Y| = m$. Suppose P is the maximizing probability of (5.2.3). Let $p_1 \leq p_2 \leq \dots \leq p_l$ be the probabilities

on the vertices in X and let $q_1 \leq q_2 \leq \dots \leq q_m$ be the probabilities on the vertices in Y . Consider the vertex of probability q_j . By Lemma 5.2.1, the minimum $F(e, P)$ value, over all edges e incident with the vertex of probability q_j , is given by $F(q_j, p_1)$ since p_1 is minimum. Thus, an edge e of $K_{l,m}$ of minimum $F(e, P)$ value has one end with probability p_1 . Now, by Lemma 5.2.1, the minimum edge incident to the vertex of probability p_1 has probability q_1 . Thus, $\min_{e \in E(K_{l,m})} F(e, P) = F(p_1, q_1)$.

Now, we show that the probabilities p_i must be equal. If there existed an index $i \in [l]$ such that $p_i < p_{i+1}$, then the average probability $\bar{p} = \frac{\sum_{j=1}^l p_j}{l}$ would satisfy $\bar{p} > p_1$. In this case, we would have $F(q_1, \bar{p}) > F(q_1, p_1)$, contradicting the maximality of P . Thus, all p_i 's must be equal as claimed. Similarly, all q_i 's must be equal. Therefore, the probability distribution that maximizes $\min_{e \in E(K_{l,m})} F(e, P)$ is of the form $P(x) = \alpha$ for all $x \in X$ and $P(y) = \frac{(1-l\alpha)}{m}$ for all $y \in Y$. ■

Corollary 5.2.3 The Sperner capacity of $K_{l,m}$, $\Sigma(\mathcal{E}(K_{l,m}))$, is the unique positive root t of the equation

$$2^{-lt} + 2^{-mt} = 1.$$

[proof] Let $K_{l,m}$ have bipartition (X, Y) , where $|X| = l$ and $|Y| = m$. By Proposition 5.2.2, the maximizing probability on $V(K_{l,m})$ is of the form $P(x) = \alpha$ for each $x \in X$ and $P(y) = \frac{1-l\alpha}{m}$ for each $y \in Y$. Let p and q be functions of α given by $p(\alpha) = \alpha$ and $q(\alpha) = \frac{1-l\alpha}{m}$, and define the function f by

$$f(\alpha) = -p(\alpha) \log_2 \left(\frac{p(\alpha)}{p(\alpha) + q(\alpha)} \right) - q(\alpha) \log_2 \left(\frac{q(\alpha)}{p(\alpha) + q(\alpha)} \right).$$

By Proposition 5.2.2, the Sperner capacity of $\mathcal{E}(K_{l,m})$ satisfies

$$\Sigma(\mathcal{E}(K_{l,m})) = \max_{\alpha} f(\alpha)$$

since $f(\alpha) = F(p(\alpha), q(\alpha))$.

To find the maximizing probability $\alpha \in (0, 1)$, we take the derivative of f with respect to α , which can be simplified to

$$f'(\alpha) = -p'(\alpha) \log_2 \left(\frac{p(\alpha)}{p(\alpha) + q(\alpha)} \right) - q'(\alpha) \log_2 \left(\frac{q(\alpha)}{p(\alpha) + q(\alpha)} \right).$$

Since $p(\alpha) = \alpha$ and $q(\alpha) = \frac{1}{m}(1 - l\alpha)$, we have $p'(\alpha) = 1$ and $q'(\alpha) = -l/m$. Thus,

$$f'(\alpha) = -\log_2 \left(\frac{p(\alpha)}{p(\alpha) + q(\alpha)} \right) + \frac{l}{m} \log_2 \left(\frac{q(\alpha)}{p(\alpha) + q(\alpha)} \right). \quad (5.2.4)$$

Therefore, $f(\alpha)$ can be rewritten in terms of its derivative as follows:

$$f(\alpha) = \alpha f'(\alpha) - \frac{1}{m} \log_2 \left(\frac{q(\alpha)}{p(\alpha) + q(\alpha)} \right).$$

If f attains an absolute maximum at $\alpha^* \in (0, 1)$, then $f'(\alpha^*) = 0$, and

$$\Sigma(\mathcal{E}(K_{l,m})) = f(\alpha^*).$$

If we let $t = \Sigma(\mathcal{E}(K_{l,m})) = f(\alpha^*)$, then

$$t = -\alpha^* f'(\alpha^*) - \frac{1}{m} \log_2 \left(\frac{q(\alpha^*)}{p(\alpha^*) + q(\alpha^*)} \right) = -\frac{1}{m} \log_2 \left(\frac{q(\alpha^*)}{p(\alpha^*) + q(\alpha^*)} \right).$$

Consequently, $-mt = \log_2 \left(\frac{q(\alpha^*)}{p(\alpha^*) + q(\alpha^*)} \right)$ and we can write

$$2^{-mt} = \frac{q(\alpha^*)}{p(\alpha^*) + q(\alpha^*)}. \quad (\star)$$

Substitute $f'(\alpha^*) = 0$ and $(\star)$ into the equation given in (5.2.4), we have

$$\log_2 \left(\frac{p(\alpha^*)}{p(\alpha^*) + q(\alpha^*)} \right) = \frac{l}{m} \log_2 \left(\frac{q(\alpha^*)}{p(\alpha^*) + q(\alpha^*)} \right) = \frac{l}{m} \log_2(2^{-mt}).$$

Thus, $\log_2 \left(\frac{p(\alpha^*)}{p(\alpha^*) + q(\alpha^*)} \right) = -lt$ and we have

$$2^{-lt} = \frac{p(\alpha^*)}{p(\alpha^*) + q(\alpha^*)}. \quad (\star\star)$$

Putting $(\star)$ together with $(\star\star)$, we get

$$2^{-mt} + 2^{-lt} = \left(\frac{q(\alpha^*)}{p(\alpha^*) + q(\alpha^*)} \right) + \left(\frac{p(\alpha^*)}{p(\alpha^*) + q(\alpha^*)} \right) = 1.$$

Thus, $t = \Sigma(\mathcal{E}(K_{l,m}))$ is a positive root of the equation $2^{-lt} + 2^{-mt} = 1$.

Let $x = 2^{-t}$ and rewrite $2^{-lt} + 2^{-mt} = 1$ as $x^l + x^m - 1 = 0$. By Descartes' Rule of Signs, $x^l + x^m - 1 = 0$ has at most one positive real root, thus $t = \Sigma(\mathcal{E}(K_{l,m}))$ is the unique positive real root of $2^{-lt} + 2^{-mt} = 1$. ■

In Table 5.2, we give the approximate probabilities in the maximizing distributions for the Sperner capacities of complete bipartite graphs, with respect to Proposition 5.2.2. These values were obtained by computer.

l	m	α	$\frac{1-l\alpha}{m}$	$\Sigma(\mathcal{E}(K_{l,m}))$
2	2	0.25	0.25	0.5
2	3	0.234485	0.17701	0.405685231376
2	4	0.223605	0.1381975	0.347120956815
2	5	0.215295	0.113882	0.306268894185
2	6	0.208615	0.0971283	0.275731544873
2	7	0.20306	0.08484	0.251825364448
2	8	0.19832	0.07542	0.232479208608
3	3	0.16667	0.16667	0.333333333333
3	4	0.15932	0.13051	0.287760787084
3	5	0.153656	0.107806	0.255632592557
3	6	0.149071	0.092131	0.23141397121
3	7	0.145235	0.080614	0.2123226659
4	4	0.125	0.125	0.25
4	5	0.120724	0.103421	0.223180302968
4	6	0.117243	0.088504	0.202842615688
5	5	0.1	0.1	0.2

Table 5.2: Maximizing distributions of Sperner capacities of $K_{l,m}$

For an alphabet graph H with no loops, we get the following bounds on the Sperner capacity of H :

Proposition 5.2.4 If H is an undirected alphabet graph with no loops, then

$$\frac{2}{|V(H)|} \leq \Sigma(\mathcal{E}(H)) \leq \frac{2}{|\chi(H)|}.$$

[proof] By Proposition 3.3.4, we have

$$\text{CAK}(n; 2, K_{|V(H)|}) \leq \text{CAK}(n; 2, H) \leq \text{CAK}(n; 2, K_{\chi(H)}).$$

By Theorem 5.1.1, we have $2/|V(H)| = \Sigma(\mathcal{E}(K_{|V(H)|}))$ and $2/\chi(H) = \Sigma(\mathcal{E}(K_{\chi(H)}))$ and the result follows. ■

5.3 Transitive tournament capacities

In this section, we define a new Sperner capacity involving transitive tournament column graphs. A slight alteration of a proof in [24] allows us to determine a formula, analogous to the limit in Theorem 5.1.2, for these capacities.

Let H be a directed alphabet graph. The *column number with respect to transitive tournament column graphs*, denoted $\text{CAK}(n; 2, \{T_L\}, H)$, is the maximum integer k for which there exists a $\text{CA}(n; 2, T_k, H)$.

The *Sperner capacity of H with respect to transitive tournaments*, denoted $\Sigma(H, \{T_L\})$, is the limit

$$\Sigma(H, \{T_L\}) = \limsup_{n \rightarrow \infty} \frac{1}{n} \log_2 \text{CAK}(n; 2, \{T_L\}, H).$$

It is clear that

$$\text{CAK}(n; 2, H) \leq \text{CAK}(n; 2, \{T_L\}, H)$$

for all n , since every $\text{CA}(n; 2, K_k, H)$ is, in particular, a $\text{CA}(n; 2, T_k, H)$. It now follows that the Sperner capacity of the family of one-arc digraphs $\mathcal{E}(H)$ satisfies

$$\Sigma(\mathcal{E}(H)) \leq \Sigma(H, \{T_L\}).$$

Corollary 5.3.1 If H is a directed alphabet graph, then

$$\max_P \min_{ab \in E(H)} F(ab, P) \leq \Sigma(H, \{T_L\}),$$

where the maximum is taken over all probability distributions P on $V(H)$.

[proof] By Theorem 5.1.2, we have

$$\max_P \min_{ab \in E(H)} F(ab, P) = \lim_{n \rightarrow \infty} \frac{1}{n} \log_2 \text{CAK}(n; 2, H).$$

Since $\text{CAK}(n; 2, H) \leq \text{CAK}(n; 2, \{T_L\}, H)$, the result follows. ■

Gargano, Körner and Vaccaro attribute the following theorem to Cohen, Körner and Simonyi [9], but give a different proof of it in [24]. Here, we rephrase it using covering array notation.

Theorem 5.3.2 (see Theorem CKS in [24]) If G is an undirected alphabet graph, then

$$\limsup_{n \rightarrow \infty} \frac{1}{n} \log_2 \text{CAK}(n; 2, G) \leq \max_P \min_{ab \in E(G)} F(ab, P),$$

where $F(ab, P) = (P_a + P_b) \cdot h(\frac{P_a}{P_a + P_b})$, and the maximum is taken over all probability distributions P on $V(G)$. ■

We adapt the proof of Theorem 5.3.2, given in [24], to accommodate transitive tournaments using the following result of Frankl [23].

Theorem 5.3.3 (Frankl’s Inequality [23]) Let $\mathcal{A} = \{A_1, \dots, A_k\}$ be a collection of r -subsets of $[n]$ and let $\mathcal{B} = \{B_1, \dots, B_k\}$ be a collection of s -subsets of $[n]$. If $A_i \cap B_i = \emptyset$ for all $i \in [k]$, and $A_i \cap B_j \neq \emptyset$ for $1 \leq i < j \leq k$, then

$$k \leq \binom{r+s}{s}. \quad \blacksquare$$

Theorem 5.3.3 can be applied to the columns of covering arrays on transitive tournament column graphs as follows. Let H be a directed alphabet graph with no loops. Let $V(H) = [v]$. Let $C_1, \dots, C_k$ denote the columns of a $\text{CA}(n; 2, T_k, H)$, where, for each $j \in [k]$, the j th column is of the form $C_j = (c_{1j}, \dots, c_{nj}) \in [v]^n$. Take an arc $ab \in E(H)$. For each column C_j , define two subsets of $[n]$: $A_j = \{i \in [n] : c_{ij} = a\}$ and $B_j = \{i \in [n] : c_{ij} = b\}$. Let $\mathcal{A} = \{A_1, \dots, A_k\}$ and let $\mathcal{B} = \{B_1, \dots, B_k\}$. Clearly, $A_i \cap B_i = \emptyset$ for all $i \in [k]$. If $i, j \in [k]$ and $i < j$, then $ij \in E(T_k)$, so columns C_i and C_j must cover the arc $ab \in E(H)$. In terms of the families $\mathcal{A}$ and $\mathcal{B}$, this means that $A_i \cap B_j \neq \emptyset$. All that remains for $\mathcal{A}$ and $\mathcal{B}$ to satisfy the conditions of Theorem 5.3.3 is to ensure that all the sets $A_i \in \mathcal{A}$ have a common cardinality and all the sets $B_i \in \mathcal{B}$ have a common cardinality.

To obtain our result on Sperner capacities with respect to transitive tournaments, we also make use of the following lemma which relates the binary entropy function to binomial coefficients.

Lemma 5.3.4 (see Lemma 2.3 in [18]) Let $0 < k < n$ be integers. If $q = k/n$, then

$$\frac{1}{(n+1)^2} 2^{nh(q)} \leq \binom{n}{k} \leq 2^{nh(q)}. \quad \blacksquare$$

We are now in a position to adapt the proof of Theorem 5.3.2 given by Gargano, Körner, and Vaccaro [24] to a proof that holds for any directed alphabet graph H and for the family of transitive tournament column graphs $\{T_L\}$. For our proof, we essentially repeat the proof in [24]; the only point where our proof differs is when we apply Frankl’s Inequality in Theorem 5.3.3—the proof in [24] applies Bollobás’s Inequality (Theorem 2.1.3) exactly where we use Frankl’s Inequality.

Theorem 5.3.5 If H is a directed alphabet graph with no loops, then

$$\Sigma(H, \{T_L\}) \leq \max_P \min_{e \in E(H)} F(e, P).$$

[proof] Let $V(H) = [v]$ and let $\widehat{\mathcal{C}} = \{C_1, \dots, C_k\}$ be the ordered collection of columns of a $\text{CA}(n; 2, T_k, H)$, where $k = \text{CAK}(n; 2, \{T_L\}, H)$ and $C_j = (c_{1j}, c_{2j}, \dots, c_{nj})$ for each $j \in [k]$.

For each $C_j \in \widehat{\mathcal{C}}$ and for each $a \in [v]$, let $n_j(a)$ denote the number of times the symbol a occurs in C_j , that is, $n_j(a) = |\{i \in [n] : c_{ij} = a\}|$. Recall that the **type** of C_j is the v -tuple $(n_j(1), n_j(2), \dots, n_j(v))$.

For each $a \in [v]$, notice that $n_j(a)$ is in the range $0 \leq n_j(a) \leq n$. Furthermore, we have $n_j(1) + n_j(2) + \dots + n_j(v-1) + n_j(v) = n$. Consequently, among all v -ary n -tuples there are at most $(n+1)^{v-1}$ possible types.

It now follows that there is a subset $\mathcal{C} \subseteq \widehat{\mathcal{C}}$ such that

$$|\mathcal{C}| \geq |\widehat{\mathcal{C}}|(n+1)^{1-v}$$

and all $C_j \in \mathcal{C}$ have a common type. For each $a \in [v]$, let $n(a)$ denote the common value of $n_j(a)$ for all $C_j \in \mathcal{C}$. By preserving the same ordering of these n -tuples as they were ordered in $\widehat{\mathcal{C}}$, we clearly have a collection of n -tuples corresponding to the columns of a $\text{CA}(n; 2, T_{|\mathcal{C}|}, H)$.

Choose any arc $ab \in E(H)$ and define two collections of subsets of $[n]$:

$$\mathcal{A} = \{A_j : C_j \in \mathcal{C}\} \text{ and } \mathcal{B} = \{B_j : C_j \in \mathcal{C}\}$$

where, for each $C_j \in \mathcal{C}$, we define $A_j = \{i \in [n] : c_{ij} = a\}$ and $B_j = \{i \in [n] : c_{ij} = b\}$. Clearly, as explained earlier, the families $\mathcal{A}$ and $\mathcal{B}$ satisfy the intersection conditions of Frankl's Inequality in Theorem 5.3.3. By virtue of $\mathcal{C}$, all $A_j \in \mathcal{A}$ have cardinality $|A_j| = n(a)$, and all $B_j \in \mathcal{B}$ have cardinality $|B_j| = n(b)$. We can thus apply Frankl's Inequality in Theorem 5.3.3 to obtain the bound

$$|\mathcal{C}| \leq \binom{n(a) + n(b)}{n(a)}.$$

Since $|\mathcal{C}| \geq |\widehat{\mathcal{C}}|(n+1)^{-v}$ we get

$$\text{CAK}(n; 2, \{T_L\}, H) = |\widehat{\mathcal{C}}| \leq (n+1)^v \binom{n(a) + n(b)}{n(a)}.$$

The arc $ab \in E(H)$ above was arbitrary, thus

$$\text{CAK}(n; 2, \{T_L\}, H) \leq (n+1)^v \min_{ab \in E(H)} \binom{n(a) + n(b)}{n(a)}.$$

For each $a \in [v]$, we now define a probability $P^*(a) = \frac{1}{n}n(a)$. Thus, $n(a) = nP^*(a)$ for each $a \in V(H)$ and our inequality becomes

$$\text{CAK}(n; 2, \{T_L\}, H) \leq (n+1)^v \min_{ab \in E(H)} \binom{n(P^*(a) + P^*(b))}{nP^*(a)}.$$

We now apply the upper bound given in Lemma 5.3.4, namely $\binom{m}{l} \leq 2^{m \cdot h(l/m)}$, and our bound on $\text{CAK}(n; 2, \{T_L\}, H)$ becomes

$$\text{CAK}(n; 2, \{T_L\}, H) \leq (n+1)^v \min_{e \in E(H)} 2^{n \cdot F(e, P^*)}.$$

Since P^* was but one possible distribution, we get an upper bound by choosing the maximizing distribution among all distributions on $V(H)$:

$$\text{CAK}(n; 2, \{T_L\}, H) \leq \max_P \min_{e \in E(H)} (n+1)^v 2^{n \cdot F(e, P)}.$$

Now,

$$\frac{1}{n} \log_2 \text{CAK}(n; 2, \{T_L\}, H) \leq \max_P \min_{e \in E(H)} \frac{v \log_2(n+1)}{n} + F(e, P),$$

hence

$$\limsup_{n \rightarrow \infty} \frac{1}{n} \log_2 \text{CAK}(n; 2, \{T_L\}, H) \leq \max_P \min_{e \in E(H)} F(e, P).$$

Consequently,

$$\Sigma(H, \{T_L\}) \leq \max_P \min_{e \in E(H)} F(e, P). \quad \blacksquare$$

We now give the formula for the Sperner capacity of a directed alphabet graph H with respect to transitive tournaments. Notice that we get the same formula as the Sperner capacity for an undirected alphabet graph, given in Theorem 5.1.2.

Corollary 5.3.6 If H is a directed alphabet graph, then

$$\Sigma(H, \{T_L\}) = \max_P \min_{ab \in E(H)} (P_a + P_b) \cdot h\left(\frac{P_a}{P_a + P_b}\right),$$

where the maximum is taken over all probability distributions P on $V(H)$.

[proof] Combine Corollary 5.3.1 with Theorem 5.3.5. \(\blacksquare\)

Chapter 6

LYM inequalities for H -intersecting collections and F -following collections

In this chapter, we develop a new method that produces LYM-like inequalities for graph-intersecting collections for any alphabet graph H . We use a permutation-counting technique that extends Katona’s technique [33] and Tarjan’s technique [59] for proving Theorem 2.1.3 (see the proof of Theorem 2.1.3 in Section 2.1 for an illustration of their technique).

For every alphabet graph H , there exists a directed “follow” digraph F that encodes the “right” set of permutations to count in order to obtain our LYM inequality for H . The relationship between H and F guarantees that “ H -intersecting” collections are “ F -following” collections, and being an F -following collection is precisely the property needed to yield a LYM inequality for H .

In Section 6.1, we introduce the problem that motivated our method, briefly outline our method, and discuss related results. In Section 6.2, we define F -following collections and show that they are equipped with a LYM-like inequality. In Section 6.3, we characterize the relationship between H -intersecting collections and F -following collections. In Section 6.4, we investigate “strong” graphs, an important class of alphabet graphs with respect to our method.

6.1 LYM inequalities for graph-intersecting collections — an overview

6.1.1 H -intersecting collections

Throughout this chapter and the next, all alphabet graphs are undirected.

A **v -packing** of $[n]$ is an ordered collection $P = (P^1, \dots, P^v)$ of v pairwise-disjoint nonempty subsets of $[n]$, that is, $P^a \cap P^b = \emptyset$ for all $a, b \in [v]$ with $a \neq b$. The subsets $P^1, \dots, P^v$ are the **classes** of P . In particular, if $P^1 \cup \dots \cup P^v = [n]$, then P is a **v -partition** of $[n]$.

Definition 6.1.1 Let $\mathcal{P} = \{P_1, \dots, P_m\}$ be a collection of v -packings of $[n]$, where $P_i = (P_i^1, \dots, P_i^v)$ for each $i \in [m]$, and let H be an alphabet graph with $V(H) = [v]$. If $P_i^a \cap P_j^b \neq \emptyset$ whenever $ab \in E(H)$ and $i \neq j$, then $\mathcal{P}$ is an **H -intersecting collection of v -packings of $[n]$** , or simply an **H -intersecting collection**.

For a fixed alphabet graph H and integer n , we denote by $m(n, H)$ the size of a largest H -intersecting collection of $|V(H)|$ -packings of $[n]$.

In general, H -intersecting collections of v -packings of $[n]$ are equivalent to v cross-intersecting set systems of $[n]$. Let $\mathcal{A}^1, \dots, \mathcal{A}^v$ be set systems on $[n]$, where, for each $a \in [v]$, we have $\mathcal{A}^a = \{A_1^a, \dots, A_m^a\}$. Two set systems $\mathcal{A}^a$ and $\mathcal{A}^b$ are **cross-intersecting** if $A_i^a \cap A_j^b \neq \emptyset$ whenever $i \neq j$.

Let $\mathcal{P} = \{P_1, \dots, P_m\}$ be a collection of v -packings of $[n]$, and set $A_i^a = P_i^a$ for all $i \in [m]$ and $a \in [v]$. If $\mathcal{P}$ is an H -intersecting collection, then $\mathcal{A}^a$ and $\mathcal{A}^b$ are cross-intersecting whenever $ab \in E(H)$.

For another perspective, consider a covering array $\text{CA}(n; 2, k, H)$ with alphabet graph H , where $V(H) = [v]$. Its columns correspond to an H -intersecting collection of v -packings of $[n]$. Each column is a v -ary n -tuple and corresponds to a packing $P = (P^1, \dots, P^v)$ — actually, a partition — where the class P^a is the set of indices where symbol a occurs in the column. In fact, two v -packings of $[n]$ are H -intersecting if and only if they correspond to v -ary n -tuples which are **H -dependent**. We use both terminologies as they help to distinguish the language of v -ary n -tuples from collections of packings (which are naturally phrased in terms of intersection).

In particular, for an alphabet graph H and integer n , we have $\text{CAK}(n; 2, H) = m(n, H)$.

It is straightforward to see that the columns of a classical covering array $\text{CA}(n; 2, k, v)$ correspond to a K_v^{loop} -intersecting collection. Equivalently, a **qualitatively independent** collection of v -partitions of $[n]$ is a K_v^{loop} -intersecting collection of v -partitions of $[n]$.

In Section 6.2, we define “ F -following” collections of v -packings of $[n]$ for a follow digraph F . In Section 6.3, we characterize when “ F -following” is equivalent to H -intersecting. Thus, “ F -following” is yet another way to view “ H -intersecting.”

It is worthwhile to emphasize the various equivalent guises for the notion of H -intersecting collections; however, throughout this chapter, we most often adopt the language of packings.

6.1.2 An extremal problem

We are interested in the following problem.

Problem 6.1.2 Given an alphabet graph H and an integer n , determine $m(n, H)$.

For all n , the only alphabet graphs for which $m(n, H)$ is known exactly are K_2 (maximum size of an antichain — see Theorem 2.1.1), K_2 with a loop on one vertex (maximum size of an intersecting antichain — see Theorem 2.1.4), and K_2 with loops on both vertices (the binary covering array number — see Theorem 2.3.3).

Recall that Gargano, Körner and Vaccaro [24, 25] completely solved a problem closely related to Problem 6.1.2. For any graph H , they proved

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log_2 m(n, H) = \max_P \min_{ab \in E(H)} (P_a + P_b) \cdot h\left(\frac{P_a}{P_a + P_b}\right), \quad (6.1.1)$$

where the maximum is taken over all probability distributions P on $V(H)$, the minimum is taken over all edges $ab \in E(H)$, and h denotes the binary entropy function.

In terms of Problem 6.1.2, knowing the limit in (6.1.1) does not help us to determine $m(n, H)$ itself — any subexponential function $f(n)$ inserted within the logarithm of this limit as a multiplicative factor of $m(n, H)$ does not alter the limit.

6.1.3 Follow digraphs and permutation-counting inequalities

For any alphabet graph H and integer n , we give a LYM inequality for H -intersecting collections of packings of $[n]$. The key to providing this LYM inequality is to associate a directed graph F , called a “follow digraph,” with H , and to count a suitable set of permutations of $[n]$ which are encoded by the arcs of F .

Definition 6.1.3 A *follow digraph* F is a directed graph having no isolated vertices, no repeated arcs, and no loops (antiparallel arcs are permitted).

Given a follow digraph F , we are interested in counting permutations with properties based on the arcs of F .

Let A and B be two disjoint nonempty subsets of $[n]$, and let $\pi = (\pi_1, \dots, \pi_n)$ be a permutation of $[n]$, where $\pi(i) = \pi_i$ for each $i \in [n]$. Recall, that π **contains** A **followed by** B if $i < j$ whenever $\pi_i \in A$ and $\pi_j \in B$. If $\{\pi_1, \pi_2, \dots, \pi_{|A|}\} = A$, then π **begins with** A . Similarly, if $\{\pi_{n+1-|A|}, \pi_{n+2-|A|}, \dots, \pi_n\} = A$, then π **ends with** A .

The goals of this chapter are to demonstrate how every follow digraph has a corresponding LYM-like inequality, to establish the connection between alphabet graphs and follow digraphs, and to use this connection to build LYM-like inequalities for H -intersecting collections for every alphabet graph H . Briefly, our method is encompassed by Theorem 6.2.9, Corollary 6.3.2, Lemma 6.3.7, and Theorem 6.4.8. For simplicity, we provide the following informal summary:

Theorem 6.1.4 (Generalized LYM Inequality for H -intersecting Collections) Let H be an alphabet graph with $V(H) = [v]$. If $\mathcal{P} = \{P_1, \dots, P_m\}$ is an H -intersecting collection of v -packings of $[n]$, then there exists a follow digraph F , with $V(F) = [v]$, such that the following inequality holds:

$$\sum_{i=1}^m \left(\begin{array}{c} \# \text{ permutations of } [n] \text{ that} \\ \text{contain } P_i^a \text{ followed by } P_i^b \\ \text{for some arc } ab \in E(F) \end{array} \right) \leq n! \quad \blacksquare$$

When we apply Theorem 6.1.4 to $H = K_2$, we obtain the well-known LYM-like inequality given in Theorem 2.1.3. Our proof of Theorem 6.1.4 is in fact a generalization of the proof technique used by Katona [33] and Tarjan [59] to prove Theorem 2.1.3 (see the proof of Theorem 2.1.3 given in Section 2.1).

The application of Theorem 6.1.4 to $H = K_2^{\text{loop}}$ yields another known LYM-like inequality for intersecting set systems:

Theorem 6.1.5 [48, 57] If $\mathcal{A} = \{A_1, \dots, A_m\}$ and $\mathcal{B} = \{B_1, \dots, B_m\}$ are two intersecting families of subsets of $[n]$ such that $A_i \cap B_j = \emptyset$ if and only if $i = j$, then

$$\sum_{i=1}^m \binom{|A_i| + |B_i|}{|A_i|}^{-1} \leq \frac{1}{2}.$$

By defining a collection of 2-packings of the form $P_i = (P_i^1, P_i^2)$, where $P_i^1 = A_i$ and $P_i^2 = B_i$ for each $i \in [m]$, it can be seen that the two families $\mathcal{A}$ and $\mathcal{B}$, given in Theorems 2.1.3 and 6.1.5, are equivalent, respectively, to K_2 - and K_2^{loop} -intersecting collections of 2-packings of $[n]$.

6.1.4 Using LYM inequalities to bound $m(n, H)$

For a given alphabet graph H , the LYM-like inequality of Theorem 6.1.4 inherently bounds $m(n, H)$. For example, the LYM Inequality (see Theorem 2.1.2) transforms into the upper bound given by Sperner's Theorem (see Theorem 2.1.1).

For each alphabet graph H , our LYM inequality, given in Theorem 6.1.4, can be transformed into an upper bound on $m(n, H)$. In Chapter 7, we spend some time making these transformations for specific small alphabet graphs H ; however, transforming our generalized LYM inequality for H -intersecting collections into an upper bound on $m(n, H)$ becomes more challenging for larger alphabet graphs H . We try to overcome this challenge using an asymptotic estimate, given in Section 7.5, although the estimate is based on some assumptions (see Premise 7.5.2).

The transformation of Theorem 6.1.4 into upper bounds on $m(n, H)$ is the second half of our method. This half of the problem is explored in Chapter 7.

6.2 F -following collections and inequalities

In this section, we define “ F -following” collections of v -packings of $[n]$. The definition itself is what gives us our LYM-like inequality. In Lemma 6.2.2, we give a general-

ized LYM inequality for F -following collections, and in Theorem 6.2.9, we provide a simplified version of our inequality.

Definition 6.2.1 Let $\mathcal{P} = \{P_1, \dots, P_m\}$ be a collection of v -packings of $[n]$, where $P_j = (P_j^1, \dots, P_j^v)$ for each $j \in [m]$. Let π be a permutation of $[n]$, and let F be a follow digraph on $V(F) = [v]$. Let $a, b \in [v]$ with $a \neq b$. If π contains P_j^a followed by P_j^b for some $ab \in E(F)$, then π **contains a P_j -following for F** . If every permutation π of $[n]$ contains a P_j -following for F for at most one $P_j \in \mathcal{P}$, then $\mathcal{P}$ is an **F -following collection**.

Let $P_j = (P_j^1, \dots, P_j^v)$ be a v -packing of $[n]$. Let $a, b \in [v]$ with $a \neq b$. Denote by $X_j(a, b)$ the set of permutations of $[n]$ that contain P_j^a followed by P_j^b . If F is a follow digraph with $V(F) = [v]$, then the union $\bigcup_{ab \in E(F)} X_j(a, b)$ is the set of permutations of $[n]$ that contain a P_j -following for F .

The next lemma is our LYM-like inequality for F -following collections. Ultimately, it will be used for H -intersecting collections, but this connection is not established until Section 6.3.

Lemma 6.2.2 (Generalized LYM Inequality for F -following Collections) Let F be a follow digraph with $V(F) = [v]$. If $\mathcal{P} = \{P_1, \dots, P_m\}$ is an F -following collection of v -packings of $[n]$, then

$$\sum_{j=1}^m \left| \bigcup_{ab \in E(F)} X_j(a, b) \right| \leq n!$$

[proof] Since $\mathcal{P}$ is an F -following collection, for each permutation π of $[n]$ there is at most one index $j \in [m]$ such that π contains a P_j -following for F . Thus, each of the $n!$ permutations of $[n]$ can be counted in at most one of the unions $\bigcup_{ab \in E(F)} X_j(a, b)$. In other words, $\{\bigcup_{ab \in E(F)} X_j(a, b) : j \in [m]\}$ is an m -packing of the set of permutations of $[n]$. Consequently, the sum of the unions $\bigcup_{ab \in E(F)} X_j(a, b)$, over all $j \in [m]$, is at most $n!$ (the total number of permutations of $[n]$). ■

For a follow digraph F and an F -following collection $\mathcal{P}$ of packings of $[n]$, let $\beta(F, \mathcal{P}, n)$ denote the left side of the inequality given in Lemma 6.2.2, that is,

$$\beta(F, \mathcal{P}, n) = \sum_{i=1}^{|\mathcal{P}|} \left| \bigcup_{ab \in E(F)} X_i(a, b) \right| = \sum_{i=1}^{|\mathcal{P}|} \left(\begin{array}{l} \# \text{ permutations of } [n] \text{ that} \\ \text{contain } P_i^a \text{ followed by } P_i^b \\ \text{for some arc } ab \in E(F) \end{array} \right) \quad (6.2.1)$$

The quantity $\beta(F, \mathcal{P}, n)$ measures the extent to which $\mathcal{P}$ captures the permutations of $[n]$. By Lemma 6.2.2, we know that $0 \leq \beta(F, \mathcal{P}, n) \leq n!$ so larger values of $\beta(F, \mathcal{P}, n)$ indicate that many permutations of $[n]$ have P_j -followings for F for some $P_j \in \mathcal{P}$. Informally, if $\beta(F, \mathcal{P}, n)$ is much smaller than $n!$, then we might hope to add another packing to the collection $\mathcal{P}$ and still maintain its F -following property. Conversely, if $\beta(F, \mathcal{P}, n)$ is close enough to $n!$, then $\mathcal{P}$ must be a maximal F -following collection: every packing in $\mathcal{P}$ contributes nontrivially to $\beta(F, \mathcal{P}, n)$ and there is a minimum possible contribution; having fewer permutations left than this minimum guarantees that we cannot add any more packings to $\mathcal{P}$ without violating the upper bound of $n!$ permutations that have a following for F .

For a fixed collection $\mathcal{P}$, our first observation regarding $\beta(F, \mathcal{P}, n)$ is that, among all follow digraphs F such that $\mathcal{P}$ is an F -following collection, the largest value for $\beta(F, \mathcal{P}, n)$ is attained for a follow digraph that is maximal among such F . Removing arcs from F never gives a better bound.

Lemma 6.2.3 Let F_1 and F_2 be follow digraphs on the same vertex set $[v]$, and let $\mathcal{P}$ be an F_2 -following collection of v -packings of $[n]$. If $E(F_1) \subseteq E(F_2)$, then $\mathcal{P}$ is an F_1 -following collection and $\beta(F_1, \mathcal{P}, n) \leq \beta(F_2, \mathcal{P}, n)$.

[proof] Suppose, to the contrary, that $\mathcal{P}$ is an F_2 -following collection but not an F_1 -following collection. Then there exists at least one permutation π of $[n]$ such that π contains P_i^a followed by P_i^b and π contains P_j^c followed by P_j^d for some arcs $ab, cd \in E(F_1)$ and for some $i \neq j$. Since $E(F_1) \subseteq E(F_2)$, the arcs ab and cd belong to $E(F_2)$, so the permutation π contradicts the fact that $\mathcal{P}$ is an F_2 following collection.

Since $E(F_1) \subseteq E(F_2)$, it is clear that $\beta(F_1, \mathcal{P}, n) \leq \beta(F_2, \mathcal{P}, n)$. ■

Let us examine $\beta(F, \mathcal{P}, n)$ further. By the Principle of Inclusion-Exclusion, we have

$$\beta(F, \mathcal{P}, n) = \sum_{j=1}^m \left| \bigcup_{ab \in E(F)} X_j(a, b) \right| = \sum_{j=1}^m \sum_{\substack{S \subseteq E(F) \\ S \neq \emptyset}} (-1)^{|S|+1} \left| \bigcap_{ab \in S} X_j(a, b) \right|. \quad (6.2.2)$$

Let $S \subseteq E(F)$. We simply write S to denote the subgraph of F induced by the arcs in S . The **transitive closure** of S in F , denoted $\hat{S}$, is defined as follows: $ab \in \hat{S}$ if and only if there is a directed path from a to b in S with $ab \in E(F)$.

Lemma 6.2.4 Let F be a follow digraph and let S and T be subsets of $E(F)$. If $S \subseteq T \subseteq \hat{S}$, then, for a $|V(F)|$ -packing P_j , we have

$$\bigcap_{ab \in S} X_j(a, b) = \bigcap_{ab \in T} X_j(a, b) = \bigcap_{ab \in \hat{S}} X_j(a, b).$$

[proof] Since $S \subseteq T \subseteq \hat{S}$, it is clear that

$$\bigcap_{ab \in S} X_j(a, b) \supseteq \bigcap_{ab \in T} X_j(a, b) \supseteq \bigcap_{ab \in \hat{S}} X_j(a, b).$$

Suppose $\pi \in \bigcap_{ab \in S} X_j(a, b)$ and let $\alpha\beta \in \hat{S}$. Since $\alpha\beta \in \hat{S}$, there exists a directed path from α to β in S , say $a_0, a_1, \dots, a_k$, where $a_0 = \alpha$ and $a_k = \beta$. Since $\pi \in \bigcap_{ab \in S} X_j(a, b)$, it is clear that π contains $P_j^{a_l}$ followed by $P_j^{a_{l+1}}$ for all l , $0 \leq l \leq k-1$. Consequently, π also contains all the followings that arise from the transitivity of a linear ordering of the sets $P_j^{a_0}, P_j^{a_1}, \dots, P_j^{a_k}$. In particular, π contains P_j^α followed by P_j^β , hence, $\pi \in X_j(\alpha, \beta)$. Therefore, $\pi \in X_j(\alpha, \beta)$ for all $\alpha\beta \in \hat{S}$ and it follows that

$$\bigcap_{ab \in S} X_j(a, b) \subseteq \bigcap_{ab \in \hat{S}} X_j(a, b). \quad \blacksquare$$

Corollary 6.2.5 Let F be a follow digraph and let $S \subseteq E(F)$. If S contains a directed cycle, then, for a $|V(F)|$ -packing P_j , we have $\bigcap_{ab \in S} X_j(a, b) = \emptyset$.

[proof] Suppose $\pi \in \bigcap_{ab \in S} X_j(a, b)$ and let $a_1, a_2, \dots, a_k, a_1$ be a directed k -cycle in S . Then, by the proof of Lemma 6.2.4, we have $\pi \in X_j(a_k, a_1) \cap X_j(a_1, a_k)$. Consequently, π contains $P_j^{a_1}$ followed by $P_j^{a_k}$ as well as $P_j^{a_k}$ followed by $P_j^{a_1}$, which is clearly impossible. Therefore, there are no permutations in $\bigcap_{ab \in S} X_j(a, b)$. $\blacksquare$

Consider the sum $\beta(F, \mathcal{P}, n)$, given in (6.2.2). By Corollary 6.2.5, subsets $S \subseteq E(F)$ for which S contains any directed cycles contribute zero to $\beta(F, \mathcal{P}, n)$. We can say more: for $S \subseteq E(F)$ with S acyclic, if $S \neq \hat{S}$, then some cancellations occur when we combine the terms of the form $|\bigcap_{ab \in T} X_j(a, b)|$ for all subsets $T \subseteq E(F)$ with $S \subseteq T \subseteq \hat{S}$; this observation will be given precisely in Lemma 6.2.6.

Given a follow digraph F and a set $S \subset E(F)$, the **transitive closure poset** of S with respect to F , denoted $p(S)$, is the collection of arc sets $\{T : S \subseteq T \subseteq \hat{S}\}$. Let $\beta[p(S)]$ denote the terms of $\beta(F, \mathcal{P}, n)$ corresponding to the poset $p(S)$, that is,

$$\beta[p(S)] = \sum_{j=1}^m \sum_{T \in p(S)} (-1)^{|T|+1} \left| \bigcap_{ab \in T} X_j(a, b) \right|.$$

Lemma 6.2.6 If F is a follow digraph and S is a subset $S \subseteq E(F)$ such that $S \neq \hat{S}$, then $\beta[p(S)] = 0$.

[proof] Let $j \in [m]$. By Lemma 6.2.4, for all T such that $S \subseteq T \subseteq \hat{S}$, the number of permutations in $\bigcap_{ab \in T} X_j(a, b)$ is a constant. For each $j \in [m]$, let x_j be that constant. For each l such that $0 \leq l \leq |\hat{S}| - |S|$, the number of subsets T with $|T| = |S| + l$ is $\binom{|\hat{S}| - |S|}{l}$.

Thus,

$$\beta[p(S)] = (-1)^{|S|+1} \sum_{j=1}^m x_j \sum_{l=0}^{|\hat{S}| - |S|} \binom{|\hat{S}| - |S|}{l} (-1)^l = (-1)^{|S|+1} \sum_{j=1}^m x_j (1 - 1)^{|\hat{S}| - |S|} = 0. \blacksquare$$

It remains to show that we can partition the set of all acyclic subsets of arcs of F into disjoint transitive closure posets. To do so, we use the transitive reduction of a directed graph and a result by Aho, Garey and Ullman [2]. Let G be a directed graph. A graph G^t is a **transitive reduction** of G if

1. there is a directed path from u to v in G^t if and only if there is a directed path from u to v in G , and
2. there is no graph with fewer arcs than G^t satisfying condition 1.

Theorem 6.2.7 (Aho, Garey, Ullman [2]) Let G be a finite directed acyclic graph, and let $T(G)$ be the set of all graphs G_i such that the transitive closure of G_i is equal to the transitive closure of G . Then there is a unique transitive reduction of G , namely $G^t = \bigcap_{G_i \in T(G)} G_i$. In particular, G^t is a subgraph of G . $\blacksquare$

For each set $S \subseteq E(F)$ such that S is acyclic, Theorem 6.2.7 tells us that S has a unique transitive reduction which we denote by S^t . Consequently, we can partition

the set of nonempty acyclic subsets of $E(F)$ into maximal transitive closure posets. Each acyclic subset $S \subseteq E(F)$ belongs to a unique maximal transitive closure poset.

Corollary 6.2.8 If $S \subseteq E(F)$ is acyclic, then S belongs to a unique maximal transitive closure poset, namely $p(S^t)$, the poset of the transitive reduction of S with respect to F .

[proof] Suppose S belongs to a transitive closure poset $p(T)$ for some acyclic subset $T \subseteq E(F)$. By the definition of transitive closure posets, we have $T \subseteq S \subseteq \widehat{T}$, hence $\widehat{S} = \widehat{T}$. By Theorem 6.2.7, since S and T are acyclic and have the same transitive closure, S and T must have the same transitive reduction $S^t = T^t$. Moreover, $\widehat{S}^t = \widehat{S}$. It now follows that $S^t \subseteq T \subseteq \widehat{T} = \widehat{S}^t$. Thus, $p(T) \subseteq p(S^t)$. Since the transitive reduction of S is unique, $p(S^t)$ is the unique maximal transitive closure poset to which S belongs. ■

We now rewrite the bound of Lemma 6.2.2 taking into account the terms of $\beta(F, \mathcal{P}, n)$ that contribute zero, as well as the terms corresponding to transitive closure posets for which Lemma 6.2.6 applies.

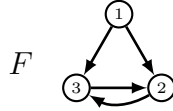
Theorem 6.2.9 Let F be a follow digraph and let $\mathcal{P} = \{P_1, \dots, P_m\}$ be an F -following collection of $|V(F)|$ -packings of $[n]$. Define $\mathfrak{S}$ to be the set of all nonempty subsets S of $E(F)$ such that S is acyclic and such that $S = S^t = \widehat{S}$. Then

$$\beta(F, \mathcal{P}, n) = \sum_{j=1}^m \left| \bigcup_{ab \in E(F)} X_j(a, b) \right| = \sum_{j=1}^m \sum_{S \in \mathfrak{S}} (-1)^{|S|+1} \left| \bigcap_{ab \in S} X_j(a, b) \right| \leq n!.$$

[proof] By Corollary 6.2.5, we may discard all terms $\left| \bigcap_{ab \in S} X_j(a, b) \right|$ for which S contains a directed cycle. By Corollary 6.2.8, each of the remaining (nonempty) subsets $S \subseteq E(F)$ belongs to a unique equivalence class corresponding to the transitive closure poset $p(S^t)$. Whenever $S^t \neq \widehat{S}$, we apply Lemma 6.2.6, yielding a combined total of zero for the terms $\beta[p(S^t)]$. The only terms of $\beta(F, \mathcal{P}, n)$ that survive correspond to subsets $S \in \mathfrak{S}$. ■

6.2.1 Example of an F -following collection and its LYM inequality

To illustrate some of the newly defined concepts, in this section, we examine a concrete example of an F -following collection and its LYM inequality. We choose a small follow digraph, but one that has enough arcs to require some nontrivial computations. Here is a follow digraph F with $V(F) = [3]$:



Here are two 3-packings of [8]:

$$P_1 = (\underbrace{\{1, 2\}}_{P_1^1}, \underbrace{\{3, 4, 5\}}_{P_1^2}, \underbrace{\{6, 7, 8\}}_{P_1^3}) \text{ and } P_2 = (\underbrace{\{4, 7\}}_{P_2^1}, \underbrace{\{1, 3, 6\}}_{P_2^2}, \underbrace{\{2, 5, 8\}}_{P_2^3})$$

We claim that $\mathcal{P} = \{P_1, P_2\}$ is an F -following collection. To verify our claim, one could exhaustively check each of the $8! = 40320$ permutations of [8] to see that each of these permutations either

1. does not contain a P_1 -following for F nor a P_2 -following for F , or
2. contains a P_1 -following for F , but does not contain a P_2 -following for F , or
3. does not contain a P_1 -following for F , but does contain a P_2 -following for F .

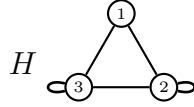
Take the permutation $\pi = (1, 2, 3, 4, 5, 6, 7, 8)$. We claim that π contains a P_1 -following for F . In fact, there are three arcs of F which justify the claim: π contains P_1^1 followed by P_1^2 , corresponding to the arc $12 \in E(F)$, and π contains P_1^1 followed by P_1^3 , corresponding to the arc $13 \in E(F)$, and π contains P_1^2 followed by P_1^3 , corresponding to the arc $23 \in E(F)$. Notice that π does not contain a P_2 -following for F . This one permutation meets the criteria for $\mathcal{P}$ being an F -following collection.

Take $\sigma = (1, 2, 3, 6, 4, 7, 5, 8)$. Check that σ contains a P_1 -following for F , corresponding to the two arcs $12, 13 \in E(F)$. Notice that σ also contains P_2^2 followed by P_2^1 , but that this is not a P_2 -following for F since $21 \notin E(F)$. Indeed, σ does not contain a P_2 -following for F .

The permutation $\rho = (5, 1, 3, 6, 4, 7, 2, 8)$ does not contain a P_1 -following for F , nor does it contain a P_2 -following for F .

The permutation $\tau = (7, 8, 4, 2, 6, 1, 5, 3)$ contains a P_2 -following for F (corresponding to the arc $12 \in E(F)$) and τ does not contain a P_1 -followings for F .

If we consider the classes of the P_1 and P_2 that intersect, we see that $\mathcal{P}$ is an H -intersecting collection for the alphabet graph H shown below:



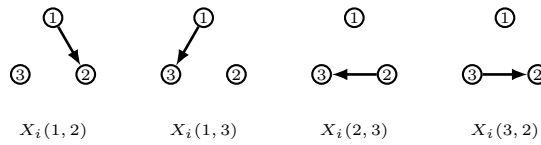
In Lemma 6.3.7, we will characterize the relationship between an alphabet graph H and a follow digraph F which guarantees that every H -intersecting collection is an F -following collection. This characterization will allow us to verify that a given collection $\mathcal{P}$ is an F -following collection without resorting to an exhaustive verification of all permutations.

Now, let us compute the LYM inequality for the given follow digraph F , using Lemma 6.2.2 first, and then by applying the cancellations of Theorem 6.2.9.

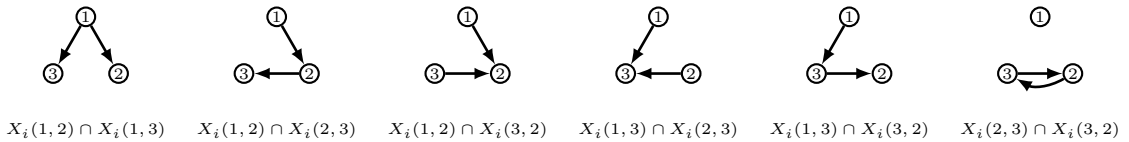
Let $\mathcal{P} = \{P_1, \dots, P_m\}$ be a collection of 3-packings of $[n]$, where, for each $i \in [m]$, we have $P_i = (P_i^1, P_i^2, P_i^3)$ and $|P_i^1| = a_i$, $|P_i^2| = b_i$, and $|P_i^3| = c_i$. If $\mathcal{P}$ is an F -following collection, then, by Lemma 6.2.2 and (6.2.2), we have

$$\beta(F, \mathcal{P}, n) = \sum_{i \in [m]} \sum_{\substack{S \subseteq E(F) \\ S \neq \emptyset}} (-1)^{|S|+1} \left| \bigcap_{ab \in S} X_i(a, b) \right| \leq n!$$

The follow digraph F has four arcs, so it has $2^4 - 1 = 15$ nonempty subsets of arcs $S \subseteq E(F)$ to sum over. We break these down by the cardinality of S . For each $i \in [m]$, the **single-arc terms** of $\beta(F, \mathcal{P}, n)$ correspond to the following 1-arc subgraphs of F :



For each $i \in [m]$, the 2-arc terms of $\beta(F, \mathcal{P}, n)$ correspond to the following 2-arc subgraphs of F :



For each $i \in [m]$, the 3-arc terms of $\beta(F, \mathcal{P}, n)$ correspond to the following 3-arc subgraphs of F :



$$X_i(1, 2) \cap X_i(1, 3) \cap X_i(2, 3)$$



$$X_i(1, 2) \cap X_i(1, 3) \cap X_i(3, 2)$$



$$X_i(1, 2) \cap X_i(2, 3) \cap X_i(3, 2)$$



$$X_i(1, 3) \cap X_i(2, 3) \cap X_i(3, 2)$$

For each $i \in [m]$, there is one 4-arc term of $\beta(F, \mathcal{P}, n)$, corresponding to F itself:



$$X_i(1, 2) \cap X_i(1, 3) \cap X_i(2, 3) \cap X_i(3, 2)$$

Now, let us give all terms of $\beta(F, \mathcal{P}, n)$, without cancellation, where permutations are counted in the same order as the subgraphs listed above.

$$\begin{aligned} & \sum_{i \in [m]} \left[\frac{n!}{\binom{a_i + b_i}{a_i}} + \frac{n!}{\binom{a_i + c_i}{a_i}} + \frac{n!}{\binom{b_i + c_i}{b_i}} + \frac{n!}{\binom{b_i + c_i}{b_i}} \right] \\ & - \left[\frac{n!}{\binom{a_i + b_i + c_i}{a_i}} + \frac{n!}{\binom{a_i + b_i + c_i}{a_i, b_i, c_i}} + \frac{n!}{\binom{a_i + b_i + c_i}{b_i}} + \frac{n!}{\binom{a_i + b_i + c_i}{c_i}} + \frac{n!}{\binom{a_i + b_i + c_i}{a_i, b_i, c_i}} + 0 \right] \\ & + \left[\frac{n!}{\binom{a_i + b_i + c_i}{a_i, b_i, c_i}} + \frac{n!}{\binom{a_i + b_i + c_i}{a_i, b_i, c_i}} + 0 + 0 \right] - 0 \end{aligned}$$

To see how the terms in the above sum arise, we will explicitly count the permutations for several sample terms.

We will count the permutations of $[n]$ in $X_i(1, 2)$; the other 1-arc terms are similar.

There are $\binom{n}{a_i + b_i}$ ways to choose $a_i + b_i$ positions for the elements of the classes P_i^1 and P_i^2 . There are $(a_i)!$ ways to arrange the elements of P_i^1 in the first a_i of these positions, and there are $(b_i)!$ ways to arrange the elements of P_i^2 in the last b_i positions. There are $(n - a_i - b_i)!$ ways to arrange the remaining elements of $[n]$. Thus,

$$|X_i(1, 2)| = \binom{n}{a_i + b_i} a_i! b_i! (n - a_i - b_i)! = \frac{n!}{\binom{a_i + b_i}{a_i}}.$$

Let us count the permutations of $[n]$ in $X_i(1, 2) \cap X_i(1, 3)$; the terms $|X_i(1, 2) \cap X_i(3, 2)|$ and $|X_i(1, 3) \cap X_i(2, 3)|$ are counted similarly.

There are $\binom{n}{a_i+b_i+c_i}$ ways to choose $a_i + b_i + c_i$ positions for the elements of the classes P_i^1 , P_i^2 , and P_i^3 . There are $(a_i)!$ ways to arrange the elements of P_i^1 in the first a_i of these positions, and there are $(b_i + c_i)!$ ways to arrange the elements of P_i^2 and P_i^3 in the last $b_i + c_i$ positions. There are $(n - a_i - b_i - c_i)!$ ways to arrange the remaining elements of $[n]$. Thus,

$$|X_i(1, 2) \cap X_i(1, 3)| = \binom{n}{a_i+b_i+c_i} a_i! (b_i + c_i)! (n - a_i - b_i - c_i)! = \frac{n!}{\binom{a_i+b_i+c_i}{a_i}}.$$

Next, let us count $|X_i(1, 2) \cap X_i(2, 3)|$; the term $|X_i(1, 3) \cap X_i(3, 2)|$ is counted similarly.

There are $\binom{n}{a_i+b_i+c_i}$ ways to choose $a_i + b_i + c_i$ positions for the elements of the classes P_i^1 , P_i^2 , and P_i^3 . There are $(a_i)!$ ways to arrange the elements of P_i^1 in the first a_i of these positions, there are $(b_i)!$ ways to arrange the elements of P_i^2 in the next b_i positions, and there are $(c_i)!$ ways to arrange the elements of P_i^3 in the last c_i positions. There are $(n - a_i - b_i - c_i)!$ ways to arrange the remaining elements of $[n]$. Thus,

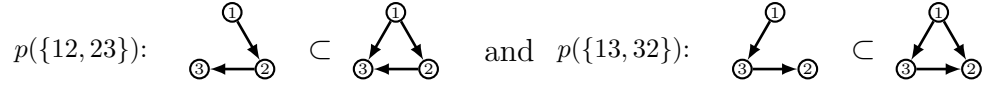
$$|X_i(1, 2) \cap X_i(2, 3)| = \binom{n}{a_i+b_i+c_i} a_i! b_i! c_i! (n - a_i - b_i - c_i)! = \frac{n!}{\binom{a_i+b_i+c_i}{a_i, b_i, c_i}}. \quad (6.2.3)$$

There are no permutations in $X_i(2, 3) \cap X_i(3, 2)$ since no permutation contains P_i^2 followed by P_i^3 and P_i^3 followed by P_i^2 . Thus, $|X_i(2, 3) \cap X_i(3, 2)| = 0$.

The cardinalities $|X_i(1, 2) \cap X_i(1, 3) \cap X_i(2, 3)|$ and $|X_i(1, 2) \cap X_i(1, 3) \cap X_i(3, 2)|$ are similar to (6.2.3), and, by Corollary 6.2.5, the cardinalities $|X_i(1, 2) \cap X_i(2, 3) \cap X_i(3, 2)|$ and $|X_i(1, 3) \cap X_i(2, 3) \cap X_i(3, 2)|$ are both zero.

Since F contains a directed cycle, the cardinality $|X_i(1, 2) \cap X_i(1, 3) \cap X_i(2, 3) \cap X_i(3, 2)|$ is zero by Corollary 6.2.5.

Notice that the terms corresponding to subsets S containing a directed cycle are zero, hence contribute nothing to $\beta(F, \mathcal{P}, n)$. The acyclic subsets $S \subseteq E(F)$ such that the transitive reduction of S is not equal to its transitive closure in F combine in transitive closure posets as follows:



By Lemma 6.2.6, the combined terms of each of the above transitive closure posets contribute zero to $\beta(F, \mathcal{P}, n)$. Below we give the remaining terms of $\beta(F, \mathcal{P}, n)$, after cancellation:

$$\sum_{i \in [m]} \frac{n!}{\binom{a_i + b_i}{a_i}} + \frac{n!}{\binom{a_i + c_i}{a_i}} + \frac{2n!}{\binom{b_i + c_i}{b_i}} - \frac{n!}{\binom{a_i + b_i + c_i}{a_i}} - \frac{n!}{\binom{a_i + b_i + c_i}{b_i}} - \frac{n!}{\binom{a_i + b_i + c_i}{c_i}}$$

Applying Theorem 6.2.9 to the above formula for $\beta(F, \mathcal{P}, n)$ (after cancellations), and dividing both sides of the resulting inequality by $n!$, we obtain the following LYM inequality for F -following collections:

$$\sum_{i \in [m]} \frac{1}{\binom{a_i + b_i}{a_i}} + \frac{1}{\binom{a_i + c_i}{a_i}} + \frac{2}{\binom{b_i + c_i}{b_i}} - \frac{1}{\binom{a_i + b_i + c_i}{a_i}} - \frac{1}{\binom{a_i + b_i + c_i}{b_i}} - \frac{1}{\binom{a_i + b_i + c_i}{c_i}} \leq 1$$

6.3 Relating H -intersecting collections and F -following collections

In this section, we establish the connection between F -following collections and H -intersecting collections.

Let H be an alphabet graph and let F be a follow digraph with $V(H) = V(F) = [v]$. If every H -intersecting collection of v -packings is also an F -following collection, then we write $H \rightsquigarrow F$. If every F -following collection of v -packings is also an H -intersecting collection, then we write $H \leftarrow F$. If a collection of v -packings is H -intersecting if and only if it is F -following, then we write $H \leftrightarrow F$.

Remark 6.3.1 Whenever the arrow notations $\rightsquigarrow$, $\leftarrow$, or $\leftrightarrow$ are used, our convention is to write the alphabet graph H to the left of the arrow, and we write the follow digraph F to the right of the arrow.

Notice that if $H \rightsquigarrow F$, then we can apply the inequality of Theorem 6.2.9 to H -intersecting collections.

Corollary 6.3.2 Let H be an alphabet graph and let $\mathcal{P} = \{P_1, \dots, P_m\}$ be an H -intersecting collection of packings of $[n]$. Let F be a follow digraph such that $V(F) = V(H)$, and define $\mathfrak{S}$ to be the set of all nonempty subsets $S \subseteq E(F)$ such that S is acyclic and such that $S = S^t = \hat{S}$. If $H \rightsquigarrow F$, then

$$\sum_{j=1}^m \left| \bigcup_{ab \in E(F)} X_j(a, b) \right| = \sum_{j=1}^m \sum_{S \in \mathfrak{S}} (-1)^{|S|+1} \left| \bigcap_{ab \in S} X_j(a, b) \right| \leq n! \quad \blacksquare$$

Here, we restate Corollary 6.3.2 in terms of families of cross-intersecting set systems; however, going forward, our results will be phrased in terms of packings.

Corollary 6.3.3 Let H be an alphabet graph with $V(H) = [v]$. Let $\mathcal{A}^1, \dots, \mathcal{A}^v$ be v families of subsets of $[n]$, where $\mathcal{A}^a = \{A_1^a, A_2^a, \dots, A_m^a\}$ for each $a \in [v]$. Suppose, for each $i \in [m]$, we have $A_i^a \cap A_i^b = \emptyset$ for all $a \neq b$, and $\mathcal{A}^a$ and $\mathcal{A}^b$ are cross-intersecting whenever $ab \in E(H)$. If F is any follow digraph such that $V(F) = V(H)$ and $H \rightsquigarrow F$, then

$$\sum_{j=1}^m \left| \bigcup_{ab \in E(F)} \{\pi : \pi \text{ contains } A_j^a \text{ followed by } A_j^b\} \right| \leq n! \quad \blacksquare$$

Our main goal for this section is to answer the following question:

Question 6.3.4 Given an alphabet graph H , for which follow digraphs F can we apply Corollary 6.3.2 to obtain the best upper bounds on the number of packings in an H -intersecting collection?

As a first step towards answering Question 6.3.4, we give necessary and sufficient conditions for $H \rightsquigarrow F$, based on the next definition and lemma.

Definition 6.3.5 Let F be a follow digraph and let a and b be two (not necessarily distinct) vertices of F . Vertices a and b are **aligned** if both a and b are sources of F , or if both a and b are sinks of F ; otherwise, a and b are **unaligned**. Since F has no isolated vertices, a and b are unaligned if $\text{indeg}_F(a) > 0$ and $\text{outdeg}_F(b) > 0$, or if $\text{outdeg}_F(a) > 0$ and $\text{indeg}_F(b) > 0$.

Let H be an alphabet graph and let F be a follow digraph such that $V(H) = V(F) = [v]$. An H -intersecting collection $\mathcal{P} = \{P_1, \dots, P_m\}$ of v -packings of $[n]$ is **minimal**

with respect to H if removing an element of a class P_i^a , for some $i \in [m]$ and some $a \in [v]$, results in a collection that is not H -intersecting. Similarly, an F -following collection $\mathcal{P} = \{P_1, \dots, P_m\}$ of v -packings of $[n]$ is **minimal with respect to** F if removing an element of a class P_i^a , for some $i \in [m]$ and some $a \in [v]$, results in a collection that is not F -following.

Lemma 6.3.6 If H is an alphabet graph with $V(H) = [v]$, then there exist two v -packings, P_1 and P_2 , such that $P_1^a \cap P_2^b \neq \emptyset$ if and only if $ab \in E(H)$. Moreover, $\{P_1, P_2\}$ is minimal with respect to H .

[proof] To construct P_1 and P_2 , it is convenient to use a ground set X , defined as follows. For each ordered pair ab of adjacent vertices of H , X contains an element x_{ab} indexed by this pair. In particular, if $ab \in E(H)$, then both x_{ab} and x_{ba} are elements of X . If aa is a loop of H , then x_{aa} is in X once.

We build two packings of X : for each $x_{ab} \in X$, put the element x_{ab} into class a of P_1 and class b of P_2 . Consequently, $\{x_{ab}\} = P_1^a \cap P_2^b$ for all ordered pairs of adjacent vertices ab of H . By the construction of P_1 and P_2 , it is clear that $P_1^a \cap P_2^b \neq \emptyset$ if and only if $ab \in E(H)$. Whenever $ab \in E(H)$, we have $\{x_{ab}\} = P_1^a \cap P_2^b$, so the minimality of $\mathcal{P}$ being H -intersecting is also clear. ■

Lemma 6.3.7 Let H be an alphabet graph and let F be a follow digraph such that $V(F) = V(H)$. Then $H \rightsquigarrow F$ if and only if we have the edge $ab \in E(H)$ whenever a and b are unaligned in F .

[proof] ($\Leftarrow$) Assume ab is an edge of H whenever a and b are unaligned in F . Let $\mathcal{P} = \{P_1, \dots, P_m\}$ be an H -intersecting collection of packings of $[n]$. If $\mathcal{P}$ is not an F -following collection, then there exist distinct packings $P_i, P_j \in \mathcal{P}$ and a permutation π of $[n]$ such that π contains P_i^a followed by P_i^b , as well as P_j^c followed by P_j^d for some arcs $ab, cd \in E(F)$. Having arcs $ab, cd \in E(F)$ means that a and d are unaligned in F . Similarly, b and c are unaligned in F . We therefore have edges $ad, bc \in E(H)$.

Let $s \in [n]$ be the index of π that P_i^a ends at, and let $t \in [n]$ be the index of π that P_j^c ends at. There are two cases: either $t \leq s$ or $t > s$. If $t \leq s$, then class P_i^b must begin at index u of π , where $u > s$, since P_i^a and P_i^b are disjoint. Consequently, we have $P_j^c \cap P_i^b = \emptyset$, which contradicts the fact that $bc \in E(H)$ and that P_i and P_j are

H -intersecting. The case when $t > s$ leads to a similar contradiction. Therefore, $\mathcal{P}$ must be an F -following collection.

($\implies$) Assume that $H \rightsquigarrow F$. Using Lemma 6.3.6, we construct $\mathcal{P} = \{P_1, P_2\}$ such that $P_1^a \cap P_2^b \neq \emptyset$ if and only if $ab \in E(H)$. Since $H \rightsquigarrow F$, we see that $\mathcal{P}$ must be an F -following collection.

If there exist unaligned vertices a and b in F (not necessarily distinct) such that $ab \notin E(H)$, then, by construction of $\mathcal{P}$, we have $P_1^a \cap P_2^b = \emptyset$. Without loss of generality, there exist vertices c and d such that ac and db are arcs of F , since a and b are unaligned. Let π be any permutation that begins with P_1^a and ends with P_2^b (such a permutation exists since P_1^a and P_2^b are disjoint). It follows that π contains P_1^a followed by P_1^c and π also contains P_2^d followed by P_2^b , contradicting the fact that $\mathcal{P}$ is an F -following collection. Therefore, $ab \in E(H)$ whenever a and b are unaligned in F . ■

Analogous to Lemma 6.3.6, for every follow digraph F there exists a minimal F -following collection.

Lemma 6.3.8 If F is a follow digraph with $V(F) = [v]$, then there exist two v -packings, P_1 and P_2 , such that $\mathcal{P} = \{P_1, P_2\}$ is an F -following collection. Moreover, $\mathcal{P}$ is minimal with respect to F .

[proof] To construct $\mathcal{P}$, we use a ground set X , defined as follows. Let the elements of X be indexed by ordered pairs of (not necessarily distinct) unaligned vertices of F . That is,

$$X = \{x_{ab} : a \text{ and } b \text{ are unaligned in } F\}.$$

To build $\mathcal{P}$, for each $x_{ab} \in X$, we put the element x_{ab} into class a of P_1 and put x_{ab} into class b of P_2 . We claim that $\mathcal{P} = \{P_1, P_2\}$ is an F -following collection. Let π be a permutation of X . If π contains a P_1 -following for F , then π contains P_1^a followed by P_1^b for some arc $ab \in E(F)$. Let cd be any arc of F (not necessarily distinct from ab). By the definition of X , we have elements x_{ad} , x_{da} , x_{bc} , and x_{cb} in X (the arcs $ab, cd \in E(F)$ provide the indegree and outdegree conditions). In particular, $x_{ad} \in P_1^a \cap P_2^d$ and $x_{bc} \in P_1^b \cap P_2^c$. Since π contains P_1^a followed by P_1^b , the element x_{ad} must occur in π before the element x_{bc} . Thus, it is impossible for π to contain P_2^c followed by P_2^d . Similarly, if π contains a P_2 -following for F , it cannot simultaneously contain a P_1 -following. Therefore, $\{P_1, P_2\}$ is an F -following collection.

If we delete an element from any class of P_1 or P_2 , then we no longer have an F -following collection: Suppose we delete an element of P_1^a , say x_{ab} . Since x_{ab} is an element of X , we know that $\text{outdeg}_F(a) > 0$ and $\text{indeg}_F(b) > 0$ or vice versa (the opposite case is similar). So, there exist arcs $a\beta, \alpha b \in E(F)$ for some $\alpha, \beta \in V(F)$. Notice that x_{ab} was the only element of X in the intersection $P_1^a \cap P_2^b$. So $P_1^a - \{x_{ab}\}$ is disjoint from P_2^b . Choose any permutation π of X that begins with $P_1^a - \{x_{ab}\}$ and ends with P_2^b . Then, π contains $P_1^a - \{x_{ab}\}$ followed by P_1^β , and π contains P_2^α followed by P_2^b . Hence, we no longer have an F -following collection. Deleting an element from some class of P_2 is similar. ■

Although the assumption $H \leftarrow F$ does not give us the means to apply Corollary 6.3.2, it gives us the means to characterize when being an H -intersecting collection is equivalent to being an F -following collection. Thus, necessary and sufficient conditions for $H \leftarrow F$ are given next.

Lemma 6.3.9 Let H be an alphabet graph and let F be a follow digraph with $V(H) = V(F) = [v]$. Then $H \leftarrow F$ if and only if vertices a and b are unaligned in F whenever $ab \in E(H)$.

[proof] ($\Leftarrow$) Assume that a and b are unaligned in F whenever $ab \in E(H)$. If $H \leftarrow F$ is false, then there exists an F -following collection $\mathcal{P} = \{P_1, \dots, P_m\}$ such that $\mathcal{P}$ is not H -intersecting. Consequently, there is an edge $ab \in E(H)$ such that $P_i^a \cap P_j^b = \emptyset$ for some $i \neq j \in [m]$. Since $ab \in E(H)$, the vertices a and b must be unaligned in F . Without loss of generality, there exist vertices $\beta \neq a$ and $\alpha \neq b$ such that $a\beta, \alpha b \in E(F)$. Define a permutation π that begins with P_i^a and ends with P_j^b (possible since P_i^a and P_j^b are disjoint). Now π contains P_i^a followed by P_i^β and π also contains P_j^α followed by P_j^b , contradicting the fact that $\mathcal{P}$ is an F -following collection. Therefore, $H \leftarrow F$ must be true.

($\Rightarrow$) Suppose there exists an edge $ab \in E(H)$ such that a and b are aligned in F . Then there are two cases: either a and b are both sources of F , or a and b are both sinks. Suppose the former and construct the F -following collection $\mathcal{P} = \{P_1, P_2\}$ given by Lemma 6.3.8. We claim that $\mathcal{P}$ is not H -intersecting. By the construction of $\mathcal{P}$, since a is a source, $P_1^a = \{x_{a\beta} \in X : \text{indeg}_F(\beta) > 0\}$. Similarly, since b is a source, $P_2^b = \{x_{\alpha b} \in X : \text{indeg}_F(\alpha) > 0\}$. As $\text{indeg}_F(a) = \text{indeg}_F(b) = 0$, we see that $P_1^a \cap P_2^b = \emptyset$, so $\mathcal{P}$ is not an H -intersecting collection. The argument when both a and b are sinks of F is similar. ■

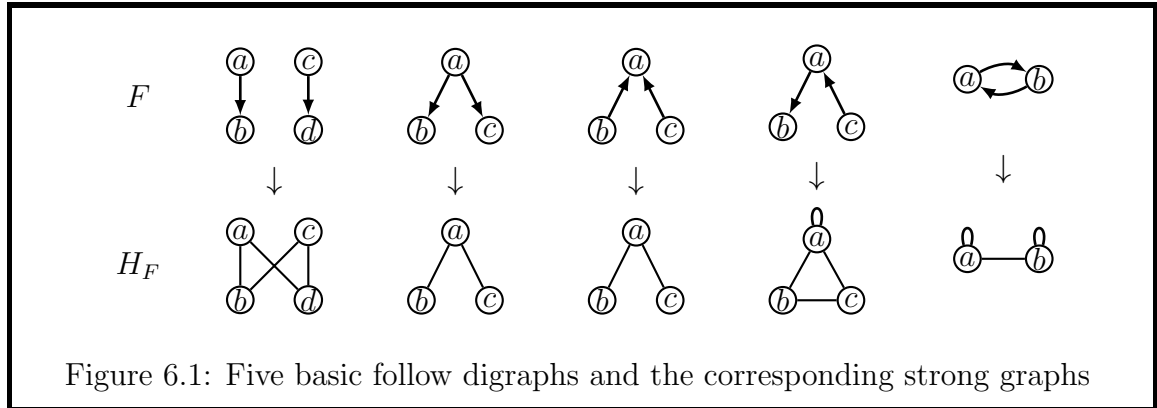
Corollary 6.3.10 Let H be an alphabet graph and let F be a follow digraph with $V(F) = V(H) = [v]$. Then $(H \rightsquigarrow F)$ if and only if $(a$ and b are unaligned in F if and only if $ab \in E(H))$. ■

Given a follow digraph F , Corollary 6.3.10 tells us that there is a unique alphabet graph H such that $H \rightsquigarrow F$. On the other hand, in the following section, we will show that if we are given an alphabet graph H , then there may any number of follow digraphs F satisfying $H \rightsquigarrow F$ (including zero).

6.4 Strong graphs

Definition 6.4.1 Let F be a follow digraph. The **strong graph** for F , denoted H_F , has $V(H_F) = V(F)$ and edge $ab \in E(H_F)$ if and only if a and b are unaligned in F .

By Corollary 6.3.10, H_F is the unique alphabet graph such that $H_F \rightsquigarrow F$. The construction of H_F is summarized in Figure 6.1. Each pair of distinct arcs in F is of one of the five types given in Figure 6.1; we also give the edges of H_F that are implied by unaligned vertices of F in each case.



Corollary 6.4.2 Let H be an alphabet graph and let F be a follow digraph such that $V(F) = V(H) = [v]$. If H_F is the strong graph for F , then

1. $H \rightsquigarrow F$ if and only if $H \supseteq H_F$,
2. $H \rightsquigarrow F$ if and only if $H \subseteq H_F$, and
3. $H \rightsquigarrow F$ if and only if $H = H_F$. ■

A **strong graph** is an alphabet graph H for which there exists a follow digraph F such that $H \Leftarrow\!\!\!\rightarrow F$. With respect to our results, strong graphs are the most relevant class of alphabet graphs, and they have a particular structure based on the following definition. Let F be a follow digraph with $V(F) = [v]$ (recall that F has no isolated vertices). The **alignment decomposition** of F is the partition (W, X, Y) of $V(F)$, where

- $W = \{w \in [v] : \text{indeg}_F(w) > 0 \text{ and } \text{outdeg}_F(w) > 0\}$,
- $X = \{x \in [v] : \text{indeg}_F(x) = 0\}$, and
- $Y = \{y \in [v] : \text{outdeg}_F(y) = 0\}$.

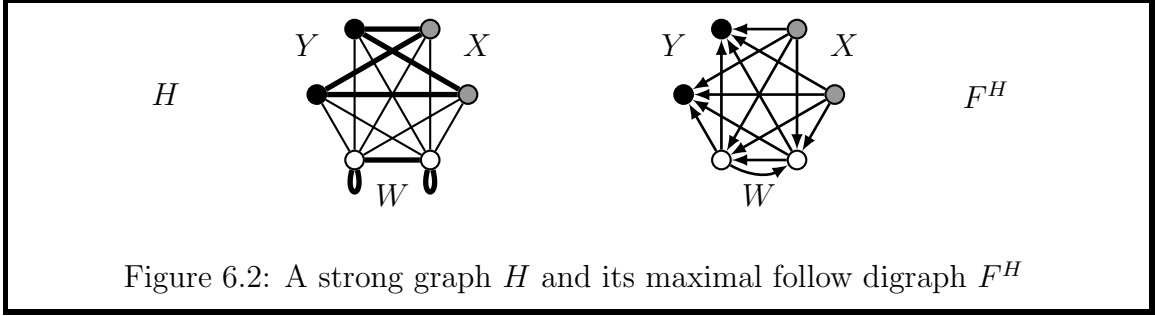
Notice that $|W| = 1$ implies $|X| \geq 1$ and $|Y| \geq 1$.

Proposition 6.4.3 An alphabet graph H is a strong graph if and only if H is the join of a complete graph with a loop on every vertex and a complete bipartite graph, where at least one of the two factors of the join has an edge.

[proof] By Corollaries 6.3.10 and 6.4.2, H is the strong graph for a follow digraph F if and only if the edges of H correspond to the unaligned pairs of vertices of F . Consider the alignment decomposition of F , (W, X, Y) . Each vertex in W is unaligned with itself and every other vertex; each vertex in X is unaligned with every vertex in $W \cup Y$; each vertex in Y is unaligned with every vertex in $W \cup X$. Equivalently, H is composed of a complete graph with loops induced by W , which is completely joined to all vertices in $X \cup Y$, and $X \cup Y$ induces a complete bipartite subgraph of H with bipartition (X, Y) . If $|W| = 1$, then the vertex in W must be adjacent in F to at least one vertex in X and another in Y . ■

We give an example in Figure 6.2 (on the left) to demonstrate the structure of a strong graph H_F based on the alignment decomposition (W, X, Y) . The set W has white vertices with loops. The sets X and Y are indicated using grey and black vertices, respectively. Notice that H_F is the join of a complete graph with a loop on each vertex and a complete bipartite graph, as prescribed by Proposition 6.4.3; the edges in each of these parts are thick edges, while thin edges indicate the join of these two parts.

Consider a strong graph $H = H_F$ and the alignment decomposition (W, X, Y) of F . Notice that X and Y are indistinguishable when we simply look at the structure of H . Which part of the complete bipartite subgraph of H represents X and which part



represents Y ? The answer depends on the particular follow digraph F , but, as we shall explain, we need not worry about this distinction.

Let F be a digraph. Build a new graph from F as follows: use the same vertex set, and for every arc of F , say ab , put the reverse-direction arc, ba , in the new graph. The directed graph we obtain is the **reversal** of F .

Remark 6.4.4 Since the relations $\rightsquigarrow$, $\leftarrow$, $\rightleftarrows$, between an alphabet graph H and a follow digraph F are based solely on unaligned pairs of vertices of F and the corresponding edges of H , it makes no difference if the direction of all arcs of F are reversed. We therefore make no distinction between a follow digraph F and its reversal.

By Remark 6.4.4, the alignment decomposition parts X and Y are interchangeable since F is interchangeable with its reversal. Let H be the strong graph for F . The **alignment decomposition** of H is the unique (up to reversal) alignment decomposition of F .

Let H be a strong graph and let (W, X, Y) be its alignment decomposition. The **maximal follow digraph** for H , denoted F^H , has vertex set $V(F^H) = V(H) = W \cup X \cup Y$, and arcs as follows:

- every ordered pair of distinct vertices $w, w' \in W$ are joined by two antiparallel arcs in F^H , namely ww' and $w'w$;
- every ordered pair of vertices $x \in X, y \in Y$ are joined by an arc xy ;
- each vertex $x \in X$ is joined to every vertex $w \in W$ by an arc xw ;
- each vertex $w \in W$ is joined to every vertex $y \in Y$ by an arc wy .

In other words, F^H is constructed by packing in as many arcs as possible while

preserving the alignment decomposition that is unique to H . The structure of F^H is demonstrated by the example in Figure 6.2.

We now highlight several interesting properties of strong graphs and their connection to maximal follow digraphs. Let $\mathcal{F}$ denote the set of follow digraphs, and let $\mathcal{H}_{\mathcal{F}}$ denote the set of strong graphs.

Theorem 6.4.5 1. Strong graphs induce a partition of $\mathcal{F}$ via the following equivalence relation: F_1 is equivalent to F_2 if and only if $H_{F_1} = H_{F_2}$.
 2. Each $H \in \mathcal{H}_{\mathcal{F}}$ defines an equivalence class, namely $[H] = \{F \in \mathcal{F} : H = H_F\}$.
 3. All $F \in [H]$ have the same alignment decomposition (up to reversal).
 4. Each class $[H]$ has a unique (up to reversal) maximal element, namely F^H , and every $F \in [H]$ is a subgraph of F^H (up to reversal).

[proof] We prove (4). Let $H \in \mathcal{H}_{\mathcal{F}}$ and consider its maximal follow digraph F^H . Clearly, $F^H \in [H]$; moreover, F^H is maximal in the sense that any pair of nonadjacent vertices, $a, b \in V(F^H)$, cannot be adjacent in any follow digraph $F \in [H]$ without violating the alignment decomposition of H . Consequently, all follow digraphs $F \in [H]$ are necessarily subgraphs of F^H (up to reversal). ■

For a strong graph $H \in \mathcal{H}_{\mathcal{F}}$, we can apply Corollary 6.3.2 for all $F \in [H]$. The relation $H \Leftarrow F$ is stronger than $H \rightsquigarrow F$, so at this point, it makes sense to differentiate the two resulting types of inequalities.

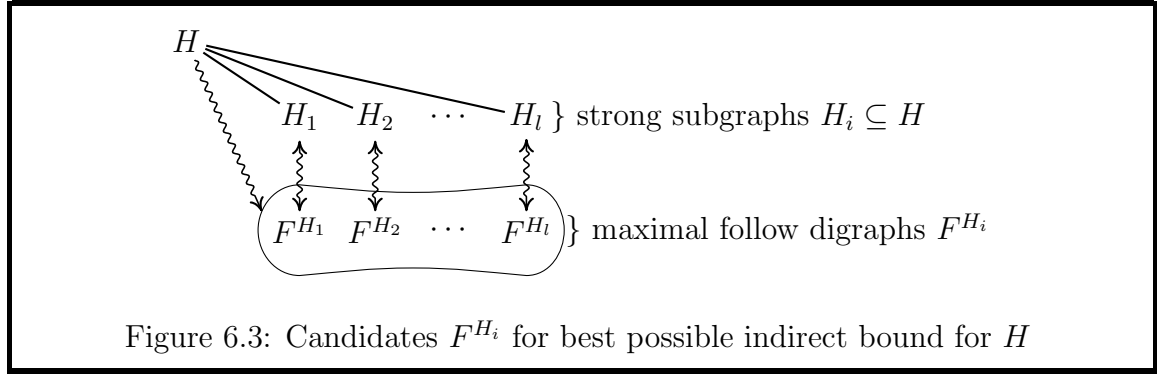
Let H be an alphabet graph and let $\mathcal{P}$ be an H -intersecting collection of packings of $[n]$. Let F be a follow digraph. If $H \rightsquigarrow F$ is true but $H \Leftarrow F$ is false, then the inequality $\beta(F, \mathcal{P}, n) \leq n!$ is an **indirect bound** for H -intersecting collections. If, on the other hand, $H \Leftarrow F$, then the inequality $\beta(F, \mathcal{P}, n) \leq n!$ is a **direct bound** for H -intersecting collections.

We now have the answer to Question 6.3.4 when the given alphabet graph H is a strong graph. In this case, F^H , by its maximality, yields the best direct bound for H -intersecting collections. Moreover, the direct bound given by F^H is better than any indirect bound for H -intersecting collections.

Corollary 6.4.6 Let $H \in \mathcal{H}_{\mathcal{F}}$ be a strong graph and let $\mathcal{P}$ be an H -intersecting collection of packings of $[n]$. Let $F \in \mathcal{F}$. If $H \rightsquigarrow F$, then

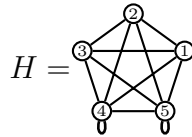
$$\beta(F, \mathcal{P}, n) \leq \beta(F^H, \mathcal{P}, n) \leq n!.$$

[**proof**] First, F has a unique strong graph, namely H_F . By Corollary 6.4.2, we have $H_F \subseteq H$. It now follows that the maximal follow digraphs for H_F and H , respectively, satisfy $F^{H_F} \subseteq F^H$ (up to reversal). This is easily checked by analyzing the alignment decompositions of H_F and H under the constraint $H_F \subseteq H$. Thus, $F \subseteq F^{H_F} \subseteq F^H$ (up to reversal). Applying Lemma 6.2.3 twice and Lemma 6.2.2 once, we get $\beta(F, \mathcal{P}, n) \leq \beta(F^{H_F}, \mathcal{P}, n) \leq \beta(F^H, \mathcal{P}, n) \leq n!$ as required. ■



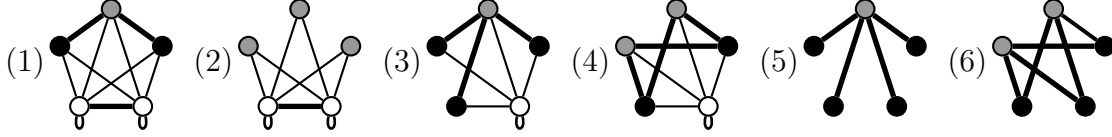
For an alphabet graph $H \notin \mathcal{H}_{\mathcal{F}}$, indirect bounds are the only option. We can produce the list of all $F \in \mathcal{F}$ that satisfy $H \rightsquigarrow F$ using Corollary 6.4.2: $H \rightsquigarrow F$ if and only if $H_F \subseteq H$. We enumerate the list of all strong graphs $H_i \in \mathcal{H}_{\mathcal{F}}$ such that $H_i \subseteq H$. For each strong subgraph $H_i \subseteq H$, we compute its maximal follow digraph F^{H_i} . By Corollary 6.4.2, we have $H \rightsquigarrow F^{H_i}$ for each strong subgraph H_i found. All subgraphs $F \subseteq F^{H_i}$ that preserve the alignment decomposition for H_i also satisfy $H \rightsquigarrow F$, but, for the purposes of optimizing our inequalities, we need only consider the maximal follow digraph F^{H_i} . Figure 6.3 summarizes this approach. Example 6.4.7 illustrates the procedure.

Example 6.4.7 Let

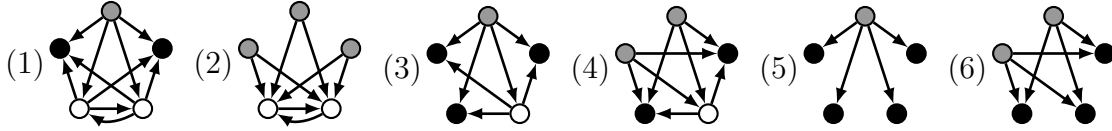


and notice that H fails to have the structure of a strong graph described in Proposition 6.4.3. Each strong subgraph of H has an alignment decomposition (W, X, Y) . The possibilities for W are $\{4, 5\}$, $\{4\}$, $\{5\}$, or $\emptyset$. In each case, we look at the induced subgraph $H - W$ and compute all possible complete bipartite graphs. Modulo vertex labels, we list all such strong subgraphs below. In each case, the set W has white

vertices with loops. The sets X and Y are indicated using grey and black vertices, respectively. Thick edges indicate edges in each of the two parts $K_{|W|}^{\text{loop}}$ or $K_{|X|,|Y|}$, while thin edges indicate the join of these two parts.



Next, we give the maximal follow digraphs for each type of strong subgraph; these are our candidates for the best possible indirect bound for H -intersecting collections.



To conclude this section, we give Theorem 6.4.8, which provides our best answer to Question 6.3.4.

Theorem 6.4.8 Let H be an alphabet graph and let $\mathcal{P}$ be an H -intersecting collection of packings of $[n]$. If H is a strong graph, then F^H yields the best direct bound for H . If H is not a strong graph, then the best indirect bound for H is given by the maximal follow digraph of a strong subgraph H_i of H , where H_i is chosen to maximize $\beta(F^{H_i}, \mathcal{P}, n)$. ■

For an alphabet graph H that is not a strong graph, Theorem 6.4.8 does not tell us whether there is a unique choice for maximizing $\beta(F, \mathcal{P}, n)$, nor do we know if there is a universally optimal candidate that works irrespective of the particular H -intersecting collection $\mathcal{P}$. We wonder whether the optimal choice is the follow digraph F with the most arcs among the list of candidates. In Section 7.5, we give an asymptotically based estimate of $\beta(F, \mathcal{P}, n)$ that supports choosing follow digraphs with as many arcs as possible.

By Theorem 6.4.8, our inequalities for H -intersecting collections are always based on a strong subgraph of the alphabet graph H in question.

Let H be a strong graph and let F^H be its maximal follow digraph. Recall from Theorem 6.2.9 that the terms of $\beta(F^H, \mathcal{P}, n)$ range over all nonempty subsets $S \subseteq E(F^H)$ such that S is acyclic and such that $S = S^t = \hat{S}$. For the maximal follow

digraph F^H , such subsets S are simply those that contain no directed walk of length two.

Theorem 6.4.9 Let $H \in \mathcal{H}_{\mathcal{F}}$ be a strong graph on $V(H) = [v]$ and let F^H be its maximal follow digraph. Define $\mathcal{T}$ to be the set of all nonempty subsets $T \subseteq E(F^H)$ such that T contains no directed walk of length two. If $\mathcal{P} = \{P_1, \dots, P_m\}$ is an H -intersecting collection of v -packings of $[n]$, then

$$\beta(F^H, \mathcal{P}, n) = \sum_{i=1}^m \sum_{T \in \mathcal{T}} (-1)^{|T|+1} \left| \bigcap_{ab \in T} X_i(a, b) \right| \leq n!$$

[proof] By Theorem 6.2.9, the terms of $\beta(F^H, \mathcal{P}, n)$ range over the set $\mathfrak{S}$ of all nonempty subsets $S \subseteq E(F^H)$ such that S is acyclic and such that $S = S^t = \hat{S}$. Since F^H is a maximal follow digraph, we claim that $\mathfrak{S} = \mathcal{T}$.

Suppose $T \in \mathcal{T}$. Then T does not contain any directed walks of length 2. It follows that T is acyclic and transitively closed in F . Therefore, $T \in \mathfrak{S}$ and $\mathcal{T} \subseteq \mathfrak{S}$.

Suppose $T \subseteq E(F^H)$ and $T \notin \mathcal{T}$. Then T contains a directed walk of length 2, say u_1, u_2, u_3 (where $u_1 u_2 \in E(F^H)$ and $u_2 u_3 \in E(F^H)$). If $u_1 = u_3$, then T contains a directed cycle, hence is not an element of $\mathfrak{S}$. Let (W, X, Y) be the alignment decomposition of F^H . We consider every possibility for the membership of the vertices u_1, u_2 and u_3 in the alignment decomposition's parts:

First, notice that the vertex u_2 must belong to W since the vertices in X are all sources and the vertices in Y are all sinks.

If $u_1, u_3 \in W$, then, since every pair of vertices in W are symmetrically adjacent, we know that $u_1 u_3 \in E(F^H)$. If $u_1 \in W$ and $u_3 \notin W$, then, since $u_2 u_3 \in E(F^H)$, it follows that $u_3 \in Y$ (the set of sinks). Consequently, $u_1 u_3 \in E(F^H)$ since every vertex in W is adjacent to all vertices in Y . If $u_1 \notin W$ and $u_3 \in W$, then u_1 must be in X (the set of sources), hence $u_1 u_3 \in E(F^H)$ since every vertex in X is adjacent to all vertices in W . If $u_1 \notin W$ and $u_3 \notin W$, then u_1 must be in X and u_3 must be in Y , hence $u_1 u_3 \in E(F^H)$ since every vertex in X is adjacent to all vertices in Y .

In all cases, $T \neq \hat{T}$ and so $T \notin \mathfrak{S}$. Therefore, $\mathfrak{S} \subseteq \mathcal{T}$. ■

6.4.1 Number of strong graphs

By Proposition 6.4.3, all strong graphs consist of two parts: a complete graph with loops completely joined to a complete bipartite graph, where at least one of these two subgraphs contains an edge joining two distinct vertices in that part. If the complete graph with loops consists of only one vertex, this vertex must be unaligned with itself in the corresponding follow digraph. Consequently, the complete bipartite part must be nontrivially bipartite, that is, contain at least one edge. Conversely, if the complete bipartite part contains no edges, then the complete graph with loops must contain at least two vertices in order for these vertices to be unaligned in the corresponding follow digraph.

The number of ways that l unlabelled vertices can be bi-partitioned is $\lfloor l/2 \rfloor + 1$ since this is the number of ways to write l as $l = i + (l - i)$ where $0 \leq i \leq \lfloor l/2 \rfloor$.

For a given number of vertices v , let c denote the number of vertices in the complete part with loops. It follows that $0 \leq c \leq v$ and the remaining $v - c$ vertices must be the complete bipartite part, which can be bi-partitioned in $\lfloor (v - c)/2 \rfloor + 1$ ways.

There are two special cases: If $c = 1$, then we do not count the bipartition with $v - 1$ vertices in one part and no vertices in the other part since this would not allow the vertex with a loop to be unaligned with itself in the corresponding follow digraph. If $c = 0$, then we do not count the bipartition with v vertices in one part and no vertices in the other part: this would produce an empty graph which is not a strong graph. For each of the above two cases, we must subtract 1 from the total.

The number of strong graphs on v vertices is thus

$$\sum_{c=0}^v (\lfloor \frac{v-c}{2} \rfloor + 1) - 2 = \sum_{l=0}^v (\lfloor \frac{l}{2} \rfloor + 1) - 2 = \frac{1}{4}v(v+1) - \frac{1}{2} \lceil \frac{v}{2} \rceil + v - 1.$$

Lemma 6.4.10 For $v \geq 2$, there are $\frac{1}{4}v(v+1) - \frac{1}{2} \lceil \frac{v}{2} \rceil + v - 1$ strong graphs on v vertices. ■

6.4.2 Small strong graphs and maximal follow digraphs

For illustrative purposes, we list all strong graphs on 2, 3, and 4 vertices, along with the corresponding maximal follow digraphs.

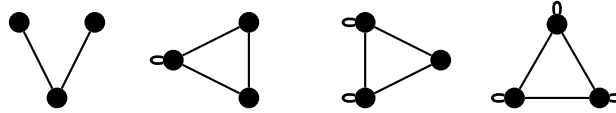
Here are the two strong graphs on 2 vertices:



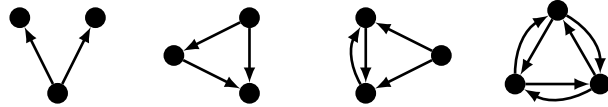
Here are the corresponding maximal follow digraphs:



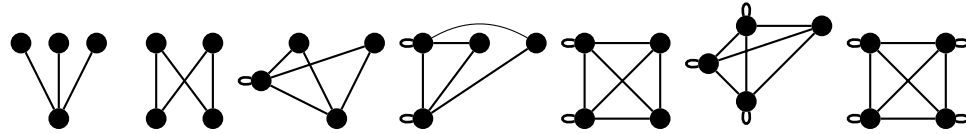
Here are the four strong graphs on 3 vertices:



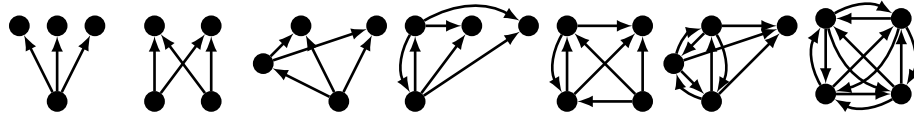
Here are the corresponding maximal follow digraphs:



Here are the seven strong graphs on 4 vertices:



Here are the corresponding maximal follow digraphs:



For an inventory of LYM inequalities for H -intersecting collections for small H , see [Appendix A](#).

Chapter 7

Bounds for covering arrays with alphabet graphs

The goal of this chapter is to transform our LYM inequalities for H -intersecting collections into upper bounds on $m(n, H)$ for several strong graphs H .

Recall that the column number for a covering array with alphabet graph H , denoted $\text{CAK}(n; 2, H)$, is the maximum number of columns k for which there exists a $\text{CA}(n; 2, k, H)$.

For a given n and alphabet graph H , the quantities $m(n, H)$ and $\text{CAK}(n; 2, H)$ are equal. Thus, we are in fact using our LYM inequalities to find upper bounds on the column number of covering arrays with strong alphabet graphs. Since K_v^{loop} is a strong graph, classical covering arrays fall into this category (recall that $\text{CAK}(n; 2, v) = \text{CAK}(n; 2, K_v^{\text{loop}})$), and we do provide improved bounds for $\text{CAK}(n; 2, v)$ in this chapter, specifically using our LYM inequality for K_3^{loop} -intersecting collections.

When reading this chapter, always consider the equivalence between $m(n, H)$ and $\text{CAK}(n; 2, H)$, but note that we continue to phrase our results in terms of collections of packings and using $m(n, H)$ rather than $\text{CAK}(n; 2, H)$.

The method we use for transforming our LYM inequalities for H -intersecting collections into upper bounds on $m(n, H)$ is summarized as follows: Using the appropriate follow digraph F , we compute $\beta(F, \mathcal{P}, n)$ in terms of the class cardinalities of the packings in $\mathcal{P}$. Recall from (6.2.2) and Theorem 6.2.9 that

$$\beta(F, \mathcal{P}, n) = \sum_{i=1}^{|\mathcal{P}|} \left(\begin{array}{c} \# \text{ permutations of } [n] \text{ that} \\ \text{contain } P_i^a \text{ followed by } P_i^b \\ \text{for some arc } ab \in E(F) \end{array} \right) = \sum_{i=1}^{|\mathcal{P}|} \sum_{\substack{S \subseteq E(F) \\ S \text{ acyclic} \\ S \neq \emptyset \\ S^t \neq S}} (-1)^{|S|+1} \left| \bigcap_{ab \in S} X_i(a, b) \right| \leq n!$$

The formula for $\beta(F, \mathcal{P}, n)$ sums over all $P_i \in \mathcal{P}$, but for each i , the formula has the same form. For a fixed $P_i \in \mathcal{P}$, we have v variables in the formula, namely $|P_i^1|, \dots, |P_i^v|$. Let $f(|P_i^1|, \dots, |P_i^v|)$ be the formula of $\beta(F, \mathcal{P}, n)$ for one fixed i , that is,

$$f(|P_i^1|, \dots, |P_i^v|) = \sum_{\substack{S \subseteq E(F) \\ S \text{ acyclic} \\ S \neq \emptyset \\ S^t \neq S}} (-1)^{|S|+1} \left| \bigcap_{ab \in S} X_i(a, b) \right|.$$

We want to find the minimum value of f over all $|P_i^1|, \dots, |P_i^v|$. Since any H -intersecting collection of v -packing of $[n]$ may be extended to an H -intersecting collection of v -partitions of $[n]$, we may assume that $|P_i^1| + \dots + |P_i^v| = n$ for all i . We find the minimum via “balancing” lemmas, wherein we prove that certain substitutions help to reduce f . For example, when is it better to make the substitutions $|P_i^a| \leftarrow |P_i^a| - 1$ and $|P_i^b| \leftarrow |P_i^b| + 1$? With adequate balancing lemmas, we are equipped with a procedure for taking any value of f and reducing to the minimum value of f . Once we have the minimum value of f , say $f_{\min}$, then for every H -intersecting collection $\mathcal{P}$ of packings of n , we have

$$|\mathcal{P}| \cdot f_{\min} \leq \beta(F, \mathcal{P}, n) \leq n!$$

From that point, the upper bound is given by $|\mathcal{P}| \leq n!/f_{\min}$.

In Section 7.1, we discuss stars. For the star on three vertices, we give the following upper bound on $m(n, S_3)$ in Theorem 7.1.14:

$$m(n, S_3) \leq \frac{1}{2-\delta} \binom{a+b}{a}$$

where $a \approx \frac{1}{2}(1 + \sqrt{5})b$, $a + 2b = n$, and $\delta = o(1)$ (the exact values of a , b , and δ are given in Theorem 7.1.14).

In Section 7.3, we provide an upper bound for $m(n, K_3^{\text{loop}})$ in Theorem 7.3.20. From this result, we derive a general bound on $m(n, K_v^{\text{loop}})$ for all $v \geq 3$ in Corollary 7.4.1. For $v \geq 3$, Corollary 7.4.1 improves a bound given by Poljak and Tuza [48] (see Theorem 2.3.4).

Although we successfully obtain the above bounds, transforming our generalized LYM inequality for H -intersecting collections into an upper bound on $m(n, H)$ becomes more challenging for larger alphabet graphs H .

Under the assumption that there is a limiting distribution of class cardinalities among the packings in optimal H -intersecting collections (this limiting distribution will be defined precisely later), in Section 7.5, we prove that, asymptotically, it suffices to consider a simplified version of our LYM inequalities with so-called “single-arc” terms. While dealing only with single-arc terms, our task of transforming our LYM inequalities into upper bounds on $m(n, H)$ is simplified; although, obtaining upper bounds using single-arc terms can nevertheless be a difficult task. The use of this single-arc simplification also suggests the question: are the assumptions we made in order to obtain the single-arc simplification reasonable?

Under these assumptions, we provide an asymptotic bound for $m(n, K_v^{\text{loop}})$ for all v in Theorem 7.6.2:

$$m(n, K_v^{\text{loop}}) \leq \frac{1}{v^2 - v} \left(2 \lfloor n/v \rfloor + 2 \right) (\lfloor n/v \rfloor + 1) (1 + o(1)).$$

If there is a limiting distribution on class cardinalities, then the above bound significantly improves the bound in Corollary 7.4.1 for large enough v and n .

7.1 Stars and the alphabet graph S_3

Stars are examples of strong graphs, and we give the inequality for star-intersecting collections next. Our convention is to label the vertices of S_v as $V(S_v) = [v]$, where the central vertex is labelled 1, and the leaves have labels from the set $\{2, \dots, v\}$.

Theorem 7.1.1 If $\mathcal{P} = \{P_1, \dots, P_m\}$ is an S_v -intersecting collection of v -packings of $[n]$, then

$$\sum_{j=1}^m \sum_{\substack{B \subseteq \{2, \dots, v\} \\ B \neq \emptyset}} \frac{(-1)^{|B|+1}}{\binom{|P_j^1| + \sum_{a \in B} |P_j^a|}{|P_j^1|}} \leq 1.$$

[**proof**] The maximal follow digraph F^{S_v} is (up to reversal) the orientation of S_v in which the central vertex is a source and the leaves are sinks. For F^{S_v} , the subsets of arcs $S \subseteq E(F^{S_v})$ satisfying the conditions of the sum given in Theorem 6.4.9 ($T \neq \emptyset$, T contains no directed walk of length 2) are simply all nonempty subsets of $E(F^{S_v})$. Each subset $T \subseteq E(F^{S_v})$ corresponds to a subset of leaves $B \subseteq \{2, \dots, v\}$, and we have

$$\beta(F^{S_v}, \mathcal{P}, n) = \sum_{i=1}^m \sum_{\substack{B \subseteq \{2, \dots, v\} \\ B \neq \emptyset}} (-1)^{|B|+1} \left| \bigcap_{a \in B} X_i(1, a) \right|.$$

It remains to count the permutations in $\bigcap_{a \in B} X_i(1, a)$ for any $B \subseteq \{2, \dots, v\}$ such that $B \neq \emptyset$. There are $\binom{n}{|P_i^1| + \sum_{a \in B} |P_i^a|}$ ways to choose positions for the elements of P_i^1 and P_i^a , $a \in B$. We have $|P_i^1|!$ ways to arrange the elements of P_i^1 in the first $|P_i^1|$ of these positions. There are $(\sum_{a \in B} |P_i^a|)!$ ways to arrange the elements of P_i^a , $a \in B$, in the remaining positions. There are $(n - |P_i^1| - \sum_{a \in B} |P_i^a|)!$ ways to arrange the remaining elements of $[n]$. Thus,

$$\begin{aligned} \left| \bigcap_{a \in B} X_i(1, a) \right| &= \binom{n}{|P_i^1| + \sum_{a \in B} |P_i^a|} |P_i^1|! \left(\sum_{a \in B} |P_i^a| \right)! \left(n - |P_i^1| - \sum_{a \in B} |P_i^a| \right)! \\ &= \frac{n!}{\binom{|P_i^1| + \sum_{a \in B} |P_i^a|}{|P_i^1|}} \end{aligned}$$

Now, dividing both sides of the inequality $\beta(F^{S_v}, \mathcal{P}, n) \leq n!$ by $n!$ yields the inequality for star-intersecting collections. ■

The application of Theorem 7.1.1 to the star S_3 is the simplest generalization of Theorem 2.1.3 from a result about collections of 2-packings to a result for collections of 3-packings. An inequality equivalent to Corollary 7.1.2 was given without proof by Körner and Simonyi [35].

Corollary 7.1.2 Let $\mathcal{P} = \{P_1, \dots, P_m\}$ be a collection of 3-packings of $[n]$ where $P_i = (P_i^1, P_i^2, P_i^3)$ for each i . Let $a_i = |P_i^1|$, $b_i = |P_i^2|$, and $c_i = |P_i^3|$ for each $i \in [m]$. If $\mathcal{P}$ is an S_3 -intersecting collection, then

$$\sum_{i=1}^m \frac{1}{\binom{a_i + b_i}{a_i}} + \frac{1}{\binom{a_i + c_i}{a_i}} - \frac{1}{\binom{a_i + b_i + c_i}{a_i}} \leq 1. \quad \blacksquare$$

Ahlsweide and Cai [1] characterize the collections for which the inequality of Corollary 7.1.2 holds with equality; however, the collections that achieve this identity do not coincide with collections that maximize $m(n, S_3)$ (except when $n = 6$). If n is even, then the construction of Ahlsweide and Cai produces an S_3 -intersecting collection of packings of $[n]$ containing $n/2$ packings, and, for this collection, the inequality of Corollary 7.1.2 is met with equality. In contrast, in Section 7.2, we investigate a construction of S_3 -intersecting collections of $[n]$ given by Körner and Simonyi consisting of approximately $(\frac{1+\sqrt{5}}{2})^n/n^3$ packings, but for which the inequality of Corollary 7.1.2 is not met with equality. Evidently, the result of Ahlsweide and Cai does not address Problem 6.1.2 when $H = S_3$.

Let $\mathcal{P} = \{P_1, \dots, P_m\}$ be a collection of 3-packings of $[n]$ where $P_i = (P_i^1, P_i^2, P_i^3)$ for each i . Let $a_i = |P_i^1|$, $b_i = |P_i^2|$, and $c_i = |P_i^3|$ for each $i \in [m]$. The expression for $\beta(F^{S_3}, \mathcal{P}, n)$ is as follows:

$$\beta(F^{S_3}, \mathcal{P}, n) = \sum_{i=1}^m \frac{n!}{\binom{a_i + b_i}{a_i}} + \frac{n!}{\binom{a_i + c_i}{a_i}} - \frac{n!}{\binom{a_i + b_i + c_i}{a_i}} \quad (7.1.1)$$

Define $f(a, b, c)$ as follows:

$$f(a, b, c) = \binom{a+b}{a}^{-1} + \binom{a+c}{a}^{-1} - \binom{a+b+c}{a}^{-1} \quad (7.1.2)$$

Throughout Section 7.1, f will denote the function defined in (7.1.2).

The expression for $\beta(F^{S_3}, \mathcal{P}, n)$, given in (7.1.1), can now be rewritten as

$$\beta(F^{S_3}, \mathcal{P}, n) = \sum_{i=1}^m n! f(a_i, b_i, c_i).$$

In an S_3 -intersecting collection of 3-packings of $[n]$, every packing $P_i \in \mathcal{P}$ must have at least one element in each of its three classes, so we may assume $a_i, b_i, c_i \geq 1$. We also have $a_i + b_i + c_i \leq n$. While maintaining the property of being S_3 -intersecting, we can add extra elements to the classes of the packings in $\mathcal{P}$ so that, for all i , the packing P_i is a partition of $[n]$; consequently, we may also assume $a_i + b_i + c_i = n$.

Thus, for each packing P_i in an S_3 -intersecting collection, the contribution of P_i to $\beta(F^{S_3}, \mathcal{P}, n)$ can be assumed to be of the following form: $n! f(a_i, b_i, c_i)$, where $a_i, b_i, c_i \geq 1$ and $a_i + b_i + c_i = n$.

For a fixed value of n , our goal for this section is to show that there exist values a , b , and c such that $a, b, c \geq 1$, $a + b + c = n$, and $f(a, b, c) \leq f(a_i, b_i, c_i)$, for all i . Once we establish these values, we will obtain the following lower bound on $\beta(F^{S_3}, \mathcal{P}, n)$:

$$|\mathcal{P}| n! f(a, b, c) \leq \sum_{i=1}^{|\mathcal{P}|} n! f(a_i, b_i, c_i) = \beta(F^{S_3}, \mathcal{P}, n). \quad (7.1.3)$$

Using the fact that $\beta(F^{S_3}, \mathcal{P}, n) \leq n!$, the bound in (7.1.3) produces an upper bound on $|\mathcal{P}|$:

$$|\mathcal{P}| \leq \frac{1}{f(a, b, c)}. \quad (7.1.4)$$

Finding the values a, b, c such that $f(a, b, c) \leq f(a_i, b_i, c_i)$ for all i will be accomplished using so-called balancing lemmas.

Our balancing lemmas will work in two stages:

1. In Section 7.1.1, we will use balancing lemmas show that the minimum value of f has $b = c$.
2. In Section 7.1.2, we will show that the minimum value of f has approximately a golden ratio between a and b .

In Section 7.1.3, we use our results on the minimum value of f to derive the upper bound on $m(n, S_3)$, given in Theorem 7.1.14.

Before we get to these results, we need some notation and a lemma.

Let a and b be positive integers. If $|a - b| \geq 2$, then a and b are called **unbalanced**. If $|a - b| \leq 1$, then a and b are called **balanced**.

For convenience, we use falling factorial notation, defined as follows: for positive integers x and n such that $x \geq n \geq 1$, the **falling factorial**, denoted $(x)_n$, is defined as

$$(x)_n = x(x-1) \cdots (x-(n-1)).$$

Many times throughout this chapter, we will use the following lemma to get exponential bounds from falling factorial expressions that frequently appear in the proofs of balancing lemmas.

Lemma 7.1.3 (Falling Factorial Fractions) Let $x, y, d \in \mathbb{Z}$, where $x \geq d$, $y > d$, and $d \geq 1$.

1. If $\frac{x}{y} < 1$, then $\left(\frac{x-d}{y-d}\right)^d \leq \frac{(x)_d}{(y)_d} \leq \left(\frac{x}{y}\right)^d$.
2. If $\frac{x}{y} > 1$, then $\left(\frac{x}{y}\right)^d \leq \frac{(x)_d}{(y)_d} \leq \left(\frac{x-d}{y-d}\right)^d$.

[proof]

1. Let i be an integer such that $1 \leq i \leq d$. If $\frac{x}{y} < 1$, then we claim that $\frac{x-(i-1)}{y-(i-1)} > \frac{x-i}{y-i}$. Since $\frac{x}{y} < 1$ implies $x < y$ and $\frac{x-i}{y-i} < 1$, we have

$$\frac{x-(i-1)}{y-(i-1)} = \frac{x-i+1}{y-i+1} > \frac{x-i+\frac{x-i}{y-i}}{y-i+1} = \frac{(x-i)(y-i)+(x-i)}{(y-i)(y-i+1)} = \frac{x-i}{y-i}.$$

Thus, when we consider $\frac{(x)_d}{(y)_d}$ as a product of “falling” fractions, the largest term is the first term $\frac{x}{y}$ and the smallest term is the last term $\frac{x-d+1}{y-d+1}$.

2. This follows from 1. by reciprocating. ■

7.1.1 Balancing leaves

Lemma 7.1.4 If a, b, c are nonnegative integers such that $c \geq b+2$, then

$$\frac{1}{\binom{a+b}{b}} + \frac{1}{\binom{a+c}{c}} \geq \frac{1}{\binom{a+b+1}{b+1}} + \frac{1}{\binom{a+c-1}{c-1}}.$$

[proof] The inequality of Lemma 7.1.4 is equivalent to $f(a, b, c) - f(a, b+1, c-1) \geq 0$, which is true as follows:

$$\begin{aligned} f(a, b, c) - f(a, b+1, c-1) &= \frac{1}{\binom{a+b}{a}} + \frac{1}{\binom{a+c}{a}} - \frac{1}{\binom{a+b+c}{a}} - \frac{1}{\binom{a+b+1}{a}} - \frac{1}{\binom{a+c-1}{a}} + \frac{1}{\binom{a+b+c}{a}} \\ &= \frac{a!b!}{(a+b)!} + \frac{a!c!}{(a+c)!} - \frac{a!(b+1)!}{(a+b+1)!} - \frac{a!(c-1)!}{(a+c-1)!} \end{aligned}$$

$$\begin{aligned}
&= \frac{a!b!}{(a+c)!} \left((a+c)_{c-b} + (c)_{c-b} - (b+1)(a+c)_{c-b-1} - (a+c)(c-1)_{c-1-b} \right) \\
&= \frac{a!b!}{(a+c)!} \left((a+c)_{c-b-1}(a+b+1) + (c)(c-1)_{c-1-b} - (b+1)(a+c)_{c-b-1} - (a+c)(c-1)_{c-1-b} \right) \\
&= \frac{a!b!}{(a+c)!} \left((a+c)_{c-b-1}(a) - (c-1)_{c-1-b}(a) \right) \\
&= a \frac{a!b!}{(a+c)!} \left((a+c)_{c-b-1} - (c-1)_{c-b-1} \right) \tag{7.1.5}
\end{aligned}$$

Since $a+c \geq c+1 > c-1$, it is clear that the expression given in (7.1.5) is greater than zero, as claimed. $\blacksquare$

Lemma 7.1.4 implies that $f(a, b, c)$ can be reduced by balancing the class cardinalities b and c whenever b and c are unbalanced. This is achieved by making the substitutions $a \leftarrow a$, $b \leftarrow b+1$, and $c \leftarrow c-1$.

A priori, we do not know what the class cardinalities a_i, b_i, c_i will be in an optimal S_3 -intersecting collection, nor does the application of Lemma 7.1.4 tell us that collections with balanced leaf-class cardinalities exist; however, our goal is not to construct S_3 -intersecting collections with balanced leaf-class cardinalities — our goal is to obtain bounds as in (7.1.3) and (7.1.4).

Suppose we apply Lemma 7.1.4 until we have a lower bound for $\beta(F^{S_3}, \mathcal{P}, n)$ with all b_i and c_i balanced. We can further reduce our lower bound by forcing $b_i = c_i$ in one of two ways: if $a_i \leq 2b_i$ then we make the substitutions $a_i \leftarrow a_i+1$, $b_i \leftarrow b_i$, $c_i \leftarrow c_i-1$; otherwise, $a_i > 2b_i$ and we make the substitutions $a_i \leftarrow a_i-1$, $b_i \leftarrow b_i+1$, $c_i \leftarrow c_i$. These cases are given in detail in the following two lemmas.

Lemma 7.1.5 Let a, b, c be positive integers such that $c = b+1$. If $a \leq 2b$, then

$$\frac{1}{\binom{a+b}{a}} + \frac{1}{\binom{a+c}{a}} - \frac{1}{\binom{a+b+c}{a}} \geq \frac{1}{\binom{a+1+b}{a+1}} + \frac{1}{\binom{a+c}{a+1}} - \frac{1}{\binom{a+b+c}{a+1}}.$$

[proof] When $c = b+1$, the inequality of Lemma 7.1.5 is equivalent to $f(a, b, b+1) \geq f(a+1, b, b)$, which is true for all $a \leq 2b$ as follows:

$$\begin{aligned}
& f(a, b, b+1) - f(a+1, b, b) \\
&= \frac{1}{\binom{a+b}{a}} + \frac{1}{\binom{a+b+1}{a}} - \frac{1}{\binom{a+2b+1}{a}} - \frac{2}{\binom{a+1+b}{a+1}} + \frac{1}{\binom{a+2b+1}{a+1}} \\
&= \frac{a!b!}{(a+b)!} + \frac{a!(b+1)!}{(a+b+1)!} - \frac{a!(2b+1)!}{(a+2b+1)!} - 2 \frac{(a+1)!b!}{(a+b+1)!} + \frac{(a+1)!(2b)!}{(a+2b+1)!} \\
&= \frac{a!b!}{(a+2b+1)!} \left((a+2b+1)_{b+1} + (b+1)(a+2b+1)_b - (2b+1)_{b+1} - 2(a+1)(a+2b+1)_b + (a+1)(2b)_b \right) \\
&= \frac{a!b!}{(a+2b+1)!} \left((a+2b+1)_b ((a+b+1) + (b+1) - 2(a+1)) + (2b)_b ((a+1) - (2b+1)) \right) \\
&= \frac{a!b!}{(a+2b+1)!} (2b-a) \left((a+2b+1)_b - (2b)_b \right) \tag{7.1.6}
\end{aligned}$$

Since $a \leq 2b$, it is clear that the expression (7.1.6) is greater than or equal to zero, as claimed. ■

Lemma 7.1.6 Let a, b, c be positive integers such that $c = b + 1$. If $a > 2b$, then

$$\frac{1}{\binom{a+b}{a}} + \frac{1}{\binom{a+c}{a}} - \frac{1}{\binom{a+b+c}{a}} \geq \frac{1}{\binom{a+b}{a-1}} + \frac{1}{\binom{a-1+c}{a-1}} - \frac{1}{\binom{a+b+c}{a-1}}.$$

[proof] When $c = b + 1$, the inequality of Lemma 7.1.6 is equivalent to $f(a, b, b+1) \geq f(a-1, b+1, b+1)$, which is true for all $a > 2b$ as follows:

$$\begin{aligned}
& f(a, b, b+1) - f(a+1, b, b) \\
&= \frac{1}{\binom{a+b}{a}} + \frac{1}{\binom{a+b+1}{a}} - \frac{1}{\binom{a+2b+1}{a}} - \frac{2}{\binom{a+b}{a-1}} + \frac{1}{\binom{a+2b+1}{a-1}} \\
&= \frac{a!b!}{(a+b)!} + \frac{a!(b+1)!}{(a+b+1)!} - \frac{a!(2b+1)!}{(a+2b+1)!} - 2 \frac{(a-1)!(b+1)!}{(a+b)!} + \frac{(a-1)!(2b+2)!}{(a+2b+1)!} \\
&= \frac{(a-1)!b!}{(a+2b+1)!} \left(a(a+2b+1)_{b+1} - a(b+1)(a+2b+1)_b - a(2b+1)_{b+1} - 2(b+1)(a+2b+1)_{b+1} + (2b+2)_{b+2} \right)
\end{aligned}$$

$$= \frac{(a-1)!b!}{(a+2b+1)!} \left((a+2b+1)_b (a^2 - 2b^2 - 4b - 2) - (2b+1)_b (a(b+1) - 2b^2 - 4b - 2) \right) \quad (7.1.7)$$

Since $(a+2b+1)_b > (2b+1)_b$, in order to prove that the expression in (7.1.7) is greater than or equal to zero, it suffices to prove $a^2 - 2b^2 - 4b - 2 \geq a(b+1) - 2b^2 - 4b - 2$; equivalently, it suffices to prove $a^2 \geq a(b+1)$ which is true since $a > 2b \geq b+1$. ■

Corollary 7.1.7 Let n, a_i, b_i , and c_i be integers such that $a_i, b_i, c_i \geq 1$ and $a_i + b_i + c_i = n$. Then there exist integers a and b such that $a, b \geq 1$, $a + 2b = n$, and

$$f(a, b, b) \leq f(a_i, b_i, c_i).$$

[proof] If $b_i = c_i$, then $a = a_i$ and $b = b_i = c_i$ satisfy the claim.

If $b_i \neq c_i$, then by Lemma 7.1.4 there exist integers b and c such that $|b - c| \leq 1$ and $f(a_i, b, c) \leq f(a_i, b_i, c_i)$. If $b = c$, then we are done; otherwise, without loss of generality, we have $b = c + 1$. In this case, we may apply Lemma 7.1.5 or Lemma 7.1.6 to complete the proof. ■

7.1.2 Golden balance of central vertex with leaves

In this section, we first show that the minimum value of f is of the form $f(a, b, b)$, for some $a, b \geq 1$ with $a + 2b = n$, such that a is within the following range:

$$\frac{1}{2}(b - 3 + \sqrt{3b^2 - 4b + 1}) < a < \frac{1}{2}(2b + 3 + \sqrt{12b^2 + 20b + 9}). \quad (7.1.8)$$

Once we establish that the minimizing values of a and b satisfy (7.1.8), we then use balancing lemmas to show that, in fact, the minimum value for f has a within the following narrower range:

$$\frac{1}{2}(b - 3 + \sqrt{5b^2 - 2b - 1}) < a < \frac{1}{2}(b + 2 + \sqrt{5b^2 + 8b + 6}). \quad (7.1.9)$$

First, we give two lemmas to show that if a is not in the range (7.1.8), then the substitutions $a \leftarrow a - 2$, $b \leftarrow b + 1$, or $a \leftarrow a + 2$, $b \leftarrow b - 1$, respectively, can further reduce the value of f .

Lemma 7.1.8 If $a \leq \frac{1}{2}(b - 3 + \sqrt{3b^2 - 4b + 1})$, then

$$\frac{2}{\binom{a+b}{a}} - \frac{1}{\binom{a+2b}{a}} \geq \frac{2}{\binom{a+2+b-1}{a+2}} - \frac{1}{\binom{a+2+2(b-1)}{a+2}}.$$

[proof] The inequality in Lemma 7.1.8 is equivalent to $f(a, b, b) \geq f(a+2, b-1, b-1)$, which is true for all $a \leq \frac{1}{2}(b - 3 + \sqrt{3b^2 - 4b + 1})$ as follows:

$$\begin{aligned} & f(a, b, b) - f(a+2, b-1, b-1) \\ &= \frac{2}{\binom{a+b}{a}} - \frac{1}{\binom{a+2b}{a}} - \frac{2}{\binom{a+b+1}{a+2}} + \frac{1}{\binom{a+2b}{a+2}} \\ &= 2 \frac{a!b!}{(a+b)!} - \frac{a!(2b)!}{(a+2b)!} - 2 \frac{(a+2)!(b-1)!}{(a+b+1)!} + \frac{(a+2)!(2b-2)!}{(a+2b)!} \\ &= \frac{a!(b-1)!}{(a+b+1)!} \left(2b(a+b+1) - \frac{(2b)_{b+1}}{(a+2b)_{b-1}} - 2(a+2)(a+1) + \frac{(a+2)(a+1)(2b-2)_{b-1}}{(a+2b)_{b-1}} \right) \end{aligned} \quad (7.1.10)$$

The expression in (7.1.10) is nonnegative if and only if

$$2ab + 2b^2 + 2b - 2a^2 - 6a - 4 - \frac{(2b)_{b-1}}{(a+2b)_{b-1}}(b^2 + b) + \frac{(2b-2)_{b-1}}{(a+2b)_{b-1}}(a^2 + 3a + 2) \geq 0. \quad (7.1.11)$$

For the inequality in (7.1.11) to hold, it suffices to satisfy the weaker inequality

$$2ab + 2b^2 + 2b - 2a^2 - 6a - 4 - (b^2 + b) \geq 0, \quad (7.1.12)$$

where we have subtracted $(b^2 + b)$ rather than $\frac{(2b)_{b-1}}{(a+2b)_{b-1}}(b^2 + b)$, and we have not bothered to add the term $\frac{(2b-2)_{b-1}}{(a+2b)_{b-1}}(a^2 + 3a + 2)$.

The inequality in (7.1.12) holds if and only if

$$2a^2 - (2b - 6)a - b^2 - b + 4 \geq 0,$$

which is true for all a such that $0 \leq a \leq \frac{1}{2}(b - 3 + \sqrt{3b^2 - 4b + 1})$. ■

Lemma 7.1.9 If $a \geq \frac{1}{2}(2b + 3 + \sqrt{12b^2 + 20b + 9})$, then

$$\frac{2}{\binom{a+b}{a}} - \frac{1}{\binom{a+2b}{a}} \geq \frac{2}{\binom{a-2+b+1}{a-2}} - \frac{1}{\binom{a-2+2(b+1)}{a-2}}.$$

[proof] The inequality of Lemma 7.1.9 is equivalent to $f(a, b, b) \geq f(a-2, b+1, b+1)$, which is true for all $a \geq \frac{1}{2}(2b + 3 + \sqrt{12b^2 + 20b + 9})$ as follows:

$$\begin{aligned} & f(a, b, b) - f(a-2, b+1, b+1) \\ &= \frac{2}{\binom{a+b}{a}} - \frac{1}{\binom{a+2b}{a}} - \frac{2}{\binom{a+b-1}{a-2}} + \frac{1}{\binom{a+2b}{a-2}} \\ &= 2 \frac{a!b!}{(a+b)!} - \frac{a!(2b)!}{(a+2b)!} - 2 \frac{(a-2)!(b+1)!}{(a+b-1)!} + \frac{(a-2)!(2b+2)!}{(a+2b)!} \\ &= \frac{(a-2)!b!}{(a+b)!} \left(2a(a-1) - \frac{a(a-1)(2b)_b}{(a+2b)_b} - 2(b+1)(a+b) + \frac{(2b+2)_{b+2}}{(a+2b)_b} \right) \quad (7.1.13) \end{aligned}$$

The expression in (7.1.13) is nonnegative if and only if

$$2a(a-1) - 2(b+1)(a+b) - \frac{(2b)_b}{(a+2b)_b} \left((a)(a-1) - (2b+2)(2b+1) \right) \geq 0. \quad (7.1.14)$$

For the inequality in (7.1.14) to hold, it suffices to satisfy the weaker inequality

$$2a(a-1) - 2(b+1)(a+b) - (a)(a-1) \geq 0, \quad (7.1.15)$$

where we have subtracted $(a)(a-1)$ rather than $\frac{(2b)_b}{(a+2b)_b}(a)(a-1)$ and we have not bothered to add the term $\frac{(2b+2)_{b+2}}{(a+2b)_b}$.

The inequality in (7.1.15) holds if and only if

$$a^2 - (2b+3)a - 2b^2 - 2b \geq 0$$

which is true for all a such that $a \geq \frac{1}{2}(2b + 3 + \sqrt{12b^2 + 20b + 9})$. ■

Corollary 7.1.10 Let n , a_i , b_i , and c_i be integers such that $a_i, b_i, c_i \geq 1$ and $a_i + b_i + c_i = n$. Then there exist integers a and b such that $a, b \geq 1$, $a + 2b = n$,

$$\frac{1}{2}(b-3 + \sqrt{3b^2 - 4b + 1}) < a < \frac{1}{2}(2b + 3 + \sqrt{12b^2 + 20b + 9})$$

and $f(a, b, b) \leq f(a_i, b_i, c_i)$.

[proof] By Corollary 7.1.7, there exist values a and b such that $f(a, b, b) \leq f(a_i, b_i, c_i)$. If $a \leq \frac{1}{2}(b - 3 + \sqrt{3b^2 - 4b + 1})$, then we may apply Lemma 7.1.8. If $a \geq \frac{1}{2}(2b + 3 + \sqrt{12b^2 + 20b + 9})$, then we may instead apply Lemma 7.1.9. $\blacksquare$

Knowing that the bounds given in (7.1.8) hold for the minimizing values of a and b , we can go back to the proofs of Lemmas 7.1.8 and 7.1.9 and reconsider some of the simplifications we made.

Lemma 7.1.11 Let n be a fixed integer and let a and b be two positive integers such that $a + 2b = n$. If $a \leq \frac{1}{2}(b - 3 + \sqrt{5b^2 - 2b - 1})$, then $f(a, b, b) \geq f(a + 2, b - 1, b - 1)$.

[proof] By Corollary 7.1.10, we may assume

$$\frac{1}{2}(b - 3 + \sqrt{3b^2 - 4b + 1}) < a < \frac{1}{2}(2b + 3 + \sqrt{12b^2 + 20b + 9}). \quad (7.1.16)$$

Recall from the proof of Lemma 7.1.8 that $f(a, b, b) \geq f(a + 2, b - 1, b - 1)$ if and only if the inequality in (7.1.11) holds, that is,

$$2ab + 2b^2 + 2b - 2a^2 - 6a - 4 - \frac{(2b)_{b-1}}{(a+2b)_{b-1}}(b^2 + b) + \frac{(2b-2)_{b-1}}{(a+2b)_{b-1}}(a^2 + 3a + 2) \geq 0. \quad (7.1.17)$$

First, observe that

$$(2ab + 2b^2 + 2b - 2a^2 - 6a - 4) \geq 1 \quad (7.1.18)$$

if and only if $2a^2 - (2b - 6)a - 2b^2 - 2b + 5 \leq 0$, which is true for all a such that $0 \leq a \leq \frac{1}{2}(b - 3 + \sqrt{5b^2 - 2b - 1})$.

Rewrite (7.1.17) as

$$2ab + 2b^2 + 2b - 2a^2 - 6a - 4 - \frac{(2b-2)_{b-1}}{(a+2b)_{b-1}} \left((2b)(2b-1) - (a+2)(a+1) \right) \geq 0. \quad (7.1.19)$$

To prove (7.1.19) holds for all $a \leq \frac{1}{2}(b - 3 + \sqrt{5b^2 - 2b - 1})$, by (7.1.18), it suffices to determine a value n_0 such that, for all $n \geq n_0$ (with a and b constrained by (7.1.8)), we have

$$\left| \frac{(2b-2)_{b-1}}{(a+2b)_{b-1}} \left((2b)(2b-1) - (a+2)(a+1) \right) \right| < 1. \quad (7.1.20)$$

We now prove (7.1.20) holds for sufficiently large n .

First, if $(2b)(2b-1) - (a+2)(a+1) \geq 0$, then

$$\begin{aligned}
& |(2b)(2b-1) - (a+2)(a+1)| \\
&= (2b)(2b-1) - (a+2)(a+1) \\
&< (2b)(2b-1) - (b^2 - b + \frac{b}{2}\sqrt{3b^2 - 4b + 1}) \quad (\text{since } a > \frac{1}{2}(b-3 + \sqrt{3b^2 - 4b + 1})) \\
&< (2b)(2b-1) - \left(1 + \frac{\sqrt{3}}{2}\right)b^2 + \left(1 + \frac{\sqrt{3}}{2}\right)b \quad (\text{since } \sqrt{3b^2 - 4b + 1} > \sqrt{3}(b-1)) \\
&= \left(3 - \frac{\sqrt{3}}{2}\right)b^2 - \left(1 - \frac{\sqrt{3}}{2}\right)b
\end{aligned}$$

Second, if $(2b)(2b-1) - (a+2)(a+1) < 0$, then

$$\begin{aligned}
& |(2b)(2b-1) - (a+2)(a+1)| \\
&= (a+2)(a+1) - (2b)(2b-1) \\
&< 4b^2 + b\sqrt{12b^2 + 20b + 9} + 11b + 3\sqrt{12b^2 + 20b + 9} + 11 - (2b)(2b-1) \\
&\quad (\text{since } a < \frac{1}{2}(2b+3 + \sqrt{12b^2 + 20b + 9})) \\
&< (4 + 2\sqrt{3})b^2 + (8\sqrt{3} + 11)b + 6\sqrt{3} + 11 - (2b)(2b-1) \\
&\quad (\text{since } \sqrt{12b^2 + 20b + 9} < 2\sqrt{3}(b+1)) \\
&= 2\sqrt{3}b^2 + (8\sqrt{3} + 13)b + 6\sqrt{3} + 11
\end{aligned}$$

In both cases, we have

$$|(2b)(2b-1) - (a+2)(a+1)| < 2\sqrt{3}b^2 + (8\sqrt{3} + 13)b + 6\sqrt{3} + 11 \quad (7.1.21)$$

Next, observe that

$$\begin{aligned}
\frac{(2b-2)_{b-1}}{(a+2b)_{b-1}} &< \left(\frac{2b-2}{a+2b}\right)^{b-1} \quad (\text{since } \frac{2b-2}{a+2b} < 1) \\
&\leq \left(\frac{2b-2}{\frac{1}{2}(b-3 + \sqrt{3b^2 - 4b + 1}) + 2b}\right)^{b-1} \quad (\text{since } a > \frac{1}{2}(b-3 + \sqrt{3b^2 - 4b + 1})) \\
&= \left(\frac{4b-4}{5b + \sqrt{3b^2 - 4b + 1} - 3}\right)^{b-1} \\
&\leq \left(\frac{4(b-1)}{5b + \sqrt{3}(b-1) - 3}\right)^{b-1} \quad (\text{since } \sqrt{3b^2 - 4b + 1} > \sqrt{3}(b-1))
\end{aligned}$$

$$\begin{aligned}
&= \left(\frac{4(b-1)}{(5+\sqrt{3})b - (3+\sqrt{3})} \right)^{b-1} \\
&< \left(\frac{4(b-1)}{(5+\sqrt{3})b - (5+\sqrt{3})} \right)^{b-1} && \text{(since } 5+\sqrt{3} > 3+\sqrt{3}\text{)} \\
&= \left(\frac{4}{5+\sqrt{3}} \right)^{b-1}
\end{aligned} \tag{7.1.22}$$

From (7.1.21) and (7.1.22), we now have the following crude bound to help us prove (7.1.20):

$$\left| \frac{(2b-2)_{b-1}}{(a+2b)_{b-1}} [(2b)(2b-1) - (a+2)(a+1)] \right| < \left(\frac{4}{5+\sqrt{3}} \right)^{b-1} \left(2\sqrt{3}b^2 + (8\sqrt{3}+13)b + 6\sqrt{3}+11 \right) \tag{7.1.23}$$

As a continuous function of $b \in \mathbb{R}$, the derivative of

$$\left(\frac{4}{5+\sqrt{3}} \right)^{b-1} \left(2\sqrt{3}b^2 + (8\sqrt{3}+13)b + 6\sqrt{3}+11 \right) \tag{7.1.24}$$

is negative for all $b \geq 2$, and for $b = 15$, one can verify that the expression in (7.1.24) is less than 1.

Consequently, for all $b \geq 15$, the expression in (7.1.24) is less than 1. From (7.1.23), the inequality in (7.1.20) holds for all $b \geq 15$.

From (7.1.16), it follows that $a < b + \frac{3}{2} + \sqrt{3}(b+1)$. Thus,

$$b + \frac{3}{2} + \sqrt{3}(b+1) + 2b > a + 2b = n. \tag{7.1.25}$$

Solving for b in (7.1.25), we see that $n \geq 75$ suffices to guarantee that $b \geq 15$, hence, for all $n \geq 75$, the inequality in (7.1.20) holds.

At this point, we have shown that Lemma 7.1.11 holds for all $n \geq 75$. For $n < 75$, we can verify by computer that $f(a, b, b) \geq f(a+2, b-1, b-1)$ for all a and b such that $a, b \geq 1$, $a+2b = n$, and $a \leq \frac{1}{2}(b-3 + \sqrt{5b^2 - 2b - 1})$. ■

Lemma 7.1.12 Let n be a fixed integer and let a and b be two positive integers such that $a+2b = n$. If $a \geq \frac{1}{2}(b+2 + \sqrt{5b^2 + 8b + 6})$, then $f(a, b, b) \geq f(a-2, b+1, b+1)$.

[proof] By Corollary 7.1.10, we may assume

$$\frac{1}{2}(b-3 + \sqrt{3b^2 - 4b + 1}) < a < \frac{1}{2}(2b+3 + \sqrt{12b^2 + 20b + 9}). \tag{7.1.26}$$

Recall from the proof of Lemma 7.1.9 that $f(a, b, b) \geq f(a-2, b+1, b+1)$ if and only if the inequality in (7.1.14) holds, that is,

$$2a(a-1) - 2(b+1)(a+b) - \frac{(2b)_b}{(a+2b)_b} \left((a)(a-1) - (2b+2)(2b+1) \right) \geq 0. \quad (7.1.27)$$

First, observe that

$$2a(a-1) - 2(b+1)(a+b) \geq 1 \quad (7.1.28)$$

if and only if $2a^2 - (2b+4)a - 2b^2 - 2b - 1 \geq 0$, which is true for all a such that $a \geq \frac{1}{2}(b+2 + \sqrt{5b^2 + 8b + 6})$.

To prove the inequality in (7.1.27) holds for all $a \geq \frac{1}{2}(b+2 + \sqrt{5b^2 + 8b + 6})$, by (7.1.28), it suffices to determine a value n_0 such that, for all $n \geq n_0$ (with a and b constrained by (7.1.8)), we have

$$\left| \frac{(2b)_b}{(a+2b)_b} \left(a(a-1) - (2b+2)(2b+1) \right) \right| < 1. \quad (7.1.29)$$

We now prove (7.1.29) holds for sufficiently large n .

First, if $a(a-1) - (2b+2)(2b+1) \geq 0$, then

$$\begin{aligned} & |a(a-1) - (2b+2)(2b+1)| \\ &= a(a-1) - (2b+2)(2b+1) \\ &< 4b^2 + b\sqrt{12b^2 + 20b + 9} + 7b + \sqrt{12b^2 + 20b + 9} + 3 - (2b+2)(2b+1) \\ &\hspace{15em} (\text{since } a < \frac{1}{2}(2b+3 + \sqrt{12b^2 + 20b + 9})) \\ &< (4 + 2\sqrt{3})b^2 + (4\sqrt{3} + 7)b + 2\sqrt{3} + 3 - (2b+2)(2b+1) \\ &\hspace{15em} (\text{since } \sqrt{12b^2 + 20b + 9} < 2\sqrt{3}(b+1)) \\ &= 2\sqrt{3}b^2 + (4\sqrt{3} + 1)b + 2\sqrt{3} + 1 \end{aligned}$$

Second, if $a(a-1) - (2b+2)(2b+1) < 0$, then

$$\begin{aligned} & |a(a-1) - (2b+2)(2b+1)| \\ &= (2b+2)(2b+1) - a(a-1) \\ &< (2b+2)(2b+1) - \left(b^2 + \frac{b}{2}\sqrt{3b^2 - 4b + 1} - 3b - 2\sqrt{3b^2 - 4b + 1} + 4 \right) \\ &\hspace{15em} (\text{since } a > \frac{1}{2}(b-3 + \sqrt{3b^2 - 4b + 1})) \end{aligned}$$

$$\begin{aligned}
&< (2b+2)(2b+1) - \left(b^2 + \frac{\sqrt{3}}{2}b(b-1) - 3b - 2\sqrt{3}b + 4\right) \\
&\quad \text{(using } \sqrt{3}(b-1) < \sqrt{3b^2 - 4b + 1} < \sqrt{3}b) \\
&= \left(3 - \frac{\sqrt{3}}{2}\right)b^2 + \left(9 + \frac{5\sqrt{3}}{2}\right)b - 2
\end{aligned}$$

In both cases, we have

$$|a(a-1) - (2b+2)(2b+1)| < 2\sqrt{3}b^2 + (4\sqrt{3}+1)b + 2\sqrt{3} + 1. \quad (7.1.30)$$

Next, observe that

$$\begin{aligned}
\frac{(2b)_b}{(a+2b)_b} &< \left(\frac{2b}{a+2b}\right)^b && \text{(since } \frac{2b}{a+2b} < 1) \\
&< \left(\frac{4b}{5b-3+\sqrt{3b^2-4b+1}}\right)^b && \text{(since } a > \frac{1}{2}(b-3+\sqrt{3b^2-4b+1})) \\
&< \left(\frac{4b}{5b-3+\sqrt{3}(b-1)}\right)^b && \text{(since } \sqrt{3b^2-4b+1} > \sqrt{3}(b-1)) \\
&= \left(\frac{4b}{5b+\sqrt{3}b-(3+\sqrt{3})}\right)^b \\
&\leq \left(\frac{4b}{6.4b}\right)^b && \text{(for all } b \geq 15 \text{ since } b \geq 15 \text{ implies } \sqrt{3}b - (3+\sqrt{3}) \geq 1.4b) \\
&= \left(\frac{5}{8}\right)^b
\end{aligned} \quad (7.1.31)$$

From (7.1.30) and (7.1.31), we now have the following crude bound to help us prove (7.1.29) (for $b \geq 15$):

$$\left| \frac{(2b)_b}{(a+2b)_b} \left(a(a-1) - (2b+2)(2b+1) \right) \right| < \left(\frac{5}{8}\right)^b \left(2\sqrt{3}b^2 + (4\sqrt{3}+1)b + 2\sqrt{3} + 1 \right) \quad (7.1.32)$$

As a continuous function of $b \in \mathbb{R}$, the derivative of

$$\left(\frac{5}{8}\right)^b \left(2\sqrt{3}b^2 + (4\sqrt{3}+1)b + 2\sqrt{3} + 1 \right) \quad (7.1.33)$$

is negative for all $b \geq 4$, and for $b = 15$, one can verify that the expression in (7.1.33) is less than 1.

Consequently, for all $b \geq 15$, the expression in (7.1.33) is less than 1. From (7.1.32), the inequality in (7.1.29) holds for all $b \geq 15$.

Solving for b in (7.1.25), we see that $n \geq 75$ suffices to guarantee that $b \geq 15$, hence, for all $n \geq 75$, the inequality in (7.1.29) holds.

At this point, we have shown that Lemma 7.1.11 holds for all $n \geq 75$. For $n < 75$, we can verify by computer that $f(a, b, b) \geq f(a - 2, b + 1, b + 1)$ for all a and b such that $a, b \geq 1$, $a + 2b = n$, and $a \geq \frac{1}{2}(b + 2 + \sqrt{5b^2 + 8b + 6})$. ■

Corollary 7.1.13 Let n , a_i , b_i , and c_i be integers such that $a_i, b_i, c_i \geq 1$ and $a_i + b_i + c_i = n$. Then there exist integers a and b such that $f(a, b, b) \leq f(a_i, b_i, c_i)$, where $a, b \geq 1$, $a + 2b = n$, and

$$\frac{1}{2}(b - 3 + \sqrt{5b^2 - 2b - 1}) < a < \frac{1}{2}(b + 2 + \sqrt{5b^2 + 8b + 6})$$

[proof] By Corollary 7.1.10, there exist integers a and b such that $a, b \geq 1$, $a + 2b = n$, and $\frac{1}{2}(b - 3 + \sqrt{3b^2 - 4b + 1}) < a < \frac{1}{2}(2b + 3 + \sqrt{12b^2 + 20b + 9})$ and $f(a, b, b) \leq f(a_i, b_i, c_i)$. If $a \leq \frac{1}{2}(b - 3 + \sqrt{5b^2 - 2b - 1})$, then we may apply Lemma 7.1.11. If $a \geq \frac{1}{2}(b + 2 + \sqrt{5b^2 + 8b + 6})$, then we may instead apply Lemma 7.1.12. ■

7.1.3 The upper bound for S_3

Using our balancing lemmas, we now transform Corollary 7.1.2 into an actual upper bound on the number of packings in an S_3 -intersecting collection.

Let φ denote the *golden mean*, that is, $\varphi = (1 + \sqrt{5})/2$.

Theorem 7.1.14 If $\mathcal{P}$ is an S_3 -intersecting collection of 3-packings of $[n]$, then

$$|\mathcal{P}| \leq \frac{1}{2 - \delta} \binom{a + b}{a} \approx \frac{1}{2} \binom{a + b}{a}$$

where $a + 2b = n$, $\delta = (2b)_b / (a + 2b)_b$, and a is in the following interval of at most three integers with $a \equiv n \pmod{2}$:

$$\left\lceil \left(\frac{2}{5}\varphi - \frac{1}{5} \right) n - \left(\frac{2}{5}\varphi + \frac{4}{5} \right) \right\rceil \leq a \leq \left\lfloor \left(\frac{2}{5}\varphi - \frac{1}{5} \right) n + \left(\frac{3}{5}\varphi + \frac{1}{5} \right) \right\rfloor.$$

Moreover, $\lim_{n \rightarrow \infty} \delta = 0$, and $\lim_{n \rightarrow \infty} a/b = \varphi$.

[proof] By Corollary 7.1.13, there exist integers a and b such that

$$|\mathcal{P}|n!f(a, b, c) = |\mathcal{P}| \left[2 \frac{n!}{\binom{a+b}{a}} - \frac{n!}{\binom{a+2b}{a}} \right] \leq \beta(F^{S_3}, \mathcal{P}, n) \leq n! \quad (7.1.34)$$

where $a, b \geq 1$ with $a + 2b = n$, and

$$\frac{1}{2}(b - 3 + \sqrt{5b^2 - 2b - 1}) < a < \frac{1}{2}(b + 2 + \sqrt{5b^2 + 8b + 6}). \quad (7.1.35)$$

From (7.1.34), we get the following upper bound on $|\mathcal{P}|$:

$$|\mathcal{P}| \leq \left[\frac{2}{\binom{a+b}{a}} - \frac{1}{\binom{a+2b}{a}} \right]^{-1} = \frac{1}{2 - \delta} \binom{a+b}{a}$$

where $\delta = (2b)_b / (a + 2b)_b$.

As $n \rightarrow \infty$, the range in (7.1.35) implies $\lim_{n \rightarrow \infty} a/b = \varphi$.

Note that the following are valid for $b \geq 1$:

$$5(b - 1)^2 < 5b^2 - 2b - 1 \quad \text{and} \quad 5(b + 1)^2 > 5b^2 + 8b + 6. \quad (7.1.36)$$

Applying (7.1.36) to the bounds on a given by (7.1.35) and substituting $b = (n - a)/2$, we get the following range for a with respect to n :

$$\left(\frac{2}{5}\varphi - \frac{1}{5}\right)n - \left(\frac{2}{5}\varphi + \frac{4}{5}\right) < a < \left(\frac{2}{5}\varphi - \frac{1}{5}\right)n + \left(\frac{3}{5}\varphi + \frac{1}{5}\right). \quad (7.1.37)$$

This places a in an interval of width $\varphi + 1 \approx 2.6$. This means that a is determined to lie in a set of at most three possible values. Actually there are at most two values, since the parity of a is constrained to be the same as n . ■

For all n , our bound in (7.1.35) implies

$$\binom{\lceil \varphi b \rceil + b - 3}{b} < \binom{a + b}{b} < \binom{\lfloor \varphi b \rfloor + b + 3}{b}.$$

Stirling's approximation is $n! \sim \sqrt{2\pi n} \left(\frac{n}{e}\right)^n$, and, using this approximation gives

$$\frac{\binom{\lceil \varphi b \rceil + b + 3}{b}}{\binom{\lfloor \varphi b \rfloor + b - 3}{b}} = O(1).$$

We also have

$$\binom{\lceil \varphi b \rceil + b - 3}{b} < \binom{\lfloor \varphi b \rfloor + b}{b} < \binom{\lfloor \varphi b \rfloor + b + 3}{b}.$$

It follows that there is a constant K such that

$$\binom{a+b}{b} \sim K \binom{\lfloor \varphi b \rfloor + b}{b}. \quad (7.1.38)$$

We also have the following inequalities, which we will refer to in the subsequent expression.

1. $\left(\frac{\varphi b - 1 + b}{b}\right)^b \leq \left(\frac{\varphi b + b}{b}\right)^b \leq \left(\frac{\varphi b + b}{b}\right)^b$
2. $\left(\frac{\varphi b - 1 + b}{b}\right)^b \leq \left(\frac{\lfloor \varphi b \rfloor + b}{b}\right)^b \leq \left(\frac{\varphi b + b}{b}\right)^b$
3. $\left(\frac{\varphi b - 1 + b}{\varphi b}\right)^{\varphi b - 1} \leq \left(\frac{\varphi b + b}{\varphi b}\right)^{\varphi b} \leq \left(\frac{\varphi b + b}{\varphi b - 1}\right)^{\varphi b}$
4. $\left(\frac{\varphi b - 1 + b}{\varphi b}\right)^{\varphi b - 1} \leq \left(\frac{\lfloor \varphi b \rfloor + b}{\lfloor \varphi b \rfloor}\right)^{\lfloor \varphi b \rfloor} \leq \left(\frac{\varphi b + b}{\varphi b - 1}\right)^{\varphi b}$

In each of the above four cases, the limit of the ratio of the outermost terms is a constant. It follows that $\left(\frac{\lfloor \varphi b \rfloor + b}{b}\right)^b \sim K_1 \left(\frac{\varphi b + b}{b}\right)^b$ and $\left(\frac{\lfloor \varphi b \rfloor + b}{\lfloor \varphi b \rfloor}\right)^{\lfloor \varphi b \rfloor} \sim K_2 \left(\frac{\varphi b + b}{\varphi b}\right)^{\varphi b}$ for some constants K_1 and K_2 .

Using Stirling's approximation and $(\varphi + 2)b \sim n$, there are constants K , K^* , K^{**} , and K^{***} such that

$$\begin{aligned} \binom{a+b}{b} &\sim K \binom{\lfloor \varphi b \rfloor + b}{b} && \text{(by (7.1.38))} \\ &\sim K \sqrt{\frac{\lfloor \varphi b \rfloor + b}{2\pi \lfloor \varphi b \rfloor b}} \frac{(\lfloor \varphi b \rfloor + b)^{\lfloor \varphi b \rfloor + b}}{b^b \lfloor \varphi b \rfloor^{\lfloor \varphi b \rfloor}} && \text{(using Stirling's approximation)} \\ &\sim K \sqrt{\frac{\lfloor \varphi b \rfloor + b}{2\pi \lfloor \varphi b \rfloor b}} \left(\frac{\lfloor \varphi b \rfloor + b}{b}\right)^b \left(\frac{\lfloor \varphi b \rfloor + b}{\lfloor \varphi b \rfloor}\right)^{\lfloor \varphi b \rfloor} \\ &\sim K^* \sqrt{\frac{\lfloor \varphi b \rfloor + b}{2\pi \lfloor \varphi b \rfloor b}} \left(\frac{\varphi b + b}{b}\right)^b \left(\frac{\varphi b + b}{\varphi b}\right)^{\varphi b} \\ &\sim K^* \sqrt{\frac{\lfloor \varphi b \rfloor + b}{2\pi \lfloor \varphi b \rfloor b}} (\varphi + 1)^b \left(\frac{\varphi + 1}{\varphi}\right)^{\varphi b} \end{aligned}$$

$$\begin{aligned}
&\sim K^* \sqrt{\frac{\lfloor \varphi b \rfloor + b}{2\pi \lfloor \varphi b \rfloor b}} \varphi^{2b} \varphi^{\varphi b} && (\text{since } \varphi + 1 = \varphi^2) \\
&\sim K^{**} \sqrt{\frac{\varphi}{2\pi b}} \varphi^{2b + \varphi b} && (\text{since } \frac{\lfloor \varphi b \rfloor + b}{\lfloor \varphi b \rfloor b} \sim k \frac{\varphi + 1}{\varphi b}) \\
&\sim K^{***} \sqrt{\frac{3\varphi + 1}{2\pi n}} \varphi^n && (\text{since } n \sim (\varphi + 2)b)
\end{aligned}$$

Therefore, there is a constant K such that

$$\binom{a+b}{a} \sim K \left(\frac{\varphi^n}{\sqrt{n}} \right) \quad (7.1.39)$$

Using (7.1.39), our upper bound, given in Theorem 7.1.14, gives

$$m(n, S_3) = O \left(\frac{\varphi^n}{\sqrt{n}} \right).$$

In contrast, a related asymptotic result of Körner and Simonyi [35] is the following:

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log_2 m(n, S_3) = \log_2 \varphi. \quad (7.1.40)$$

For any subexponential function $f(n)$, we have

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log_2 (f(n) \varphi^n) = \log_2 \varphi.$$

Thus, knowing the limit in (7.1.40) does not imply $m(n, S_3) = O \left(\frac{\varphi^n}{\sqrt{n}} \right)$.

7.2 Constructions for S_3 -intersecting collections

For $n \geq 1$, let f_n denote the n th **Fibonacci number**, where $f_1 = 1$, $f_2 = 1$, and for $n \geq 3$, we have $f_n = f_{n-1} + f_{n-2}$.

In their proof of the limit in (7.1.40), Körner and Simonyi gave a construction of an S_3 -intersecting collection of 3-partitions of $[n]$ yielding the following lower bound on $m(n, S_3)$:

$$m(n, S_3) \geq \frac{f_{n+1}}{n^2(n+1)^2}. \quad (7.2.1)$$

Körner and Simonyi used the bound in (7.2.1) to prove

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log_2 m(n, S_3) \geq \log_2 \varphi. \quad (7.2.2)$$

Using the argument of Körner and Simonyi, the bound in (7.2.1) can be slightly refined to

$$m(n, S_3) \geq \frac{8}{n^3} (f_{n+1} - 1),$$

although, for their purposes, this additional precision is unnecessary since the logarithm in (7.2.2) makes any polynomial factor of $m(n, S_3)$ unimportant.

For the construction, Körner and Simonyi begin by taking all ternary n -tuples $\vec{x} = (x_1, \dots, x_n) \in [3]^n$ such that

$$x_1 \neq 3, x_n \neq 2, \text{ and, for each } i \in [n-1], \text{ we have } x_i = 2 \text{ if and only if } x_{i+1} = 3. \quad (\star)$$

These ternary n -tuples correspond bijectively to binary $(n-1)$ -tuples having no consecutive ones. It is well-known that the number of binary n -tuples with no consecutive ones is equal to the Fibonacci number f_{n+2} , a fact that can be verified using induction on n . Thus, Körner and Simonyi begin with f_{n+1} ternary n -tuples.

We discard the n -tuple $\vec{1} = (1, \dots, 1)$ since it cannot be an element of an S_3 -intersecting collection, hence we begin with $f_{n+1} - 1$ ternary n -tuples subject to $(\star)$. Denote by $\mathcal{C}$ this set of ternary n -tuples. For each $\vec{x} \in \mathcal{C}$, the **weight** of $\vec{x}$, denoted $w(\vec{x})$, is defined as the number of times the symbol 2 appears as an entry of $\vec{x}$. The weight $w(\vec{x})$ can take on any value between 1 and $\lfloor n/2 \rfloor$, since at most every second entry of $\vec{x} \in \mathcal{C}$ could be a 2. Thus, there is a subset $\mathcal{C}^* \subseteq \mathcal{C}$ such that all elements in $\mathcal{C}^*$ have the same weight and

$$|\mathcal{C}^*| \geq \frac{2}{n} |\mathcal{C}|.$$

For each $\vec{x} \in \mathcal{C}^*$, define the **index-weight** of $\vec{x}$, denoted $\lambda(\vec{x})$, to be the sum

$$\lambda(\vec{x}) = \sum_{\substack{i \in [n] \\ x_i = 2}} i.$$

The smallest possible index-weight of an n -tuple $\vec{x} \in \mathcal{C}^*$ is 1 and the largest possible index-weight is $n^2/4$ (which is achieved by the n -tuple where every second entry is a 2). We can thus find a subset $\mathcal{C}^{**} \subseteq \mathcal{C}^*$ such that every $\vec{x} \in \mathcal{C}^{**}$ has the same index-weight and

$$|\mathcal{C}^{**}| \geq \frac{4}{n^2} |\mathcal{C}^*| \geq \frac{8}{n^3} (f_{n+1} - 1).$$

In the following lemma, we summarize the properties of the construction given by Körner and Simonyi [35] (see the proof of Theorem 1 in [35]).

Lemma 7.2.1 Let $\mathcal{C} \subset [3]^n$ be a collection of ternary n -tuples such that, for each $\vec{x} \in \mathcal{C}$, we have $\vec{x} = (x_1, \dots, x_n)$. If

1. for all $\vec{x} \in \mathcal{C}$ we have $x_1 \neq 3$, $x_n \neq 2$,
2. for all $\vec{x} \in \mathcal{C}$ and for each $i \in [n-1]$, we have $x_i = 2$ if and only if $x_{i+1} = 3$,
3. $w(\vec{x})$ is the same weight for all $\vec{x} \in \mathcal{C}$, and
4. $\lambda(\vec{x})$ is the same index-weight for all $\vec{x} \in \mathcal{C}$,

then $\mathcal{C}$ is an S_3 -intersecting collection. ■

Here, we give a construction of an S_3 -intersecting collection of ternary n -tuples based on Lemma 7.2.1.

Corollary 7.2.2 Let n be a fixed integer. If a and b are positive integers such that $a + 2b = n$, then there exists an S_3 -intersecting collection $\mathcal{C}^*$ such that

$$|\mathcal{C}^*| \geq \binom{a+b}{a} (nb - 2b^2 + 1)^{-1}.$$

[proof] We give the construction in terms of 3-ary n -tuples. Let $\mathcal{C} \subset [2]^{a+b}$ be the set of all binary $(a+b)$ -tuples with weight b (note that we are using symbols from the alphabet $\{1, 2\}$). Clearly $|\mathcal{C}| = \binom{a+b}{b}$. For each $\vec{x} \in \mathcal{C}$, we blow up $\vec{x}$ into a 3-ary n -tuple $\vec{x}' \in [3]^n$ as follows. In each entry where $\vec{x}$ has the symbol 2, we replace this 2 by two entries in $\vec{x}'$, namely a 2 followed by a 3. Let $\mathcal{C}' \subset [3]^n$ denote this collection. For $\vec{x}' \in \mathcal{C}'$, the minimum possible index-weight is $\lambda(\vec{x}') = 1 + 3 + \dots + 2b - 1 = b^2$ and the maximum possible index-weight is $\lambda(\vec{x}') = n - 1 + n - 3 + \dots + n - (2b - 1) = nb - b^2$. In total, there are at most $nb - 2b^2 + 1$ possible index-weights of elements of $\mathcal{C}'$. Thus, there exists a subset $\mathcal{C}^* \subseteq \mathcal{C}'$ such that all n -tuples in $\mathcal{C}^*$ have the same index-weight, and

$$|\mathcal{C}^*| \geq (nb - 2b^2 + 1)^{-1} |\mathcal{C}'| = (nb - 2b^2 + 1)^{-1} \binom{a+b}{a}.$$

Clearly, $\mathcal{C}^*$ satisfies the conditions of Lemma 7.2.1, hence $\mathcal{C}^*$ is an S_3 -intersecting collection. ■

We now use a balancing lemma to prove that, for a fixed positive integer n , the binomial coefficient $\binom{a+b}{a}$ subject to $a + 2b = n$ is maximized when $a \approx n/\sqrt{5}$.

Lemma 7.2.3 Let n be a fixed positive integer and let a and b be positive integers such that $a + 2b = n$. The binomial coefficient

$$\binom{a+b}{a} = \binom{\frac{n+a}{2}}{\frac{n-a}{2}}$$

is maximized when the integer a is in the range

$$\left\lceil \frac{1}{5}(-7 + \sqrt{5n^2 + 10n + 9}) \right\rceil \leq a \leq \left\lfloor \frac{1}{5}(3 + \sqrt{5n^2 + 10n + 9}) \right\rfloor. \quad (\star)$$

For each n , either there is a unique value of a that maximizes $\binom{(n+a)/2}{(n-a)/2}$, or there are two values of a that both give the same maximum.

Moreover, $\lim_{n \rightarrow \infty} n/a = \sqrt{5}$ and $\lim_{n \rightarrow \infty} a/b = \varphi$.

[proof] Since $a + 2b = n$ and n is fixed, the integer a must always have the same parity as n . Start with any such a where $1 \leq a \leq n$. If $a \leq \frac{1}{5}(-7 + \sqrt{5n^2 + 10n + 9})$, then we show that the promotion $a \leftarrow a + 2$ can only increase $\binom{(n+a)/2}{(n-a)/2}$. To see this is true, observe that

$$\binom{\frac{n+a+2}{2}}{\frac{n-a-2}{2}} - \binom{\frac{n+a}{2}}{\frac{n-a}{2}} \geq 0 \text{ if and only if } \binom{\frac{n+a}{2}}{\frac{n-a}{2}} \left[\frac{\binom{\frac{n+a+2}{2}}{\frac{n-a}{2}}}{(a+2)(a+1)} - 1 \right] \geq 0.$$

This is true if and only if $5a^2 + 14a - n^2 - 2n + 8 \leq 0$, which, in turn, is true for all a such that $0 \leq a \leq \frac{1}{5}(-7 + \sqrt{5n^2 + 10n + 9})$.

Note that $a = \frac{1}{5}(-7 + \sqrt{5n^2 + 10n + 9})$ implies $\binom{\frac{n+a+2}{2}}{\frac{n-a-2}{2}} = \binom{\frac{n+a}{2}}{\frac{n-a}{2}}$.

Similarly, if $a \geq \frac{1}{5}(3 + \sqrt{5n^2 + 10n + 9})$, then the demotion $a \leftarrow a - 2$ can only increase $\binom{(n+a)/2}{(n-a)/2}$. We have

$$\binom{\frac{n+a-2}{2}}{\frac{n-a+2}{2}} - \binom{\frac{n+a}{2}}{\frac{n-a}{2}} \geq 0 \text{ if and only if } \binom{\frac{n+a}{2}}{\frac{n-a}{2}} \left[\frac{(a)(a-1)}{\binom{\frac{n+a}{2}}{\frac{n-a+2}{2}}} - 1 \right] \geq 0.$$

This is true if and only if $5a^2 - 6a - n^2 - 2n \geq 0$, which, in turn, is true for all a such that $a \geq \frac{1}{5}(3 + \sqrt{5n^2 + 10n + 9})$.

Note that $a = \frac{1}{5}(3 + \sqrt{5n^2 + 10n + 9})$ implies $\binom{\frac{n+a-2}{2}}{\frac{n-a+2}{2}} = \binom{\frac{n+a}{2}}{\frac{n-a}{2}}$.

Thus, the value of a that maximizes $\binom{(n+a)/2}{(n-a)/2}$ satisfies

$$\frac{1}{5}(-7 + \sqrt{5n^2 + 10n + 9}) \leq a \leq \frac{1}{5}(3 + \sqrt{5n^2 + 10n + 9}). \quad (7.2.3)$$

If $\frac{1}{5}(-7 + \sqrt{5n^2 + 10n + 9})$ is not an integer, then neither is $\frac{1}{5}(3 + \sqrt{5n^2 + 10n + 9})$, and conversely. For such values of n , there is a unique integer a that satisfies (7.2.3) and has the same parity as n .

If (as is the case when $n = 20$) $\frac{1}{5}(-7 + \sqrt{5n^2 + 10n + 9})$ is an integer, then so is $\frac{1}{5}(3 + \sqrt{5n^2 + 10n + 9})$, and conversely. If these integers have the same parity as n , then we have two maximizing values of a , and, by our notes above, both these options for a give the same maximum.

From (7.2.3) it follows that $\lim_{n \rightarrow \infty} \frac{a}{n} = \frac{1}{\sqrt{5}}$. Since $a + 2b = n$, it also follows that $\lim_{n \rightarrow \infty} \frac{a}{b} = \varphi$. ■

Applying the maximizing values of a and b given by Lemma 7.2.3, we get the best possible $\binom{a+b}{b}$ for the construction of Corollary 7.2.2. Using $b \sim n/(\varphi + 2)$, we have $(nb - b^2 + 1)^{-1} \sim \frac{5}{n^2 + 5}$. Similar to (7.1.39), the maximizing values of a and b given by Lemma 7.2.3 satisfy $\binom{a+b}{a} \sim K(\varphi^n/\sqrt{n})$, for some constant K . Thus, our lower bound given in Corollary 7.2.2 behaves asymptotically as

$$(nb - b^2 + 1)^{-1} \binom{a+b}{a} \sim K \frac{\varphi^n}{n^{5/2}}.$$

Since, for all $n \geq 0$, we have $5(n+1)^2 < 5n^2 + 10n + 9 < 5(n+2)^2$, the range for a given in Lemma 7.2.3 can be simplified to

$$\frac{2\sqrt{5}-7}{5} + \frac{n-1}{\sqrt{5}} = -\frac{7}{5} + \frac{n+1}{\sqrt{5}} < a < \frac{3}{5} + \frac{n+2}{\sqrt{5}} = \frac{n-1}{\sqrt{5}} + \frac{6}{5}\varphi. \quad (7.2.4)$$

Compare the range for a given in (7.2.4) to the range for a given in (7.1.37). The latter can be rewritten as

$$\left\lfloor \frac{n-1}{\sqrt{5}} \right\rfloor \leq a \leq \left\lfloor \frac{n-1}{\sqrt{5}} + \varphi \right\rfloor,$$

but the values of a and b must also satisfy the range given in Corollary 7.1.13. It is interesting to remark the similarity in these ranges.

In Table 7.1, we give the values of a and b subject to the range for a given in (7.1.37) and (7.2.4) — for the values of n given in the table, the values of a and b coincide

n	a	b	$\binom{a+b}{b}$	δ	L.B.	$m(n, S_3)$	U.B.
3	1	1	2	$\frac{2}{3}$	1	1	1
4	2	1	3	$\frac{1}{2}$	1	2	2
5	3	1	4	$\frac{2}{5}$	1	2	2
6	2	2	6	$\frac{2}{5}$	1	3	3
7	3	2	10	$\frac{2}{7}$	1	4	5
8	4	2	15	$\frac{3}{14}$	2	6	8
9	5	2	21	$\frac{1}{6}$	2	9	11
10	4	3	35	$\frac{1}{6}$	2		19
11	5	3	56	$\frac{4}{33}$	3		29
12	6	3	84	$\frac{1}{11}$	3		44
13	5	4	126	$\frac{14}{143}$	4		66
14	6	4	210	$\frac{10}{143}$	6		108
15	7	4	330	$\frac{8}{39}$	8		169
16	8	4	495	$\frac{1}{26}$	11		252
17	7	5	792	$\frac{9}{221}$	13		404
18	8	5	1287	$\frac{1}{34}$	20		653
19	9	5	2002	$\frac{7}{323}$	29		1011
20	8	6	3003	$\frac{77}{3230}$	36		1519
20	10	5	3003	$\frac{21}{1292}$	40		1513

Table 7.1: Data for $m(n, S_3)$

for Theorem 7.1.14 and Lemma 7.2.3. For $n = 20$, there are two options; in this case, $(-7 + \sqrt{5n^2 + 10n + 9})/5$ is an even integer and so is $(3 + \sqrt{5n^2 + 10n + 9})/5$, and both these options for a give the same maximum value for $\binom{a+b}{a}$.

In Table 7.1, we also summarize the bounds for $m(n, S_3)$ for $3 \leq n \leq 20$. For each n , we give $\binom{a+b}{b}$ and $\delta = (2b)_b/(n)_b$. The lower bound L.B. denotes $\binom{a+b}{a}(nb - 2b^2 - 1)^{-1}$, and the upper bound U.B. denotes $(2 - \delta)^{-1}\binom{a+b}{a}$. For $3 \leq n \leq 9$, we have exact values for $m(n, S_3)$. These initial values of $m(n, S_3)$ appear to match the Fibonacci-based sequence $f_{n-3} + 1$; however, since $f_n \sim \varphi^n/\sqrt{5}$, our upper bound given in Theorem 7.1.14 indicates that this cannot be expected as n grows, and $f_{n-3} + 1$ is too large starting from $n = 20$.

7.3 The Alphabet graph K_3^{loop}

Complete graphs with loops are strong graphs, and they are of special interest since K_v^{loop} -intersecting collections correspond to qualitatively independent collections. Thus, $m(n, K_v^{\text{loop}}) = m(n, v) = \text{CAK}(n; 2, v)$. In this section, we give the generalized LYM inequality of Theorem 6.4.9 for K_3^{loop} , and derive an upper bound for $m(n, K_3^{\text{loop}})$.

Corollary 7.3.1 Let $\mathcal{P} = \{P_1, \dots, P_m\}$ be a collection of 3-packings of $[n]$ where $P_i = (P_i^1, P_i^2, P_i^3)$ for each i . If $\mathcal{P}$ is a K_3^{loop} -intersecting collection, then

$$\sum_{i=1}^m \frac{1}{\binom{a_i + b_i}{a_i}} + \frac{1}{\binom{b_i + c_i}{b_i}} + \frac{1}{\binom{a_i + c_i}{c_i}} - \frac{1}{\binom{a_i + b_i + c_i}{a_i}} - \frac{1}{\binom{a_i + b_i + c_i}{b_i}} - \frac{1}{\binom{a_i + b_i + c_i}{c_i}} \leq \frac{1}{2}$$

where $a_i = |P_i^1|$, $b_i = |P_i^2|$, and $c_i = |P_i^3|$ for each $i = 1, \dots, m$.

[proof] Let $F = F^{K_3^{\text{loop}}}$ and let $\mathcal{T}$ denote the set of all nonempty subsets T of $E(F)$ such that T contains no directed walk of length 2. By Theorem 6.4.9, we have

$$\beta(F, \mathcal{P}, n) = \sum_{i=1}^m \sum_{T \in \mathcal{T}} (-1)^{|T|+1} \left| \bigcap_{ab \in T} X_i(a, b) \right| \leq n! \quad \left(\text{where } F = \begin{array}{c} \textcircled{1} \\ \curvearrowright \quad \curvearrowleft \\ \textcircled{3} \quad \textcircled{2} \end{array} \right).$$

There are only two types of subsets T in $\mathcal{T}$: those with one arc, and those with two arcs incident with a common vertex (either both in-neighbours or both out-neighbours).

To illustrate how the subsets in $\mathcal{T}$ contribute to $\beta(F, \mathcal{P}, n)$, we count one term of each type: The term $|X_i(1, 2)|$ corresponds to the arc $(1, 2) \in E(F)$ and we have

$$|X_i(1, 2)| = n! \binom{a_i + b_i}{a_i}^{-1}.$$

The term $|X_i(1, 2) \cap X_i(1, 3)|$ corresponds to the two arcs $(1, 2), (1, 3) \in E(F)$ and we have

$$|X_i(1, 2) \cap X_i(1, 3)| = n! \binom{a_i + b_i + c_i}{a_i}^{-1}.$$

The other ten terms of T are counted similarly. Since every subset $T \in \mathcal{T}$ can be paired with its reversal, the formula for $\beta(F, \mathcal{P}, n)$ has two sets of six terms repeated. Dividing both sides of the inequality $\beta(F, \mathcal{P}, n) \leq n!$ by $2n!$ gives rise to the factor of $1/2$ on the right side of the inequality given in Corollary 7.3.1 ■

The formula for our inequality for K_3^{loop} -intersecting collections is slightly more complicated than the formula for the star S_3 given in Corollary 7.1.2; however, with appropriate balancing lemmas, we transform it into an upper bound on $m(n, K_3^{\text{loop}})$.

Analogous to the function $f(a, b, c)$ defined in (7.1.2) for S_3 , for $a, b, c \in \mathbb{N}$, redefine f for K_3^{loop} as follows.

$$f(a, b, c) = \frac{1}{\binom{a+b}{a}} + \frac{1}{\binom{b+c}{b}} + \frac{1}{\binom{a+c}{c}} - \frac{1}{\binom{a+b+c}{a}} - \frac{1}{\binom{a+b+c}{b}} - \frac{1}{\binom{a+b+c}{c}}. \quad (7.3.1)$$

Throughout Section 7.3, f will denote the function defined in (7.3.1).

In terms of the function f , defined in (7.3.1), the inequality in Corollary 7.3.1 is equivalent to the following inequality:

$$\beta(F^{K_3^{\text{loop}}}, \mathcal{P}, n) = \sum_{i=1}^{|\mathcal{P}|} 2n! f(a_i, b_i, c_i) \leq n! \quad (7.3.2)$$

For $n \geq 3$, define

$$\bar{f}(n) = \begin{cases} f(n/3, n/3, n/3), & \text{if } n \equiv 0 \pmod{3}; \\ f(\lceil n/3 \rceil, \lfloor n/3 \rfloor, \lfloor n/3 \rfloor), & \text{if } n \equiv 1 \pmod{3}; \\ f(\lceil n/3 \rceil, \lceil n/3 \rceil, \lfloor n/3 \rfloor), & \text{if } n \equiv 2 \pmod{3}. \end{cases}$$

In order to transform Corollary 7.3.1 into an upper bound on $m(n, K_3^{\text{loop}})$ we will prove that

$$\bar{f}(n) \leq f(a_i, b_i, c_i) \quad (7.3.3)$$

for all integers a_i, b_i, c_i such that $a_i, b_i, c_i \geq 1$ and $a_i + b_i + c_i = n$. Once we establish (7.3.3), we will obtain the following lower bound, based on (7.3.2):

$$|\mathcal{P}| 2n! \bar{f}(n) \leq \sum_{i=1}^{|\mathcal{P}|} 2n! f(a_i, b_i, c_i) = \beta(F^{K_3^{\text{loop}}}, \mathcal{P}, n) \leq n! \quad (7.3.4)$$

From (7.3.4), we will obtain the following upper bound which is given explicitly in Theorem 7.3.20:

$$m(n, K_3^{\text{loop}}) \leq \frac{1}{2\bar{f}(n)}$$

Since f is invariant under permutations of a, b, c , we may assume throughout that $a \geq b \geq c$.

The goal of this section is to prove $\bar{f}(n) \leq f(a, b, c)$ for all integers a, b, c such that $a \geq b \geq c \geq 1$ and $a + b + c = n$. We use a combination of balancing lemmas and case-analysis to achieve our goal. Many of these results involve lengthy calculations. The remainder of this section is organized as follows:

- In Section 7.3.1, we give a lemma that shows that the two smallest values among a, b , and c , cannot be too far apart.
- In Section 7.3.2, we show that having one of a, b , and c large enough implies $\bar{f}(n) \leq f(a, b, c)$.
- In Section 7.3.3, we show that having b and c small enough implies $\bar{f}(n) \leq f(a, b, c)$.
- In Section 7.3.4, we show that averaging the two most extreme values a and c helps to reduce f when $a > b \geq \frac{1}{2}(a + c)$.
- In Section 7.3.5, we show that $\bar{f}(n) \leq f(a, b, c)$ when b is equal to $\lfloor n/3 \rfloor$.
- In Section 7.3.6, we show that $\bar{f}(n) \leq f(a, b, c)$ when a equals b and both are greater than $\lfloor n/3 \rfloor$.
- In Section 7.3.7, we show that $\bar{f}(n) \leq f(a, b, c)$ for several special cases of values a, b , and c .
- In Section 7.3.8, we assemble the results of the preceding sections in order to achieve our goal: $\bar{f}(n) \leq f(a, b, c)$ for all $a, b, c \geq 1$ such that $a + b + c = n$. In Theorem 7.3.20, we give the resulting upper bound on $m(n, K_3^{\text{loop}})$.

Remark 7.3.2 Often, certain steps in the proofs of our balancing lemmas apply only when n is sufficiently large (the specific thresholds are given in detail in the proofs). In all such cases, we have verified by computer for all small values of n below the particular threshold that $\bar{f}(n) \leq f(a, b, c)$ for all $a \geq b \geq c \geq 1$ such that $a + b + c = n$.

7.3.1 Balancing smallest values

Lemma 7.3.3 Let n, a, b , and c be integers such that $a \geq b \geq c \geq 1$ and $a + b + c = n$. If $a \geq b > c$ and $b \geq 3(c + 1)/2$, then $f(a, b, c) \geq f(a, b - 1, c + 1)$.

[proof] Assuming $b \geq 3(c+1)/2$, it follows that $b \geq c+2$. We have

$$\begin{aligned}
& f(a, b, c) - f(a, b-1, c+1) \\
&= \frac{1}{\binom{a+b}{a}} + \frac{1}{\binom{b+c}{b}} + \frac{1}{\binom{a+c}{c}} - \frac{1}{\binom{a+b+c}{a}} - \frac{1}{\binom{a+b+c}{b}} - \frac{1}{\binom{a+b+c}{c}} \\
&\quad - \left[\frac{1}{\binom{a+b-1}{a}} + \frac{1}{\binom{b+c}{b-1}} + \frac{1}{\binom{a+c+1}{c+1}} - \frac{1}{\binom{a+b+c}{a}} - \frac{1}{\binom{a+b+c}{b-1}} - \frac{1}{\binom{a+b+c}{c+1}} \right] \\
&= -\frac{a}{b} \binom{a+b}{b}^{-1} + \frac{b-c-1}{b} \binom{b+c}{b}^{-1} + \frac{a}{a+c+1} \binom{a+c}{c}^{-1} + \frac{a+c+1-b}{b} \binom{a+b+c}{b}^{-1} - \frac{a+b-c-1}{a+b} \binom{a+b+c}{c}^{-1} \\
&\geq \left[\frac{a}{a+c+1} \binom{a+c}{c}^{-1} - \frac{a+b-c-1}{a+b} \binom{a+b+c}{c}^{-1} \right] + \left[\frac{b-c-1}{b} \binom{b+c}{b}^{-1} - \frac{a}{b} \binom{a+b}{b}^{-1} \right]. \tag{7.3.5}
\end{aligned}$$

We now prove that the expression in (7.3.5) is nonnegative:

Notice that

$$\frac{a}{a+c+1} \binom{a+c}{c}^{-1} \geq \frac{a+b-c-1}{a+b} \binom{a+b+c}{c}^{-1} \tag{7.3.6}$$

if and only if

$$\frac{a}{(a+1)} \frac{(a+b+c)_c}{(a+c+1)_c} \frac{(a+b)}{(a+b-c-1)} \geq 1.$$

Since $\frac{a+b+c}{a+c+1} > 1$ and $b \geq c+2 \geq 3$, we have $\frac{a+b}{a+b-c-1} \geq \frac{a+3}{a+1} \geq \frac{a+1}{a}$, which suffices to prove that the inequality in (7.3.6) holds.

Next, notice that

$$\frac{b-c-1}{b} \binom{b+c}{b}^{-1} \geq \frac{a}{b} \binom{a+b}{b}^{-1} \tag{7.3.7}$$

if and only if

$$\frac{(b-c-1)(a+b)_b}{a(b+c)_b} = \frac{(a+1)}{a} \frac{(b-c-1)}{(c+1)} \frac{(a+b)}{(c+2)} \frac{(a+b-1)_{b-2}}{(b+c)_{b-2}} \geq 1.$$

Since $a+b \geq 2(c+2)$ and $b \geq 3(c+1)/2$, we have $\frac{(a+b)}{(c+2)} \frac{(b-c-1)}{(c+1)} \geq 2 \left(\frac{1}{2}\right)$, which suffices to prove that the inequality in (7.3.7) holds.

Therefore, the expression in (7.3.5) is nonnegative and $f(a, b, c) \geq f(a, b-1, c+1)$, as claimed. $\blacksquare$

In summary, if the two smallest values are too far apart, as in $b \geq 3(c+1)/2$, then we can apply the substitutions $b \leftarrow b-1$ and $c \leftarrow c+1$ until $b < 3(c+1)/2$; by Lemma 7.3.3, these substitutions can only help us to reduce the value of f .

7.3.2 One very large value

Lemma 7.3.4 Let n, a, b , and c be integers such that $a \geq b \geq c \geq 1$ and $a+b+c = n$. If $a > \lceil 2n/3 \rceil$, then $\bar{f}(n) \leq f(a, b, c)$.

[proof] Since $a > \lceil 2n/3 \rceil$ and $a+b+c = n$, it follows that $b+c \leq \lfloor n/3 \rfloor$. We assume $b \geq c$. Regardless of the value of $n \pmod 3$, we have

$$\begin{aligned}
 f(a, b, c) - \bar{f}(n) &\geq \binom{a+b}{a}^{-1} + \binom{a+c}{c}^{-1} + \binom{b+c}{c}^{-1} - \binom{n}{a}^{-1} - \binom{n}{b}^{-1} - \binom{n}{c}^{-1} - 3 \binom{2\lfloor \frac{n}{3} \rfloor}{\lfloor \frac{n}{3} \rfloor}^{-1} + 3 \binom{n}{\lceil \frac{n}{3} \rceil}^{-1} \\
 &\geq \left[\binom{b+c}{c}^{-1} - \binom{n}{a}^{-1} - 3 \binom{2\lfloor \frac{n}{3} \rfloor}{\lfloor \frac{n}{3} \rfloor}^{-1} \right] + \left[\binom{a+b}{a}^{-1} - \binom{n}{b}^{-1} \right] + \left[\binom{a+c}{c}^{-1} - \binom{n}{c}^{-1} \right].
 \end{aligned} \tag{7.3.8}$$

We now prove that the expression in (7.3.8) is nonnegative.

By Lemma 7.3.3, we may assume that $c > \frac{2}{3}b - 1$. Observe that

$$\begin{aligned}
 \binom{n}{a}^{-1} &= \frac{(a)_{a-b}(b+c)_b}{(a+b+c)_{a-b}(2b+c)_b} \binom{b+c}{b}^{-1} \\
 &\leq \left(\frac{b+c}{2b+c} \right)^b \binom{b+c}{b}^{-1} && \text{(by Lemma 7.1.3)} \\
 &< \left(\frac{b+c}{2b+\frac{2}{3}b-1} \right)^b \binom{b+c}{b}^{-1} && \text{(since } c > \frac{2}{3}b - 1) \\
 &\leq \left(\frac{2b}{\frac{8}{3}b-1} \right)^b \binom{b+c}{b}^{-1} && \text{(since } c \leq b) \\
 &= \left(\frac{6b}{8b-3} \right)^b \binom{b+c}{b}^{-1}
 \end{aligned}$$

$$\begin{aligned}
&\leq \left(\frac{6b}{7b}\right)^3 \binom{b+c}{b}^{-1} && (\text{for all } b \geq 3) \\
&< \frac{2}{3} \binom{b+c}{b}^{-1}.
\end{aligned}$$

Next, observe that

$$\begin{aligned}
3 \binom{2\lfloor n/3 \rfloor}{\lfloor n/3 \rfloor}^{-1} &= 3 \frac{\binom{\lfloor n/3 \rfloor}{\lfloor \lfloor n/3 \rfloor / 2 \rfloor} \binom{\lfloor n/3 \rfloor}{\lceil \lfloor n/3 \rfloor / 2 \rceil}}{\binom{2\lfloor n/3 \rfloor}{\lfloor \lfloor n/3 \rfloor / 2 \rfloor} \binom{\lceil 3\lfloor n/3 \rfloor / 2 \rceil}{\lceil \lfloor n/3 \rfloor / 2 \rceil}} \binom{\lfloor n/3 \rfloor}{\lfloor \lfloor n/3 \rfloor / 2 \rfloor}^{-1} \\
&\leq 3 \left(\frac{1}{2}\right)^{\lfloor \lfloor n/3 \rfloor / 2 \rfloor} \left(\frac{2}{3}\right)^{\lceil \lfloor n/3 \rfloor / 2 \rceil} \binom{\lfloor n/3 \rfloor}{\lfloor \lfloor n/3 \rfloor / 2 \rfloor}^{-1} && (\text{by Lemma 7.1.3}) \\
&\leq 3 \left(\frac{1}{3}\right)^2 \binom{\lfloor n/3 \rfloor}{\lfloor \lfloor n/3 \rfloor / 2 \rfloor}^{-1} && (\text{for all } n \geq 12) \\
&\leq \frac{1}{3} \binom{b+c}{b}^{-1}. && (\text{since } a > \lceil 2n/3 \rceil \text{ implies } b+c \leq \lfloor n/3 \rfloor)
\end{aligned}$$

Thus, for all $n \geq 12$ with $b \geq 3$, we have shown

$$\binom{b+c}{b}^{-1} - 3 \binom{2\lfloor \frac{n}{3} \rfloor}{\lfloor \frac{n}{3} \rfloor}^{-1} - \binom{n}{a}^{-1} \geq 0.$$

Clearly, $\binom{a+b}{a}^{-1} \geq \binom{n}{b}^{-1}$ and $\binom{a+c}{a}^{-1} \geq \binom{n}{c}^{-1}$. These inequalities suffice to prove that the expression in (7.3.8) is nonnegative for all $n \geq 12$ with $b \geq 3$.

The expression in (7.3.8) is nonnegative for the special cases when $b = c = 2$, or $b = 2, c = 1$, or $b = c = 1$, as follows:

- If $b = c = 2$, then $\binom{b+c}{b}^{-1} = \binom{4}{2}^{-1} \geq 3 \binom{2\lfloor n/3 \rfloor}{\lfloor n/3 \rfloor}^{-1} + \binom{n}{n-4}^{-1}$ for all $n \geq 12$.
- If $b = 2$ and $c = 1$, then $\binom{b+c}{b}^{-1} = \binom{3}{2}^{-1} \geq 3 \binom{2\lfloor n/3 \rfloor}{\lfloor n/3 \rfloor}^{-1} + \binom{n}{n-3}^{-1}$ for all $n \geq 12$.
- If $b = c = 1$, then $\binom{b+c}{b}^{-1} = \binom{2}{1}^{-1} \geq 3 \binom{2\lfloor n/3 \rfloor}{\lfloor n/3 \rfloor}^{-1} + \binom{n}{n-2}^{-1}$ for all $n \geq 12$.

Finally, for all n such that $3 \leq n < 12$, we can verify by computer that this lemma is true. ■

In summary, if we have one very large value, say $a > \lceil 2n/3 \rceil$, then by Lemma 7.3.4 it follows that $\bar{f}(n) \leq f(a, b, c)$.

7.3.3 Two small values

Lemma 7.3.5 Let n, a, b , and c be integers such that $a \geq b \geq c \geq 1$ and $a+b+c = n$. If $c \leq b < \lfloor n/3 \rfloor$, then $\bar{f}(n) \leq f(a, b, c)$.

[proof] By Lemma 7.3.4, if $a > \lceil 2n/3 \rceil$, then $\bar{f}(n) \leq f(a, b, c)$. We may thus assume $a \leq \lceil 2n/3 \rceil$.

Regardless of the value of $n \pmod 3$, we have

$$\begin{aligned}
 & f(a, b, c) - \bar{f}(n) \\
 & \geq \binom{a+b}{a}^{-1} + \binom{a+c}{c}^{-1} + \binom{b+c}{c}^{-1} - \binom{n}{a}^{-1} - \binom{n}{b}^{-1} - \binom{n}{c}^{-1} - 3 \binom{2\lfloor \frac{n}{3} \rfloor}{\lfloor \frac{n}{3} \rfloor}^{-1} + 3 \binom{n}{\lceil \frac{n}{3} \rceil}^{-1} \\
 & = \left[\binom{b+c}{c}^{-1} - 3 \binom{2\lfloor \frac{n}{3} \rfloor}{\lfloor \frac{n}{3} \rfloor}^{-1} \right] + \left[3 \binom{n}{\lceil \frac{n}{3} \rceil}^{-1} - \binom{n}{a}^{-1} \right] + \left[\binom{a+b}{a}^{-1} - \binom{n}{b}^{-1} \right] + \left[\binom{a+c}{c}^{-1} - \binom{n}{c}^{-1} \right] \\
 & \tag{7.3.9}
 \end{aligned}$$

We now prove that the expression in (7.3.9) is nonnegative.

Since $c \leq b < \lfloor \frac{n}{3} \rfloor$, we have

$$\begin{aligned}
 \binom{b+c}{b}^{-1} &= \frac{(2\lfloor \frac{n}{3} \rfloor)(2\lfloor \frac{n}{3} \rfloor - 1)}{(\lfloor \frac{n}{3} \rfloor)(\lfloor \frac{n}{3} \rfloor)} \frac{(2\lfloor \frac{n}{3} \rfloor - 2)_{2\lfloor \frac{n}{3} \rfloor - 2 - (b+c)}}{(\lfloor \frac{n}{3} \rfloor - 1)_{\lfloor \frac{n}{3} \rfloor - 1 - b} (\lfloor \frac{n}{3} \rfloor - 1)_{\lfloor \frac{n}{3} \rfloor - 1 - c}} \left(\binom{2\lfloor \frac{n}{3} \rfloor}{\lfloor \frac{n}{3} \rfloor} \right)^{-1} \\
 &\geq 3 \left(\binom{2\lfloor \frac{n}{3} \rfloor}{\lfloor \frac{n}{3} \rfloor} \right)^{-1} \tag{for all $n \geq 6$ }
 \end{aligned}$$

Since $\lfloor \frac{n}{3} \rfloor \leq a \leq \lceil \frac{2n}{3} \rceil$, we have $\lfloor \frac{n}{3} \rfloor \leq n - a$, and it follows that

$$\binom{n}{\lfloor n/3 \rfloor}^{-1} \geq \binom{n}{a}^{-1}.$$

We claim that

$$3 \binom{n}{\lceil n/3 \rceil}^{-1} > \binom{n}{\lfloor n/3 \rfloor}^{-1}. \tag{7.3.10}$$

To see our claim is true consider the possible values of $n \pmod 3$.

- If $n \equiv 0 \pmod{3}$, then $3 \binom{n}{\lceil n/3 \rceil}^{-1} = 3 \binom{n}{\lfloor n/3 \rfloor}^{-1}$.
- If $n \equiv 1 \pmod{3}$, then $3 \binom{n}{\lceil n/3 \rceil}^{-1} = 3 \binom{\lfloor n/3 \rfloor + 1}{2\lfloor n/3 \rfloor + 1} \binom{n}{\lfloor n/3 \rfloor}^{-1} > \frac{3}{2} \binom{n}{\lfloor n/3 \rfloor}^{-1}$.
- If $n \equiv 2 \pmod{3}$, then $3 \binom{n}{\lceil n/3 \rceil}^{-1} = 3 \binom{\lfloor n/3 \rfloor + 1}{2\lfloor n/3 \rfloor + 2} \binom{n}{\lfloor n/3 \rfloor}^{-1} = \frac{3}{2} \binom{n}{\lfloor n/3 \rfloor}^{-1}$.

In all cases,

$$3 \binom{n}{\lceil n/3 \rceil}^{-1} > \binom{n}{\lfloor n/3 \rfloor}^{-1} \geq \binom{n}{a}^{-1}.$$

Clearly, $\binom{a+b}{a}^{-1} \geq \binom{n}{b}^{-1}$ and $\binom{a+c}{a}^{-1} \geq \binom{n}{c}^{-1}$. Thus, the expression in (7.3.8) is nonnegative for all $n \geq 6$. The cases $3 \leq n \leq 5$ are easily verified by computer. ■

To summarize, if we have two small values, say $c \leq b < \lfloor n/3 \rfloor$, then by Lemma 7.3.5 it follows that $\bar{f}(n) \leq f(a, b, c)$.

7.3.4 Averaging extreme values

The next two lemmas are special cases, followed by a third more general “averaging” lemma.

Lemma 7.3.6 Let $n = 3x$. If $x \geq 2$, then $\bar{f}(n) \leq f(x+1, x, x-1)$.

[proof] In this case, $\bar{f}(n) = f(x, x, x)$ and we have

$$\begin{aligned}
 & f(x+1, x, x-1) - \bar{f}(n) \\
 &= f(x+1, x, x-1) - f(x, x, x) \\
 &= \binom{2x+1}{x}^{-1} + \binom{2x-1}{x}^{-1} + \binom{2x}{x-1}^{-1} - 3 \binom{2x}{x}^{-1} + 2 \binom{3x}{x}^{-1} - \binom{3x}{x+1}^{-1} - \binom{3x}{x-1}^{-1} \\
 &= \frac{x!x!}{(2x)!} \left(\frac{x+1}{2x+1} + \frac{2x}{x} + \frac{x+1}{x} - 3 \right) + \frac{x!(2x)!}{(3x)!} \left(2 - \frac{x+1}{2x} - \frac{2x+1}{x} \right) \\
 &= \binom{3x}{x}^{-1} \left(\frac{(3x)_x(x^2+3x+1)}{(2x)_x(2x+1)(x)} - \frac{x+3}{2x} \right) \\
 &\geq \binom{3x}{x}^{-1} \left(\frac{3}{2} \frac{(x^2+3x+1)}{(2x+1)(x)} - \frac{x+3}{2x} \right) \quad (\text{since } \frac{(3x)_x}{(2x)_x} \geq \frac{3}{2}). \tag{7.3.11}
 \end{aligned}$$

Since $3(x^2+3x+1) \geq (x+3)(2x+1)$, we see that the expression in (7.3.11) is nonnegative. Therefore, $\bar{f}(n) \leq f(x+1, x, x-1)$. ■

Lemma 7.3.7 Let $n = 3x + 2$. If $x \geq 1$, then $f(x + 2, x + 1, x - 1) \geq \bar{f}(n)$.

[proof] In this case, $\bar{f}(n) = f(x + 1, x + 1, x)$ and we have

$$\begin{aligned}
 & f(x + 2, x + 1, x - 1) - \bar{f}(n) \\
 &= f(x + 2, x + 1, x - 1) - f(x + 1, x + 1, x) \\
 &= \binom{2x+3}{x+2}^{-1} + \binom{2x+1}{x+2}^{-1} + \binom{2x}{x+1}^{-1} - \binom{2x+2}{x+1}^{-1} - 2\binom{2x+1}{x+1}^{-1} \\
 &\quad + \binom{3x+2}{x}^{-1} + 2\binom{3x+2}{x+1}^{-1} - \binom{3x+2}{x+2}^{-1} - \binom{3x+2}{x+1}^{-1} - \binom{3x+2}{x-1}^{-1} \\
 &\geq \left[\binom{2x}{x+1}^{-1} - 2\binom{2x+1}{x+1}^{-1} \right] + \left[\binom{2x+1}{x+2}^{-1} - \binom{2x+2}{x+1}^{-1} \right] \\
 &\quad + \left[\binom{3x+2}{x}^{-1} - \binom{3x+2}{x+2}^{-1} \right] + \left[\binom{2x+3}{x+2}^{-1} - \binom{3x+2}{x-1}^{-1} \right] \tag{7.3.12}
 \end{aligned}$$

We now show (7.3.12) is nonnegative. Observe the following three inequalities:

1. $\binom{2x}{x+1}^{-1} = \frac{2x+1}{x} \binom{2x+1}{x+1}^{-1} > 2\binom{2x+1}{x+1}^{-1}$
2. $\binom{2x+1}{x+2}^{-1} = \frac{2(x+2)}{x} \binom{2x+2}{x+1}^{-1} > \binom{2x+2}{x+1}^{-1}$
3. $\binom{3x+2}{x}^{-1} = \frac{4x+2}{x+2} \binom{3x+2}{x+2}^{-1} > \binom{3x+2}{x+2}^{-1}$

One further observation will prove that the expression in (7.3.12) is nonnegative for all $n \geq 26$: We have

$$\binom{2x+3}{x+2}^{-1} = \frac{(3x+2)(3x+1)_{x-2}(x+1)(x)}{(2x+3)_{x-2}(x+5)(x+4)(x+3)} \binom{3x+2}{x-1}^{-1}. \tag{7.3.13}$$

It follows from (7.3.13) that $\binom{2x+3}{x+2}^{-1} \geq \binom{3x+2}{x-1}^{-1}$ if and only if

$$\frac{(3x+2)(3x+1)_{x-2}(x+1)(x)}{(2x+3)_{x-2}(x+5)(x+4)(x+3)} \geq 1. \tag{7.3.14}$$

For all $x \geq 8$, we have $(3x+2)(x+1)(x) \geq (x+5)(x+4)(x+3)$, thus, for all $x \geq 8$, the inequality in (7.3.14) holds. For $1 \leq x \leq 7$, we can verify by computer that $\bar{f}(3x+2) \leq f(x+2, x+1, x-1)$, as claimed. ■

Lemma 7.3.8 Let n, a, b , and c be integers such that $a > b \geq c \geq 1$ and $a+b+c = n$. If $b \geq \lceil \frac{a+c}{2} \rceil$, then $f(a, b, c) \geq f(\lceil \frac{a+c}{2} \rceil, b, \lfloor \frac{a+c}{2} \rfloor)$.

[proof] Write $d = \frac{1}{2}(a+c)$ and $c = \lfloor d \rfloor - t$ and $a = \lceil d \rceil + t$, for some $t \geq 1$. Thus, $f(a, b, c) = f(\lceil d \rceil + t, b, \lfloor d \rfloor - t)$ and we must show $f(\lceil d \rceil + t, b, \lfloor d \rfloor - t) \geq f(\lceil d \rceil, b, \lfloor d \rfloor)$.

If $t = 1$ and $\lceil d \rceil = \lfloor d \rfloor = d$, then $a = d+1$, $b = d$, and $c = d-1$. In this case, by Lemma 7.3.6, we have $f(a, b, c) = f(d+1, d, d-1) \geq f(d, d, d) = f(\lceil \frac{a+c}{2} \rceil, b, \lfloor \frac{a+c}{2} \rfloor)$.

If $t = 1$ and $\lceil d \rceil = \lfloor d \rfloor + 1$, then $a = \lfloor d \rfloor + 2$, $b = \lfloor d \rfloor + 1$, and $c = \lfloor d \rfloor - 1$. In this case, by Lemma 7.3.7, we have $f(a, b, c) = f(\lfloor d \rfloor + 2, \lfloor d \rfloor + 1, \lfloor d \rfloor - 1) \geq f(\lfloor d \rfloor + 1, \lfloor d \rfloor + 1, \lfloor d \rfloor) = f(\lceil \frac{a+c}{2} \rceil, b, \lfloor \frac{a+c}{2} \rfloor)$.

Now, we may assume $t \geq 2$. We have

$$\begin{aligned}
& f(a, b, c) - f(\lceil \frac{a+c}{2} \rceil, b, \lfloor \frac{a+c}{2} \rfloor) \\
&= f(\lceil d \rceil + t, b, \lfloor d \rfloor - t) - f(\lceil d \rceil, b, \lfloor d \rfloor) \\
&= \binom{b + \lceil d \rceil + t}{b}^{-1} + \binom{b + \lfloor d \rfloor - t}{b}^{-1} + \binom{\lceil d \rceil + \lfloor d \rfloor}{\lfloor d \rfloor - t}^{-1} - \binom{b + \lceil d \rceil}{b}^{-1} \\
&\quad - \binom{b + \lfloor d \rfloor}{b}^{-1} - \binom{\lceil d \rceil + \lfloor d \rfloor}{\lceil d \rceil}^{-1} + \binom{b + \lceil d \rceil + \lfloor d \rfloor}{\lceil d \rceil}^{-1} + \binom{b + \lceil d \rceil + \lfloor d \rfloor}{\lfloor d \rfloor}^{-1} \\
&\quad - \binom{b + \lceil d \rceil + \lfloor d \rfloor}{\lceil d \rceil + t}^{-1} - \binom{b + \lceil d \rceil + \lfloor d \rfloor}{\lfloor d \rfloor - t}^{-1} \\
&\geq \left[\binom{b + \lfloor d \rfloor - t}{b}^{-1} - \binom{b + \lfloor d \rfloor}{b}^{-1} - \binom{b + \lceil d \rceil}{b}^{-1} - \binom{\lceil d \rceil + \lfloor d \rfloor}{\lceil d \rceil}^{-1} \right] \\
&\quad + \left[\binom{\lceil d \rceil + \lfloor d \rfloor}{\lfloor d \rfloor - t}^{-1} - \binom{b + \lceil d \rceil + \lfloor d \rfloor}{\lfloor d \rfloor - t}^{-1} \right] + \left[\binom{b + \lceil d \rceil + t}{b}^{-1} - \binom{b + \lceil d \rceil + \lfloor d \rfloor}{\lceil d \rceil + t}^{-1} \right] \\
&\hspace{15em} (7.3.15)
\end{aligned}$$

First,

$$\begin{aligned}
\binom{b + \lfloor d \rfloor - t}{b}^{-1} &= \frac{(b + \lfloor d \rfloor)(b + \lfloor d \rfloor - 1)(b + \lfloor d \rfloor - 2)_{t-2}}{(\lfloor d \rfloor)(\lfloor d \rfloor - 1)(\lfloor d \rfloor - 2)_{t-2}} \binom{b + \lfloor d \rfloor}{b}^{-1} \\
&> 4 \frac{(b + \lfloor d \rfloor - 2)_{t-2}}{(\lfloor d \rfloor - 2)_{t-2}} \binom{b + \lfloor d \rfloor}{b}^{-1} \quad (\text{since } b \geq \lceil d \rceil) \\
&> 2 \binom{b + \lfloor d \rfloor}{b}^{-1} + 2 \frac{(b + \lfloor d \rfloor - 2)_{t-2}}{(\lfloor d \rfloor - 2)_{t-2}} \binom{b + \lfloor d \rfloor}{b}^{-1}
\end{aligned}$$

$$\geq \binom{b + \lfloor d \rfloor}{b}^{-1} + \binom{b + \lceil d \rceil}{b}^{-1} + 2 \frac{(b + \lfloor d \rfloor - 2)_{t-2}}{(\lfloor d \rfloor - 2)_{t-2}} \binom{b + \lfloor d \rfloor}{b}^{-1}.$$

Second, notice that the last term of the preceding expression satisfies

$$\begin{aligned} & 2 \frac{(b + \lfloor d \rfloor - 2)_{t-2}}{(\lfloor d \rfloor - 2)_{t-2}} \binom{b + \lfloor d \rfloor}{b}^{-1} \\ &= 2 \frac{(b + \lfloor d \rfloor - 2)_{t-2}}{(\lfloor d \rfloor - 2)_{t-2}} \frac{(b)_{b - \lceil d \rceil}}{(b + \lfloor d \rfloor)_{b - \lceil d \rceil}} \binom{\lceil d \rceil + \lfloor d \rfloor}{\lceil d \rceil}^{-1} \\ &\geq 2^{t-1} \frac{(b)_{b - \lceil d \rceil}}{(b + \lfloor d \rfloor)_{b - \lceil d \rceil}} \binom{\lceil d \rceil + \lfloor d \rfloor}{\lceil d \rceil}^{-1} \quad \left(\text{since } \frac{(b + \lfloor d \rfloor - 2)_{t-2}}{(\lfloor d \rfloor - 2)_{t-2}} \geq \left(\frac{b + \lfloor d \rfloor - 2}{\lfloor d \rfloor - 2} \right)^{t-2} \geq 2^{t-2} \right) \\ &\geq 2^{t-1} \left(\frac{1}{2} \right)^{b - \lceil d \rceil} \binom{\lceil d \rceil + \lfloor d \rfloor}{\lceil d \rceil}^{-1} \quad \left(\text{since } \frac{(b)_{b - \lceil d \rceil}}{(b + \lfloor d \rfloor)_{b - \lceil d \rceil}} \geq \left(\frac{\lceil d \rceil}{\lceil d \rceil + \lfloor d \rfloor} \right)^{b - \lceil d \rceil} \geq \left(\frac{1}{2} \right)^{b - \lceil d \rceil} \right) \\ &\geq \binom{\lceil d \rceil + \lfloor d \rfloor}{\lceil d \rceil}^{-1} \quad (\text{since } a > b \text{ implies } t - 1 \geq b - \lceil d \rceil). \end{aligned}$$

By the above two observations, we have shown that

$$\binom{b + \lfloor d \rfloor - t}{b}^{-1} \geq \binom{b + \lfloor d \rfloor}{b}^{-1} + \binom{b + \lceil d \rceil}{b}^{-1} + \binom{\lceil d \rceil + \lfloor d \rfloor}{\lceil d \rceil}^{-1}.$$

We also have $\binom{\lceil d \rceil + \lfloor d \rfloor}{\lfloor d \rfloor - t}^{-1} > \binom{b + \lceil d \rceil + \lfloor d \rfloor}{\lfloor d \rfloor - t}^{-1}$ and $\binom{b + \lceil d \rceil + t}{b}^{-1} > \binom{b + \lceil d \rceil + \lfloor d \rfloor}{\lceil d \rceil + t}^{-1}$. Therefore, the expression in (7.3.15) is nonnegative for all $t \geq 2$. $\blacksquare$

In summary, in order to reduce f , we can replace the two most extreme values a and c by their average (rounded appropriately) so long as the third value b satisfies $b \geq \frac{a+c}{2}$.

7.3.5 One value equals $\lfloor n/3 \rfloor$

Lemma 7.3.9 Let n, a, b , and c be integers such that $a, b, c \geq 1$ and $a + b + c = n$. If $c = b = \lfloor n/3 \rfloor \leq a$, then $\bar{f}(n) \leq f(a, b, c)$.

[proof] In this case, depending on the value of $n \pmod{3}$, we know $a \in \{\lfloor n/3 \rfloor, \lfloor n/3 \rfloor + 1, \lfloor n/3 \rfloor + 2\}$.

If $n \equiv 0 \pmod{3}$ or $n \equiv 1 \pmod{3}$, then $a = \lfloor n/3 \rfloor$ or $a = \lfloor n/3 \rfloor + 1$, respectively. In these cases, we are done since we already have $f(a, b, c) = \bar{f}(n)$ by definition.

If $n \equiv 2 \pmod{3}$, then $a = \lfloor n/3 \rfloor + 2$. In this case, we show $f(\lfloor n/3 \rfloor + 2, \lfloor n/3 \rfloor, \lfloor n/3 \rfloor) \geq \bar{f}(n)$, as follows:

Write $x = \lfloor n/3 \rfloor$.

$$\begin{aligned}
& f(\lfloor n/3 \rfloor + 2, \lfloor n/3 \rfloor, \lfloor n/3 \rfloor) - \bar{f}(n) \\
&= f(x+2, x, x) - f(x+1, x+1, x) \\
&= 2 \binom{2x+2}{x}^{-1} + \binom{2x}{x}^{-1} - 2 \binom{3x+2}{x}^{-1} - \binom{3x+2}{x+2}^{-1} \\
&\quad - 2 \binom{2x+1}{x}^{-1} - \binom{2x+2}{x+1}^{-1} + 2 \binom{3x+2}{x+1}^{-1} + \binom{3x+2}{x}^{-1} \\
&= \left[\binom{2x+2}{x}^{-1} + \binom{2x}{x}^{-1} - 2 \binom{2x+1}{x}^{-1} - \binom{3x+2}{x+2}^{-1} \right] \\
&\quad + \left[2 \binom{3x+2}{x+1}^{-1} - \binom{3x+2}{x}^{-1} \right] + \left[\binom{2x+2}{x}^{-1} - \binom{2x+2}{x+1}^{-1} \right] \quad (7.3.16)
\end{aligned}$$

We claim that the expression in (7.3.16) is nonnegative.

First,

$$\begin{aligned}
\binom{2x+2}{x}^{-1} + \binom{2x}{x}^{-1} - 2 \binom{2x+1}{x}^{-1} &= \frac{x!(x+1)!}{(2x+1)!} \left(\frac{x+2}{2x+2} + \frac{2x+1}{x+1} - 2 \right) \\
&= \frac{x!(x+1)!}{(2x+1)!} \left(\frac{1}{2} \left(1 - \frac{1}{x+1} \right) \right) \\
&\geq \frac{x!(x+1)!}{(2x+1)!} \left(\frac{1}{4} \right) \quad (\text{for all } x \geq 1)
\end{aligned}$$

Second, the last term in the preceding expression satisfies

$$\frac{x!(x+1)!}{(2x+1)!} \left(\frac{1}{4} \right) - \binom{3x+2}{x+2}^{-1} = \frac{x!(x+1)!}{(2x+1)!} \left(\frac{1}{4} - \frac{(x+2)(2x)_x}{(3x+2)(3x+1)_x} \right) \geq 0$$

(for all $x \geq 2$).

Third, $2 \binom{3x+2}{x+1}^{-1} - \binom{3x+2}{x}^{-1} = 0$.

Fourth, $\binom{2x+2}{x}^{-1} - \binom{2x+2}{x+1}^{-1} = \frac{1}{x+1} \binom{2x+2}{x+1}^{-1} > 0$.

The above four observations prove that the expression in (7.3.16) is nonnegative for all $x \geq 2$. If $x = 1$, then we can verify that $\bar{f}(5) \leq f(3, 1, 1)$. Thus, we have shown that $\bar{f}(n) \leq f(x+2, x, x)$, as claimed.

In all cases, whenever $b = c = \lfloor n/3 \rfloor$, we have $\bar{f}(n) \leq f(a, b, c)$. ■

Lemma 7.3.10 Let n, a, b , and c be integers such that $a, b, c \geq 1$ and $a + b + c = n$. If $c = \lfloor n/3 \rfloor - 1$ and $b = \lfloor n/3 \rfloor \leq a$, then $\bar{f}(n) \leq f(a, b, c)$.

[proof] In this case, depending on the value of $n \pmod 3$, we know $a \in \{\lfloor n/3 \rfloor + 1, \lfloor n/3 \rfloor + 2, \lfloor n/3 \rfloor + 3\}$.

If $n \equiv 0 \pmod 3$, then $a = \lfloor n/3 \rfloor + 1$. In this case, by Lemma 7.3.6, we have $\bar{f}(n) \leq f(\lfloor n/3 \rfloor + 1, \lfloor n/3 \rfloor, \lfloor n/3 \rfloor - 1) = f(a, b, c)$.

Write $x = \lfloor n/3 \rfloor$.

If $n \equiv 1 \pmod 3$, then $a = \lfloor n/3 \rfloor + 2 = x + 2$. Since $x - 1 = c \geq 1$, we have $x \geq 2$. In this case, we have

$$\begin{aligned}
 & f(x+2, x, x-1) - f(x+1, x, x) \\
 &= \binom{2x+2}{x}^{-1} + \binom{2x+1}{x-1}^{-1} + \binom{2x-1}{x}^{-1} - \binom{3x+1}{x+2}^{-1} - \binom{3x+1}{x}^{-1} - \binom{3x+1}{x-1}^{-1} \\
 &\quad - 2\binom{2x+1}{x}^{-1} - \binom{2x}{x}^{-1} + \binom{3x+1}{x+1}^{-1} + 2\binom{3x+1}{x}^{-1} \\
 &\geq \left[\binom{2x+2}{x}^{-1} + \binom{2x-1}{x}^{-1} - 2\binom{2x+1}{x}^{-1} - \binom{2x}{x}^{-1} \right] \\
 &\quad + \left[\binom{3x+1}{x+1}^{-1} - \binom{3x+1}{x+2}^{-1} \right] + \left[\binom{2x+1}{x-1}^{-1} - \binom{3x+1}{x-1}^{-1} \right] \tag{7.3.17}
 \end{aligned}$$

From the next three observations, it will follow that the expression in (7.3.17) is nonnegative for all $x \geq 2$:

First,

$$\begin{aligned}
 & \binom{2x+2}{x}^{-1} + \binom{2x-1}{x}^{-1} - 2\binom{2x+1}{x}^{-1} - \binom{2x}{x}^{-1} \\
 &= \frac{x!x!}{(2x)!} \left(\frac{(x+2)(x+1)}{(2x+2)(2x+1)} + \frac{2x}{x} - 2\left(\frac{x+1}{2x+1}\right) - 1 \right) \\
 &= \frac{x!x!}{(2x)!} \left(\frac{x}{4x+2} \right) \geq 0 \tag{for all } x \geq 1
 \end{aligned}$$

Second,

$$\binom{3x+1}{x+1}^{-1} - \binom{3x+1}{x+2}^{-1} = \frac{(x+1)!(2x)!}{(3x+1)!} \left(1 - \frac{x+2}{2x}\right) \geq 0 \quad (\text{for all } x \geq 2)$$

Third,
$$\binom{2x+1}{x-1}^{-1} > \binom{3x+1}{x-1}^{-1}.$$

By the above three observations, the expression in (7.3.17) is nonnegative for all $x \geq 2$, which completes the proof that $\bar{f}(n) \leq f(\lfloor n/3 \rfloor + 2, \lfloor n/3 \rfloor, \lfloor n/3 \rfloor - 1)$.

If $n \equiv 2 \pmod{3}$, then $a = \lfloor n/3 \rfloor + 3 = x + 3$. In this case, we have

$$\begin{aligned} & f(x+3, x, x-1) - f(x+1, x+1, x) \\ &= \binom{2x+3}{x}^{-1} + \binom{2x+2}{x-1}^{-1} + \binom{2x-1}{x}^{-1} - \binom{3x+2}{x+3}^{-1} - \binom{3x+2}{x}^{-1} - \binom{3x+2}{x-1}^{-1} \\ &\quad - 2\binom{2x+1}{x+1}^{-1} - \binom{2x+2}{x+1}^{-1} + 2\binom{3x+2}{x+1}^{-1} + \binom{3x+2}{x}^{-1} \\ &= \left[\binom{2x+3}{x}^{-1} + \binom{2x-1}{x}^{-1} - 2\binom{2x+1}{x+1}^{-1} - \binom{2x+2}{x+1}^{-1} \right] \\ &\quad + \left[2\binom{3x+2}{x+1}^{-1} - \binom{3x+2}{x+3}^{-1} \right] + \left[\binom{2x+2}{x-1}^{-1} - \binom{3x+2}{x-1}^{-1} \right] \quad (7.3.18) \end{aligned}$$

From the next three observations, it will follow that the expression in (7.3.18) is nonnegative for all $x \geq 1$:

First,

$$\begin{aligned} & \binom{2x+3}{x}^{-1} + \binom{2x-1}{x}^{-1} - 2\binom{2x+1}{x+1}^{-1} - \binom{2x+2}{x+1}^{-1} \\ &= \frac{x!(x+1)!}{(2x+1)!} \left(\frac{(x+3)(x+2)}{(2x+3)(2x+2)} + \frac{(2x+1)(2x)}{(x+1)(x)} - 2 - \frac{x+1}{2x+2} \right) \\ &> \frac{x!(x+1)!}{(2x+1)!} \left(\frac{1}{4} + \frac{(2x+1)(2x)}{(x+1)(x)} - 2 - \frac{x+1}{2x+2} \right) \\ &= \frac{x!(x+1)!}{(2x+1)!} \left(\frac{7x-1}{4x+4} \right) > 0 \quad (\text{for all } x \geq 1) \end{aligned}$$

Second, for all $x \geq 1$, we have

$$2 \binom{3x+2}{x+1}^{-1} - \binom{3x+2}{x+3}^{-1} = \frac{(x+1)!(2x+1)!}{(3x+2)!} \left(2 - \frac{(x+3)(x+2)}{(2x)(2x+1)} \right) \geq 0.$$

Third,
$$\binom{2x+2}{x-1}^{-1} - \binom{3x+2}{x-1}^{-1} > 0.$$

From these three observations, it follows that (7.3.18) is nonnegative for all $x \geq 1$.

For all three possibilities for a , we have shown that $\bar{f}(n) \leq f(a, \lfloor n/3 \rfloor, \lfloor n/3 \rfloor - 1)$, as claimed. ■

Lemma 7.3.11 Let n, a, b , and c be integers such that $a, b, c \geq 1$ and $a + b + c = n$. If $c \leq b = \lfloor n/3 \rfloor \leq a$, then $\bar{f}(n) \leq f(a, b, c)$.

[proof] If $c = \lfloor n/3 \rfloor$ or $c = \lfloor n/3 \rfloor - 1$, then $\bar{f}(n) \leq f(a, b, c)$ by Lemma 7.3.9 or Lemma 7.3.10, respectively.

Now, suppose $c \leq \lfloor n/3 \rfloor - 2$ and $b = \lfloor n/3 \rfloor$. In this case, regardless of the value of $n \pmod 3$, we have

$$\begin{aligned} & f(a, \lfloor n/3 \rfloor, c) - \bar{f}(n) \\ & \geq \binom{a + \lfloor n/3 \rfloor}{a}^{-1} + \binom{a + c}{c}^{-1} + \binom{c + \lfloor n/3 \rfloor}{\lfloor n/3 \rfloor}^{-1} - \binom{n}{a}^{-1} - \binom{n}{\lfloor n/3 \rfloor}^{-1} - \binom{n}{c}^{-1} \\ & \quad - 3 \binom{2\lfloor n/3 \rfloor}{\lfloor n/3 \rfloor}^{-1} + 3 \binom{n}{\lceil n/3 \rceil}^{-1} \\ & = \left[\binom{c + \lfloor n/3 \rfloor}{\lfloor n/3 \rfloor}^{-1} - 3 \binom{2\lfloor n/3 \rfloor}{\lfloor n/3 \rfloor}^{-1} \right] + \left[3 \binom{n}{\lceil n/3 \rceil}^{-1} - \binom{n}{\lfloor n/3 \rfloor}^{-1} \right] \\ & \quad + \left[\binom{a + \lfloor n/3 \rfloor}{a}^{-1} - \binom{n}{a}^{-1} \right] + \left[\binom{c + \lfloor n/3 \rfloor}{\lfloor n/3 \rfloor}^{-1} - \binom{n}{c}^{-1} \right] \end{aligned} \tag{7.3.19}$$

We now show that the expression in (7.3.19) is nonnegative, which suffices to prove $\bar{f}(n) \leq f(a, b, c)$.

Since $c \leq \lfloor n/3 \rfloor - 2$, we have
$$\binom{c + \lfloor n/3 \rfloor}{\lfloor n/3 \rfloor}^{-1} \geq \binom{2\lfloor n/3 \rfloor - 2}{\lfloor n/3 \rfloor}^{-1}.$$

Moreover,

$$\begin{aligned} \binom{2\lfloor n/3 \rfloor - 2}{\lfloor n/3 \rfloor}^{-1} - 3 \binom{2\lfloor n/3 \rfloor}{\lfloor n/3 \rfloor}^{-1} &= \frac{(\lfloor n/3 \rfloor)!(\lfloor n/3 \rfloor - 2)!}{(2\lfloor n/3 \rfloor - 2)!} \left(1 - 3 \frac{(\lfloor n/3 \rfloor)(\lfloor n/3 \rfloor - 1)}{(2\lfloor n/3 \rfloor)(2\lfloor n/3 \rfloor - 1)} \right) \\ &> \frac{(\lfloor n/3 \rfloor)!(\lfloor n/3 \rfloor - 2)!}{(2\lfloor n/3 \rfloor - 2)!} \left(1 - 3 \left(\frac{1}{2} \right) \left(\frac{1}{2} \right) \right) > 0. \end{aligned}$$

Therefore
$$\binom{c + \lfloor n/3 \rfloor}{\lfloor n/3 \rfloor}^{-1} \geq 3 \binom{2\lfloor n/3 \rfloor}{\lfloor n/3 \rfloor}^{-1}.$$

From (7.3.10) in Lemma 7.3.5, we know $3 \binom{n}{\lfloor n/3 \rfloor}^{-1} \geq \binom{n}{\lfloor n/3 \rfloor}^{-1}$. It is clear that $\binom{a + \lfloor n/3 \rfloor}{a}^{-1} \geq \binom{n}{a}^{-1}$ and $\binom{c + \lfloor n/3 \rfloor}{c}^{-1} \geq \binom{n}{c}^{-1}$, which completes the proof that the expression in (7.3.19) is nonnegative. $\blacksquare$

In summary, if one of the values equals $\lfloor n/3 \rfloor$, then $\bar{f}(n) \leq f(a, b, c)$.

7.3.6 Two largest values are equal

Lemma 7.3.12 Let a, b, c , and n be integers such that $n \equiv 0 \pmod{3}$, $a \geq b \geq c \geq 1$ and $a + b + c = n$. If $a = b > n/3$, then $\bar{f}(n) \leq f(a, b, c)$.

[proof] Write $x = n/3$ and $a = b = x + y$ for some $y \geq 1$. Since $n \equiv 0 \pmod{3}$ we have $c = n - 2a = x - 2y$. In this case, $f(a, b, c) = f(x + y, x + y, x - 2y)$ and $\bar{f}(n) = f(x, x, x)$. Thus,

$$\begin{aligned} f(a, b, c) - \bar{f}(n) &= f(x + y, x + y, x - 2y) - f(x, x, x) \\ &= 2 \binom{2x - y}{x + y}^{-1} + \binom{2x + 2y}{x + y}^{-1} - 2 \binom{3x}{x + y}^{-1} - \binom{3x}{x - 2y}^{-1} - 3 \binom{2x}{x}^{-1} + 3 \binom{3x}{x}^{-1} \\ &\geq \left[3 \binom{3x}{x}^{-1} - 2 \binom{3x}{x + y}^{-1} \right] + \left[2 \binom{2x - y}{x + y}^{-1} - 3 \binom{2x}{x}^{-1} - \binom{3x}{x - 2y}^{-1} \right] \quad (7.3.20) \end{aligned}$$

It suffices to show that (7.3.20) is nonnegative.

First, since $x < x + y < 2x$, we have $3 \binom{3x}{x}^{-1} > 2 \binom{3x}{x + y}^{-1}$.

Second,

$$2 \binom{2x - y}{x + y}^{-1} - 3 \binom{2x}{x}^{-1} = \binom{2x - y}{x + y}^{-1} \left(2 - 3 \frac{\binom{x}{y} \binom{x - y}{y}}{\binom{2x}{y} \binom{x + y}{y}} \right)$$

$$\begin{aligned}
&\geq \binom{2x-y}{x+y}^{-1} \left(2 - 3 \frac{\binom{x}{y}}{\binom{2x}{y}} \right) \\
&\geq \binom{2x-y}{x+y}^{-1} \left(2 - 3 \left(\frac{1}{2} \right)^y \right). \tag{7.3.21}
\end{aligned}$$

Third, the expression in (7.3.21) satisfies

$$\left(2 - 3 \left(\frac{1}{2} \right)^y \right) \binom{2x-y}{x+y}^{-1} - \binom{3x}{x-2y}^{-1} = \binom{3x}{x-2y}^{-1} \left(\left(2 - 3 \left(\frac{1}{2} \right)^y \right) \frac{\binom{3x}{x+y}}{\binom{2x+2y}{x+y}} - 1 \right). \tag{7.3.22}$$

Since $3x = n > a + b = 2x + 2y$ and $2 - 3 \left(\frac{1}{2} \right)^y > 1$ for all $y \geq 2$, we see that the expression in (7.3.22) is nonnegative for all $y \geq 2$.

If $y = 1$, then

$$\left(2 - 3 \left(\frac{1}{2} \right)^y \right) \frac{\binom{3x}{x+y}}{\binom{2x+2y}{x+y}} = \left(\frac{1}{2} \right) \frac{\binom{3x}{x+1}}{\binom{2x+2}{x+1}}. \tag{7.3.23}$$

In this case, the expression in (7.3.23) is greater than or equal to 1 for all $x \geq 4$.

Thus, for all $x \geq 4$, the expression in (7.3.20) is nonnegative. For $1 \leq x \leq 3$ we can verify by computer that $\bar{f}(n) = \bar{f}(3x) \leq f(a, b, c)$, as claimed. $\blacksquare$

Lemma 7.3.13 Let a, b, c , and n be integers such that $n \equiv 1 \pmod{3}$, $a \geq b \geq c \geq 1$ and $a + b + c = n$. If $a = b \geq \lfloor n/3 \rfloor + 1$, then $\bar{f}(n) \leq f(a, b, c)$.

[proof] Write $x = \lfloor n/3 \rfloor$ and $a = b = x + y$ for some $y \geq 1$. Since $n \equiv 1 \pmod{3}$ we have $c = n - 2a = x - 2y + 1$. In this case, $f(a, b, c) = f(x + y, x + y, x - 2y + 1)$ and $\bar{f}(n) = f(x + 1, x, x)$.

If $y = 1$, then $f(a, b, c) = f(x + 1, x + 1, x - 1)$ and we have

$$\begin{aligned}
&f(a, b, c) - \bar{f}(n) \\
&= f(x + 1, x + 1, x - 1) - f(x + 1, x, x) \\
&= 2 \binom{2x}{x+1}^{-1} + \binom{2x+2}{x+1}^{-1} - 2 \binom{3x+1}{x+1}^{-1} - \binom{3x+1}{x-1}^{-1} \\
&\quad - 2 \binom{2x+1}{x}^{-1} - \binom{2x}{x}^{-1} + 2 \binom{3x+1}{x}^{-1} + \binom{3x+1}{x+1}^{-1}
\end{aligned}$$

$$\begin{aligned}
&\geq \left[2 \binom{2x}{x+1}^{-1} + \binom{3x+1}{x}^{-1} - 2 \binom{2x+1}{x}^{-1} - \binom{2x}{x}^{-1} - \binom{3x+1}{x-1}^{-1} \right] \\
&\quad + \left[\binom{3x+1}{x}^{-1} - \binom{3x+1}{x+1}^{-1} \right] \tag{7.3.24}
\end{aligned}$$

We now show that the expression in (7.3.24) is nonnegative:

First,

$$\begin{aligned}
2 \binom{2x}{x+1}^{-1} - 2 \binom{2x+1}{x}^{-1} - \binom{2x}{x}^{-1} &= \frac{(x+1)!(x-1)!}{(2x)!} \left(2 - \frac{2x}{2x+1} - \frac{x}{x+1} \right) \\
&= \frac{x!(x-1)!}{(2x+1)!} (3x+2)
\end{aligned}$$

The last term in the preceding expression satisfies

$$\begin{aligned}
&\frac{x!(x-1)!}{(2x+1)!} (3x+2) - \binom{3x+1}{x-1}^{-1} + \binom{3x+1}{x}^{-1} \\
&= \frac{x!(x-1)!}{(2x+1)!} (3x+2) - \frac{(x-1)!(2x+2)!}{(3x+1)!} \left(1 - \frac{x}{2x+2} \right) \\
&= \frac{x!(x-1)!}{(2x+1)!} (3x+2) - \frac{(x-1)!(2x+2)!}{(3x+1)!} \left(\frac{x+2}{2x+2} \right) \\
&= \frac{x!(x-1)!}{(2x+1)!} \left(3x+2 - \frac{(x+2)(2x+1)_{x+1}}{(3x+1)_x} \right). \tag{7.3.25}
\end{aligned}$$

The expression in (7.3.25) is nonnegative if and only if $\frac{(2x+1)_{x+1}}{(3x+2)_{x+1}} \leq \frac{1}{x+2}$, which is true for all $x \geq 1$.

Thus,

$$2 \binom{2x}{x+1}^{-1} + \binom{3x+1}{x}^{-1} - 2 \binom{2x+1}{x}^{-1} - \binom{2x}{x}^{-1} - \binom{3x+1}{x-1}^{-1} > 0$$

$$\text{Second, } \binom{3x+1}{x}^{-1} > \binom{3x+1}{x+1}^{-1}.$$

Therefore, the expression in (7.3.24) is nonnegative, as claimed.

Now, we may assume $y \geq 2$. In this case, we have

$$f(a, b, c) - \bar{f}(n)$$

$$\begin{aligned}
&= f(x+y, x+y, x-2y+1) - f(x+1, x, x) \\
&= \binom{2x+2y}{x+y}^{-1} + 2 \binom{2x-y+1}{x+y}^{-1} - 2 \binom{3x+1}{x+y}^{-1} - \binom{3x+1}{x-2y+1}^{-1} \\
&\quad - 2 \binom{2x+1}{x}^{-1} - \binom{2x}{x}^{-1} + 2 \binom{3x+1}{x}^{-1} + \binom{3x+1}{x+1}^{-1} \\
&\geq \left[2 \binom{3x+1}{x}^{-1} - 2 \binom{3x+1}{x+y}^{-1} \right] + \left[\binom{2x-y+1}{x+y}^{-1} - 2 \binom{2x+1}{x}^{-1} - \binom{2x}{x}^{-1} \right] \\
&\quad + \left[\binom{2x-y+1}{x+y}^{-1} - \binom{3x+1}{x-2y+1}^{-1} \right]. \tag{7.3.26}
\end{aligned}$$

We must show that the expression in (7.3.26) is nonnegative.

First, observe that $2 \binom{3x+1}{x}^{-1} \geq 2 \binom{3x+1}{x+y}^{-1}$.

Second,

$$\begin{aligned}
&\binom{2x-y+1}{x+y}^{-1} - 2 \binom{2x+1}{x}^{-1} - \binom{2x}{x}^{-1} \\
&= \frac{(x+y)!(x-2y+1)!}{(2x-y+1)!} \left(1 - 2 \frac{(x+1)_y(x-y+1)_y}{(x+y)_y(2x+1)_y} - \frac{(x)_{y-1}(x-y+1)_y}{(2x)_{y-1}(x+y)_y} \right) \\
&\geq \frac{(x+y)!(x-2y+1)!}{(2x-y+1)!} \left(1 - 2 \frac{(x-y+1)_y}{(2x+1)_y} - \frac{(x)_{y-1}}{(2x)_{y-1}} \right) \\
&\geq \frac{(x+y)!(x-2y+1)!}{(2x-y+1)!} \left(1 - 2 \left(\frac{1}{2}\right)^y - \left(\frac{1}{2}\right)^{y-1} \right) \geq 0 \quad (\text{for all } y \geq 2).
\end{aligned}$$

Third, $\binom{2x-y+1}{x+y}^{-1} = \binom{2x-y+1}{x-2y+1}^{-1} > \binom{3x+1}{x-2y+1}^{-1}$.

By the above three observations, we see that the expression in (7.3.26) is nonnegative. Thus, $\bar{f}(n) \leq f(a, b, c)$, as claimed ■

Lemma 7.3.14 Let a, b, c , and n be integers such that $n \equiv 2 \pmod{3}$, $a \geq b \geq c \geq 1$ and $a + b + c = n$. If $a = b \geq \lfloor n/3 \rfloor + 1$, then $\bar{f}(n) \leq f(a, b, c)$.

[proof] Write $x = \lfloor n/3 \rfloor$ and $a = b = x + y$ for some $y \geq 1$. Since $n \equiv 2 \pmod{3}$ we have $c = n - 2a = x - 2y + 2$. In this case, $f(a, b, c) = f(x+y, x+y, x-2y+2)$ and $\bar{f}(n) = f(x+1, x+1, x)$.

If $y = 1$, then $f(x + y, x + y, x - 2y + 2) = \bar{f}(n)$, by definition, so we are done.

Now, we may assume $y \geq 2$. In this case, we have

$$\begin{aligned}
& f(a, b, c) - \bar{f}(n) \\
&= f(x + y, x + y, x - 2y + 2) - f(x + 1, x + 1, x) \\
&= 2 \binom{2x - y + 2}{x + y}^{-1} + \binom{2x + 2y}{x + y}^{-1} - 2 \binom{3x + 2}{x + y}^{-1} - \binom{3x + 2}{x - 2y + 2}^{-1} \\
&\quad - 2 \binom{2x + 1}{x + 1}^{-1} - \binom{2x + 2}{x + 1}^{-1} + 2 \binom{3x + 2}{x + 1}^{-1} + \binom{3x + 2}{x}^{-1} \\
&> \left[2 \binom{3x + 2}{x + 1}^{-1} - 2 \binom{3x + 2}{x + y}^{-1} \right] + \left[\binom{2x - y + 2}{x + y}^{-1} - 2 \binom{2x + 1}{x + 1}^{-1} \right] \\
&\quad + \left[\binom{2x - y + 2}{x + y}^{-1} - \binom{2x + 2}{x + 1}^{-1} - \binom{3x + 2}{x - 2y + 2}^{-1} \right] \tag{7.3.27}
\end{aligned}$$

First, $2 \binom{3x + 2}{x + 1}^{-1} \geq 2 \binom{3x + 2}{x + y}^{-1}$.

Second,

$$\begin{aligned}
\binom{2x - y + 2}{x + y}^{-1} - 2 \binom{2x + 1}{x + 1}^{-1} &= \binom{2x - y + 2}{x + y}^{-1} \left(1 - 2 \frac{(x)_{y-1} (x - y + 1)_{y-1}}{(2x + 1)_{y-1} (x + y)_{y-1}} \right) \\
&> \binom{2x - y + 2}{x + y}^{-1} \left(1 - 2 \left(\frac{1}{2} \right)^{y-1} \right) \geq 0 \tag{7.3.28}
\end{aligned}$$

Third,

$$\begin{aligned}
\binom{2x - y + 2}{x + y}^{-1} - \binom{2x + 2}{x + 1}^{-1} &= \binom{2x - y + 2}{x + y}^{-1} \left(1 - \frac{(x + 1)_y (x - y + 1)_{y-1}}{(2x + 2)_y (x + y)_{y-1}} \right) \\
&> \binom{2x - y + 2}{x + y}^{-1} \left(1 - \left(\frac{1}{2} \right)^y \right) \\
&> \frac{3}{4} \binom{2x - y + 2}{x + y}^{-1}. \tag{7.3.29}
\end{aligned}$$

Now, the expression in (7.3.29) satisfies

$$\frac{3}{4} \binom{2x - y + 2}{x + y}^{-1} - \binom{3x + 2}{x - 2y + 2}^{-1} = \frac{(x + y)! (x - 2y + 2)!}{(2x - y + 2)!} \left(\frac{3}{4} - \frac{(2x + 2y)_{x+y}}{(3x + 2)_{x+y}} \right) \tag{7.3.30}$$

The expression in (7.3.30) is nonnegative if and only if $\frac{(2x+2y)_{x+y}}{(3x+2)_{x+y}} \leq \frac{3}{4}$, which is true, as follows:

$$\begin{aligned}
 \frac{(2x+2y)_{x+y}}{(3x+2)_{x+y}} &= \frac{(2x+2y)_{3y-2}(2x-y+2)_{x-2y+2}}{(3x+2)_{x-2y+2}(2x+2y)_{3y-2}} \\
 &= \frac{(2x-y+2)_{x-2y+2}}{(3x+2)_{x-2y+2}} \\
 &\leq \left(\frac{2x-y+2}{3x+2} \right)^{x-2y+2} && \text{(by Lemma 7.1.3)} \\
 &< \left(\frac{2}{3} \right)^{x-2y+2} && \text{(since } y \geq 2) \\
 &< \frac{3}{4} && \text{(since } x-2y+2 = c \geq 1).
 \end{aligned}$$

Thus, the expression in (7.3.30) is indeed nonnegative. This together with (7.3.29) shows that, for $y \geq 2$, we have

$$\binom{2x-y+2}{x+y}^{-1} - \binom{2x+2}{x+1}^{-1} - \binom{3x+2}{x-2y+2}^{-1} \geq 0.$$

We have now shown that the expression in (7.3.27) is nonnegative for all $y \geq 2$. Thus, $f(a, b, c) - \bar{f}(n) \geq 0$, as claimed. $\blacksquare$

Corollary 7.3.15 If $a = b \geq \lfloor n/3 \rfloor \geq c$, then $\bar{f}(n) \leq f(a, b, c)$.

[proof] If $a = b = \lfloor n/3 \rfloor$, then $c = \lfloor n/3 \rfloor$ and we have $f(a, b, c) = \bar{f}(n)$, by definition. Otherwise, $a = b \geq \lfloor n/3 \rfloor + 1$, and the result follows from Lemmas 7.3.12, 7.3.13, and 7.3.14. $\blacksquare$

7.3.7 Three special cases

Lemma 7.3.16 If $n = 3x + 2$, then $\bar{f}(n) \leq f(x+2, x, x)$.

[proof] In this case, $\bar{f}(n) = f(x+1, x+1, x)$ and we have

$$\begin{aligned}
 &f(x+2, x, x) - \bar{f}(n) \\
 &= f(x+2, x, x) - f(x+1, x+1, x) \\
 &= 2 \binom{2x+2}{x}^{-1} + \binom{2x}{x}^{-1} - 2 \binom{3x+2}{x}^{-1} - \binom{3x+2}{x+2}^{-1}
 \end{aligned}$$

$$\begin{aligned}
& -2 \binom{2x+1}{x+1}^{-1} - \binom{2x+2}{x+1}^{-1} + 2 \binom{3x+2}{x+1}^{-1} + \binom{3x+2}{x}^{-1} \\
& = \left[2 \binom{2x+2}{x}^{-1} + \binom{2x}{x}^{-1} - 2 \binom{2x+1}{x+1}^{-1} - \binom{2x+2}{x+1}^{-1} - \binom{3x+2}{x}^{-1} \right] \\
& \quad + \left[2 \binom{3x+2}{x+1}^{-1} - \binom{3x+2}{x+2}^{-1} \right] \tag{7.3.31}
\end{aligned}$$

We now show that the expression in (7.3.31) is nonnegative.

First,

$$\begin{aligned}
& 2 \binom{2x+2}{x}^{-1} + \binom{2x}{x}^{-1} - 2 \binom{2x+1}{x+1}^{-1} - \binom{2x+2}{x+1}^{-1} \\
& = \frac{x!x!}{(2x+2)!} \left(2(x+2)(x+1) + (2x+2)(2x+1) - 2(x+1)(2x+2) - (x+1)(x+1) \right) \\
& = \frac{(x+1)!(x+1)!}{(2x+2)!}. \tag{7.3.32}
\end{aligned}$$

Next, the expression in (7.3.32) satisfies

$$\frac{(x+1)!(x+1)!}{(2x+2)!} - \binom{3x+2}{x}^{-1} = \frac{(x+1)!(x+1)!}{(2x+2)!} \left(1 - \frac{(2x+2)_{x+1}}{(x+1)(3x+2)_x} \right). \tag{7.3.33}$$

The expression in (7.3.33) is nonnegative if and only if $\frac{(2x+2)_x}{(3x+2)_x} \leq \frac{x+1}{x+2}$, which is true for all $x \geq 4$ since

$$\frac{(2x+2)_x}{(3x+2)_x} \leq \left(\frac{2x+2}{3x+2} \right)^x < \frac{1}{3} \leq 1 - \frac{1}{x+2} = \frac{x+1}{x+2}.$$

Finally,

$$2 \binom{3x+2}{x+1}^{-1} - \binom{3x+2}{x+2}^{-1} = \frac{(x+1)!(2x)!}{(3x+2)!} \left(2(2x+1) - (x+2) \right) > 0.$$

The above observations prove $\bar{f}(n) \leq f(x+2, x, x)$ for all $x \geq 4$ (hence for all $n \geq 14$ such that $n \equiv 2 \pmod{3}$). For each n such that $3 \leq n \leq 13$ and $n \equiv 2 \pmod{3}$, we can verify by computer that $\bar{f}(n) \leq f(x+2, x, x)$. ■

Lemma 7.3.17 If $n = 3x + 1$, then $\bar{f}(n) \leq f(x + 2, x, x - 1)$.

[proof] In this case, $\bar{f}(n) = f(x + 1, x, x)$ and we have

$$\begin{aligned}
 & f(x + 2, x, x - 1) - \bar{f}(n) \\
 &= f(x + 2, x, x - 1) - f(x + 1, x, x) \\
 &= \binom{2x+2}{x}^{-1} + \binom{2x-1}{x}^{-1} + \binom{2x+1}{x-1}^{-1} - \binom{3x+1}{x+2}^{-1} - \binom{3x+1}{x}^{-1} - \binom{3x+1}{x-1}^{-1} \\
 &\quad - 2\binom{2x+1}{x}^{-1} - \binom{2x}{x}^{-1} + 2\binom{3x+1}{x}^{-1} + \binom{3x+1}{x+1}^{-1} \\
 &\geq \left[\binom{2x-1}{x}^{-1} + \binom{2x+1}{x-1}^{-1} - 2\binom{2x+1}{x}^{-1} - \binom{2x}{x}^{-1} \right] \\
 &\quad + \left[\binom{2x+2}{x}^{-1} - \binom{3x+1}{x-1}^{-1} \right] + \left[\binom{3x+1}{x}^{-1} - \binom{3x+1}{x+2}^{-1} \right] \tag{7.3.34}
 \end{aligned}$$

We now show that the expression in (7.3.34) is nonnegative.

First,

$$\begin{aligned}
 & \binom{2x-1}{x}^{-1} + \binom{2x+1}{x-1}^{-1} - 2\binom{2x+1}{x}^{-1} - \binom{2x}{x}^{-1} \\
 &= \frac{x!(x-1)!}{(2x-1)!} \left(1 + \frac{(x+2)(x+1)}{(2x+1)(2x)} - \frac{2(x+1)(x)}{(2x+1)(2x)} - \frac{x}{2x} \right) \\
 &= \frac{x!(x-1)!}{(2x-1)!} \left(\frac{1}{2} - \frac{(x+1)(x-2)}{(2x+1)(2x)} \right) \tag{7.3.35}
 \end{aligned}$$

The expression in (7.3.35) is nonnegative if and only if $\frac{(x+1)(x-2)}{(2x+1)(2x)} \leq \frac{1}{2}$, which is true for all $x \geq 1$.

Second,

$$\binom{2x+2}{x}^{-1} - \binom{3x+1}{x-1}^{-1} = \frac{x!(x+2)!}{(2x+2)!} \left(1 - \frac{(2x+2)_x}{x(3x+1)_{x-1}} \right) \tag{7.3.36}$$

The expression in (7.3.36) is nonnegative if and only if $\frac{(2x+2)_{x-1}}{(3x+1)_{x-1}} \leq \frac{x}{x+3}$, which is true for all $x \geq 4$ since

$$\frac{(2x+2)_{x-1}}{(3x+1)_{x-1}} \leq \left(\frac{2x+2}{3x+1} \right)^{x-1} < \frac{1}{2} < 1 - \frac{3}{x+3} = \frac{x}{x+3} \quad (\text{for all } x \geq 4)$$

Third, for all $x \geq 1$ we have

$$\binom{3x+1}{x}^{-1} - \binom{3x+1}{x+2}^{-1} = \frac{x!(2x-1)!}{(3x+1)!} \left((2x+1)(2x) - (x+2)(x+1) \right) \geq 0.$$

The above three observations prove that $\bar{f}(n) \leq f(x+2, x, x-1)$ for all $x \geq 4$. For $1 \leq x \leq 3$, we can verify by computer that $\bar{f}(3x+1) \leq f(x+2, x, x-1)$. $\blacksquare$

Lemma 7.3.18 If $n = 3x + 2$, then $\bar{f}(n) \leq f(x+3, x, x-1)$.

[proof] In this case $\bar{f}(n) = f(x+1, x+1, x)$ and we have

$$\begin{aligned} & f(x+3, x, x-1) - \bar{f}(n) \\ &= f(x+3, x, x-1) - f(x+1, x+1, x) \\ &= \binom{2x+3}{x}^{-1} + \binom{2x+2}{x-1}^{-1} + \binom{2x-1}{x}^{-1} - \binom{3x+2}{x+3}^{-1} - \binom{3x+2}{x}^{-1} - \binom{3x+2}{x-1}^{-1} \\ &\quad - 2\binom{2x+1}{x}^{-1} - \binom{2x+2}{x+1}^{-1} + 2\binom{3x+2}{x+1}^{-1} + \binom{3x+2}{x}^{-1} \\ &\geq \left[\binom{2x-1}{x}^{-1} - 2\binom{2x+1}{x}^{-1} - \binom{2x+2}{x+1}^{-1} \right] + \left[\binom{2x+3}{x}^{-1} - \binom{3x+2}{x+3}^{-1} \right] \\ &\quad + \left[\binom{2x+2}{x-1}^{-1} - \binom{3x+2}{x-1}^{-1} \right] \end{aligned} \tag{7.3.37}$$

We now prove that the expression in (7.3.37) is nonnegative. We have

$$\begin{aligned} & \binom{2x-1}{x}^{-1} - 2\binom{2x+1}{x}^{-1} - \binom{2x+2}{x+1}^{-1} \\ &= \frac{x!(x-1)!}{(2x-1)!} \left(1 - \frac{2(x+1)(x)}{(2x+1)(2x)} - \frac{(x+1)(x+1)(x)}{(2x+2)(2x+1)(2x)} \right) \\ &= \frac{x!(x-1)!}{(2x-1)!} \left(1 - \frac{3(x+1)}{4(2x+1)} \right) > 0 \quad (\text{for all } x \geq 1). \end{aligned}$$

Furthermore, $\binom{2x+3}{x}^{-1} = \binom{2x+3}{x+3}^{-1} > \binom{3x+2}{x+3}^{-1}$ and $\binom{2x+2}{x-1}^{-1} > \binom{3x+2}{x-1}^{-1}$. Therefore, $\bar{f}(3x+2) \leq f(x+3, x, x-1)$, as claimed. $\blacksquare$

7.3.8 The upper bound on $m(n, K_3^{\text{loop}})$

Corollary 7.3.19 If n, a, b , and c are integers such that $a, b, c \geq 1$ and $a + b + c = n$, then $\bar{f}(n) \leq f(a, b, c)$.

[proof] Since $f(a, b, c)$ is invariant under permutations of a, b , and c , we may assume without loss of generality that $a \geq b \geq c$.

If $a > \lceil 2n/3 \rceil$, then, by Lemma 7.3.4, we have $\bar{f}(n) \leq f(a, b, c)$. Now, we may assume $c \leq b \leq a \leq \lceil 2n/3 \rceil$. If it also the case that $c \leq b < \lfloor n/3 \rfloor$, then by Lemma 7.3.5, we have $\bar{f}(n) \leq f(a, b, c)$.

At this point, we may assume $c \leq \lfloor n/3 \rfloor \leq b \leq a \leq \lceil 2n/3 \rceil$. If $b = \lfloor n/3 \rfloor$, then, by Lemma 7.3.11, we have $\bar{f}(n) \leq f(a, b, c)$. Thus we may now assume $c \leq \lfloor n/3 \rfloor < b \leq a \leq \lceil 2n/3 \rceil$. If $c = \lfloor n/3 \rfloor$, then $b = a = \lfloor n/3 \rfloor + 1$, and in this case, $f(a, b, c) = \bar{f}(n)$, by definition.

Now, we may assume $c < \lfloor n/3 \rfloor < b \leq a \leq \lceil 2n/3 \rceil$. If $a = b \geq \lfloor n/3 \rfloor + 1$, then, by Corollary 7.3.15, we have $\bar{f}(n) \leq f(a, b, c)$.

Finally, we may assume $c < \lfloor n/3 \rfloor < b < a \leq \lceil 2n/3 \rceil$. Since $b \geq \lfloor n/3 \rfloor + 1$, we have $a + c = n - b \leq 2\lfloor n/3 \rfloor + 1$. Consequently, the average of a and c satisfies $\lceil \frac{a+c}{2} \rceil \leq \lfloor n/3 \rfloor + 1 \leq b$. Thus, by Lemma 7.3.8, we have $f(a, b, c) \geq f(\lceil d \rceil, b, \lfloor d \rfloor)$, where $d = \frac{a+c}{2}$. It remains to show that $\bar{f}(n) \leq f(\lceil d \rceil, b, \lfloor d \rfloor)$ for which we consider three possibilities for the value of $\lceil d \rceil$:

- If $\lceil d \rceil = \lfloor n/3 \rfloor + 1$, then, since $b \geq \lceil d \rceil = \lfloor n/3 \rfloor + 1$, we must have $f(\lceil d \rceil, b, \lfloor d \rfloor) = \bar{f}(n)$.
- If $\lceil d \rceil = \lfloor n/3 \rfloor$, then either $\lfloor d \rfloor = \lfloor n/3 \rfloor$ or $\lfloor d \rfloor = \lfloor n/3 \rfloor - 1$. We consider both cases:
 1. If $\lfloor d \rfloor = \lfloor n/3 \rfloor = \lceil d \rceil$, then $b \in \{\lfloor n/3 \rfloor + 1, \lfloor n/3 \rfloor + 2\}$. If $b = \lfloor n/3 \rfloor + 1$, then $f(\lceil d \rceil, b, \lfloor d \rfloor) = f(\lfloor n/3 \rfloor, \lfloor n/3 \rfloor + 1, \lfloor n/3 \rfloor) = \bar{f}(n)$. If $b = \lfloor n/3 \rfloor + 2$, then, by Lemma 7.3.16, we have $\bar{f}(n) \leq f(\lfloor n/3 \rfloor, \lfloor n/3 \rfloor + 2, \lfloor n/3 \rfloor) = f(\lceil d \rceil, b, \lfloor d \rfloor)$.
 2. If $\lfloor d \rfloor = \lfloor n/3 \rfloor - 1$, then $b \in \{\lfloor n/3 \rfloor + 1, \lfloor n/3 \rfloor + 2, \lfloor n/3 \rfloor + 3\}$. If $b = \lfloor n/3 \rfloor + 1$, then, by Lemma 7.3.6, we have $\bar{f}(n) \leq f(\lfloor n/3 \rfloor, \lfloor n/3 \rfloor + 1, \lfloor n/3 \rfloor - 1) = f(\lceil d \rceil, b, \lfloor d \rfloor)$. If $b = \lfloor n/3 \rfloor + 2$, then, by Lemma 7.3.17, we have $\bar{f}(n) \leq f(\lfloor n/3 \rfloor, \lfloor n/3 \rfloor + 2, \lfloor n/3 \rfloor - 1) = f(\lceil d \rceil, b, \lfloor d \rfloor)$. If $b = \lfloor n/3 \rfloor + 3$,

then, by Lemma 7.3.18, we have $\bar{f}(n) \leq f(\lfloor n/3 \rfloor, \lfloor n/3 \rfloor + 3, \lfloor n/3 \rfloor - 1) = f(\lceil d \rceil, b, \lfloor d \rfloor)$.

- If $\lceil d \rceil < \lfloor n/3 \rfloor$, then we have two small values: $\lfloor d \rfloor \leq \lceil d \rceil < \lfloor n/3 \rfloor < b \leq \lceil 2n/3 \rceil$. By Lemma 7.3.5, we have $\bar{f}(n) \leq f(b, \lceil d \rceil, \lfloor d \rfloor)$.

Thus, for all a, b, c such that $a \geq b \geq c \geq 1$ and $a + b + c = n$, we have shown $\bar{f}(n) \leq f(a, b, c)$, as claimed. $\blacksquare$

Theorem 7.3.20 For all $n \geq 3$, we have

$$m(n, K_3^{\text{loop}}) \leq \frac{1}{2\bar{f}(n)} = \begin{cases} \frac{1}{6 - \delta_{n,0}} \binom{\lfloor 2n/3 \rfloor}{\lfloor n/3 \rfloor} & \text{if } n \equiv 0 \pmod{3}, \\ \frac{1}{4 + \delta_{n,1}} \binom{\lfloor 2n/3 \rfloor}{\lfloor n/3 \rfloor} & \text{if } n \equiv 1 \pmod{3}, \\ \frac{1}{5 - \delta_{n,2}} \binom{\lfloor 2n/3 \rfloor}{\lfloor n/3 \rfloor} & \text{if } n \equiv 2 \pmod{3}, \end{cases}$$

where, in each case, $\delta_{n,r}$ is a function that tends to zero as n grows.

[proof] If $\mathcal{P}$ is a K_3^{loop} -intersecting collection of 3-packings of $[n]$, then, by Corollaries 7.3.1 and 7.3.19, we have

$$|\mathcal{P}| 2n! \bar{f}(n) \leq \beta(F^{K_3^{\text{loop}}}, \mathcal{P}, n) \leq n!$$

whence

$$m(n, K_3^{\text{loop}}) \leq \frac{1}{2\bar{f}(n)}.$$

If $n \equiv 0 \pmod{3}$, then

$$\begin{aligned} m(n, K_3^{\text{loop}}) &\leq \frac{1}{2\bar{f}(n)} = \frac{1}{2} \left(\frac{3}{\binom{2n/3}{n/3}} - \frac{3}{\binom{n}{n/3}} \right)^{-1} = \frac{1}{2} \left(\frac{\binom{2n/3}{n/3} \binom{n}{n/3}}{3 \binom{n}{n/3} - 3 \binom{2n/3}{n/3}} \right) \\ &= \frac{1}{6 \left(1 - \frac{\binom{2n/3}{n/3}}{\binom{n}{n/3}} \right)} \binom{2n/3}{n/3} \end{aligned}$$

This gives $\delta_{n,0} = \frac{6(2n/3)_{n/3}}{(n)_{n/3}}$.

If $n \equiv 1 \pmod{3}$ then, $\lfloor 2n/3 \rfloor = 2\lfloor n/3 \rfloor$ and $\bar{f}(n) = f(\lfloor n/3 \rfloor + 1, \lfloor n/3 \rfloor, \lfloor n/3 \rfloor)$, and we have

$$\begin{aligned}
 m(n, K_3^{\text{loop}}) &\leq \frac{1}{2\bar{f}(n)} = \frac{1}{2} \left(\frac{2}{\binom{2\lfloor n/3 \rfloor + 1}{\lfloor n/3 \rfloor}} + \frac{1}{\binom{2\lfloor n/3 \rfloor}{\lfloor n/3 \rfloor}} - \frac{2}{\binom{n}{\lfloor n/3 \rfloor}} - \frac{1}{\binom{n}{\lfloor n/3 \rfloor + 1}} \right)^{-1} \\
 &= \frac{1}{2} \left(\frac{2}{\binom{2\lfloor n/3 \rfloor + 1}{\lfloor n/3 \rfloor + 1} \binom{2\lfloor n/3 \rfloor + 1}{\lfloor n/3 \rfloor}} + \frac{1}{\binom{2\lfloor n/3 \rfloor}{\lfloor n/3 \rfloor}} - \frac{2}{\binom{n}{\lfloor n/3 \rfloor}} - \frac{1}{\binom{2\lfloor n/3 \rfloor + 1}{x+1} \binom{n}{\lfloor n/3 \rfloor + 1}} \right)^{-1} \\
 &= \frac{1}{2} \left(\frac{\left(2 + \frac{1}{2\lfloor n/3 \rfloor + 1}\right) \binom{n}{\lfloor n/3 \rfloor} - \left(1.5 - \frac{1}{4x+2}\right) \binom{2\lfloor n/3 \rfloor}{\lfloor n/3 \rfloor}}{\binom{2\lfloor n/3 \rfloor}{\lfloor n/3 \rfloor} \binom{n}{\lfloor n/3 \rfloor}} \right)^{-1} \\
 &= \left[\frac{1}{4 + \frac{2}{2\lfloor n/3 \rfloor + 1} - \left(3 - \frac{1}{2\lfloor n/3 \rfloor + 1}\right) \frac{\binom{2\lfloor n/3 \rfloor}{\lfloor n/3 \rfloor}}{\binom{n}{\lfloor n/3 \rfloor}}} \right] \binom{2\lfloor n/3 \rfloor}{\lfloor n/3 \rfloor}
 \end{aligned}$$

This gives $\delta_{n,1} = \frac{2}{2\lfloor n/3 \rfloor + 1} - \left(3 - \frac{1}{2\lfloor n/3 \rfloor + 1}\right) \frac{(2\lfloor n/3 \rfloor)_{\lfloor n/3 \rfloor}}{(n)_{\lfloor n/3 \rfloor}}$.

If $n \equiv 2 \pmod{3}$ then, $\lfloor 2n/3 \rfloor = 2\lfloor n/3 \rfloor + 1$ and $\bar{f}(n) = f(\lfloor n/3 \rfloor + 1, \lfloor n/3 \rfloor + 1, \lfloor n/3 \rfloor)$, and we have

$$\begin{aligned}
 m(n, K_3^{\text{loop}}) &\leq \frac{1}{2\bar{f}(n)} = \frac{1}{2} \left(\frac{2}{\binom{2\lfloor n/3 \rfloor + 1}{\lfloor n/3 \rfloor}} + \frac{1}{\binom{2\lfloor n/3 \rfloor + 2}{\lfloor n/3 \rfloor + 1}} - \frac{2}{\binom{n}{\lfloor n/3 \rfloor + 1}} - \frac{1}{\binom{n}{\lfloor n/3 \rfloor}} \right)^{-1} \\
 &= \frac{1}{2} \left(\frac{2}{\binom{2\lfloor n/3 \rfloor + 1}{\lfloor n/3 \rfloor}} + \frac{1}{2\binom{2\lfloor n/3 \rfloor + 1}{\lfloor n/3 \rfloor}} - \frac{2}{2\binom{n}{\lfloor n/3 \rfloor}} - \frac{1}{\binom{n}{\lfloor n/3 \rfloor}} \right)^{-1}
 \end{aligned}$$

$$= \frac{1}{2} \left(\frac{2.5 \binom{n}{\lfloor n/3 \rfloor} - 2 \binom{2\lfloor n/3 \rfloor + 1}{\lfloor n/3 \rfloor}}{\binom{2\lfloor n/3 \rfloor + 1}{\lfloor n/3 \rfloor} \binom{n}{\lfloor n/3 \rfloor}} \right)^{-1} = \frac{1}{5 - 4 \frac{\binom{2\lfloor n/3 \rfloor + 1}{\lfloor n/3 \rfloor}}{\binom{n}{\lfloor n/3 \rfloor}}} \binom{2\lfloor n/3 \rfloor + 1}{\lfloor n/3 \rfloor}$$

This gives $\delta_{n,2} = \frac{4(2\lfloor n/3 \rfloor + 1) \lfloor n/3 \rfloor}{\binom{n}{\lfloor n/3 \rfloor}}$. ■

7.4 A new upper bound on $m(n, K_v^{\text{loop}})$

Poljak and Tuza [48] gave the upper bound

$$m(n, K_v^{\text{loop}}) \leq \frac{1}{2} \binom{\lfloor 2n/v \rfloor}{\lfloor n/v \rfloor}$$

by applying Theorem 6.1.5 to the K_2^{loop} -intersecting collection of packings of $[n]$ obtained from a K_v^{loop} -intersecting collection by selecting the two classes of smallest cardinality from each packing.

For $v = 3$, Theorem 7.3.20 improves their bound by using our generalized LYM inequality for K_3^{loop} which takes into account all three classes from each packing in a K_3^{loop} -intersecting collection.

Following the proof of Poljak and Tuza, we use our bound for $m(n, K_3^{\text{loop}})$ in place of Theorem 6.1.5 to improve the bound on $m(n, K_v^{\text{loop}})$ for all $v \geq 3$.

Corollary 7.4.1 If $v \geq 3$, then

$$m(n, K_v^{\text{loop}}) \leq \begin{cases} \frac{1}{6 - \delta_{\lfloor 3n/v \rfloor, 0}} \binom{\lfloor 2n/v \rfloor}{\lfloor n/v \rfloor}, & \text{if } \lfloor 3n/v \rfloor \equiv 0 \pmod{3}, \\ \frac{1}{4 + \delta_{\lfloor 3n/v \rfloor, 1}} \binom{\lfloor 2n/v \rfloor}{\lfloor n/v \rfloor}, & \text{if } \lfloor 3n/v \rfloor \equiv 1 \pmod{3}, \\ \frac{1}{5 - \delta_{\lfloor 3n/v \rfloor, 2}} \binom{\lfloor 2n/v \rfloor}{\lfloor n/v \rfloor}, & \text{if } \lfloor 3n/v \rfloor \equiv 2 \pmod{3}, \end{cases} \quad (7.4.1)$$

where, in each case, $\delta_{\lfloor 3n/v \rfloor, r}$ is a function that tends to zero as n grows.

[proof] Let $\mathcal{P} = \{P_1, \dots, P_m\}$ be a maximum K_v^{loop} -intersecting collection of v -packings of $[n]$, and let $m = m(n, K_v^{\text{loop}})$. From each packing $P_i \in \mathcal{P}$, choose the three classes of smallest cardinality, say $P_i^{a_i}, P_i^{b_i}, P_i^{c_i}$.

It follows that, for all $i \in [m]$, we have $|P_i^{a_i}| + |P_i^{b_i}| + |P_i^{c_i}| \leq 3n/v$; if not, then $|P_i^{a_i}| + |P_i^{b_i}| + |P_i^{c_i}| > 3n/v$ and, assuming $|P_i^{a_i}| \leq |P_i^{b_i}| \leq |P_i^{c_i}|$, we would also have $|P_i^{c_i}| > n/v$. If this were true, then it would follow that

$$\sum_{a \in [v]} |P_i^a| \geq |P_i^{a_i}| + |P_i^{b_i}| + |P_i^{c_i}| + (v-3)|P_i^{c_i}| > \frac{3n}{v} + (v-3)\frac{n}{v} = n$$

which is a contradiction.

Consequently, for all $i \in [m]$ we have $|P_i^{a_i}| + |P_i^{b_i}| + |P_i^{c_i}| \leq \lfloor 3n/v \rfloor$; furthermore, the collection $\mathcal{P}' = \{P'_1, \dots, P'_m\}$, where $P'_i = (P_i^{a_i}, P_i^{b_i}, P_i^{c_i})$ for each $i \in [m]$, forms a K_3^{loop} -intersecting collection of 3-packings of $\lfloor 3n/v \rfloor$.

Thus, $m \leq m(\lfloor 3n/v \rfloor, K_3^{\text{loop}}) \leq \frac{1}{2f(\lfloor 3n/v \rfloor)}$, and the bound now follows from Theorem 7.3.20. ■

Given v , for all $n \geq 22v/3$, our upper bound given in Corollary 7.4.1 satisfies

$$m(n, K_v^{\text{loop}}) < \frac{1}{4} \binom{\lfloor 2n/v \rfloor}{\lfloor n/v \rfloor}.$$

In this simplified form, it is easy to see that our bound improves the bound given by Poljak and Tuza by a factor greater than 2, for all n and v such that $n \geq 22v/3$.

7.5 The single-arc asymptotic estimate of $\beta(F, \mathcal{P}, n)$

Given a follow digraph F and an F -following collection $\mathcal{P}$, the exact terms of $\beta(F, \mathcal{P}, n)$ are tedious to compute, except for intersections $\bigcap_{ab \in S} X_i(a, b)$ with relatively simple subsets of arcs. Even for small follow digraphs for which $\beta(F, \mathcal{P}, n)$ is easily computed, the transformation of $\beta(F, \mathcal{P}, n)$ into an upper bound is quite challenging, as the previous sections demonstrated.

For these reasons, we prefer to estimate $\beta(F, \mathcal{P}, n)$ in some simpler way. In this section, we derive an estimate for $\beta(F, \mathcal{P}, n)$ based on its behaviour as n grows. Asymptotically, we will show that it suffices to consider only the single-arc terms of $\beta(F, \mathcal{P}, n)$; however, our asymptotic analysis is necessarily based on assumptions about how maximum F -following collections behave as $n \rightarrow \infty$. Whether these assumptions are realistic depends on the structure of F .

Let F be a fixed follow digraph with $V(F) = [v]$. To consider the limiting behaviour of $\beta(F, \mathcal{P}, n)$, we consider an infinite sequence of F -following collections, denoted $\{\mathcal{P}_n\}_{n=1}^\infty$. The n th F -following collection of our sequence, $\mathcal{P}_n$, is a maximum F -following collection of v -packings of $[n]$. Let m_n denote its cardinality, that is, $m_n = |\mathcal{P}_n|$, and we have $m_n \geq |\mathcal{P}|$ for all F -following collections $\mathcal{P}$ of $[n]$. We write $\mathcal{P}_n$ as $\mathcal{P}_n = \{P_{n,1}, \dots, P_{n,m_n}\}$, where each of its v -packings of $[n]$, $P_{n,i} \in \mathcal{P}_n$, is of the form $P_{n,i} = (P_{n,i}^1, P_{n,i}^2, \dots, P_{n,i}^v)$. This is our usual notation for F -following collections of v -packings of $[n]$, with the additional subscript n attached to all its components. Correspondingly, we use the notation $X_{n,i}(a, b)$ to denote the set of permutations of $[n]$ that contain $P_{n,i}^a$ followed by $P_{n,i}^b$.

Remark 7.5.1 Throughout the remainder of this section, let F be a fixed follow digraph with $V(F) = [v]$, and let $\{\mathcal{P}_n\}_{n=1}^\infty$ be a sequence of F -following collections as described above.

Our aim is to estimate $\beta(F, \mathcal{P}_n, n)$ using so-called single-arc terms. Let β_1 denote the following sum

$$\beta_1 = \sum_{i=1}^{m_n} \sum_{\substack{S \subseteq E(F) \\ |S|=1}} \left| \bigcap_{ab \in S} X_{n,i}(a, b) \right| = \sum_{i=1}^{m_n} \sum_{ab \in E(F)} |X_{n,i}(a, b)|.$$

We refer to β_1 as the *single-arc terms* of $\beta(F, \mathcal{P}, n)$. To justify the single-arc estimate, we will prove $\lim_{n \rightarrow \infty} \beta(F, \mathcal{P}_n, n) / \beta_1 = 1$, based on the following premise.

Premise 7.5.2 For each $a \in [v]$, there is a constant $p_a \in (0, 1)$ such that $\sum_{a \in [v]} p_a = 1$, and the following property holds: for every $\varepsilon > 0$ there exists n_ε such that for all $a \in [v]$, for all $n \geq n_\varepsilon$, and for all $i \in [m_n]$, where $n \geq n_\varepsilon$, we have

$$n(p_a - \varepsilon) < |P_{n,i}^a| < n(p_a + \varepsilon).$$

In Premise 7.5.2, we assume that there is a limiting distribution $p_a \in (0, 1)$ for each $a \in [v]$ such that the cardinalities of class a of all packings $P_{n,i} \in \mathcal{P}_n$ converge uniformly to a fixed proportion of n , namely p_a .

Consider the terms of $\beta(F, \mathcal{P}_n, n)$ as given in Theorem 6.2.9. Each term corresponds to a nonempty subset of arcs $S \subseteq E(F)$ such that S is acyclic, S is transitively closed in F , and S is equal to its own transitive reduction. The term of $\beta(F, \mathcal{P}_n, n)$ corresponding to S is $(-1)^{|S|+1} \left| \bigcap_{ab \in S} X_{n,i}(a, b) \right|$.

We focus on three types of subsets $S \subseteq E(F)$: the single-arc subsets, two-arc subsets, and subsets of size at least three, where in each case the subsets must satisfy the transitivity conditions above and induce an acyclic subgraph of F . We then show that all two-arc terms are dominated by the one-arc terms, and furthermore, any term with three or more arcs is less than each of the terms corresponding to its two-arc subsets. This will tell us that, for large n , the single-arc terms provide a reasonable estimate for $\beta(F, \mathcal{P}_n, n)$.

When $S \subseteq E(F)$ has exactly two arcs, there are three possibilities to consider (subject to transitivity conditions and being acyclic): $S = \{ab, cd\}$ where a, b, c, d are all distinct, $S = \{ab, ac\}$ where b and c are distinct, or $S = \{ba, ca\}$ where b and c are distinct. In the latter two cases, we have $|X_{n,i}(a, b) \cap X_{n,i}(a, c)| = |X_{n,i}(b, a) \cap X_{n,i}(c, a)|$, thus, there really are only two types of two-arc subsets to consider with respect to their contribution to $\beta(F, \mathcal{P}_n, n)$.

By choosing an appropriate arc from each two-arc subset S , we now prove that the chosen single-arc term dominates the term corresponding to S . Lemma 7.5.3 and Lemma 7.5.4 correspond to the types of two-arc subsets mentioned above, respectively.

Lemma 7.5.3 Let $ab, cd \in E(F)$, where a, b, c , and d are distinct. If Premise 7.5.2 holds, then

$$\lim_{n \rightarrow \infty} \frac{|X_{n,i}(a, b) \cap X_{n,i}(c, d)|}{|X_{n,j}(a, b)|} = 0,$$

where $i, j \in \{1, \dots, m_n\}$ for each n .

[proof] By Premise 7.5.2, for every $\varepsilon > 0$ there exists an n_ε such that for all $a \in [v]$, for all $n \geq n_\varepsilon$, for all $i \in [m_n]$, $n \geq n_\varepsilon$, we have

$$\lceil p_a n - \varepsilon n \rceil \leq |P_{n,i}^a| \leq \lfloor p_a n + \varepsilon n \rfloor.$$

Using the fact that $\binom{r+s}{r} \leq \binom{r'+s'}{r'}$ whenever $r \leq r'$ and $s \leq s'$, we have the following bounds for all $a \in [v]$, for all $n \geq n_\varepsilon$, and for all $i \in [m_n]$, $n \geq n_\varepsilon$:

$$\binom{\lceil p_a n - \varepsilon n \rceil + \lceil p_b n - \varepsilon n \rceil}{\lceil p_a n - \varepsilon n \rceil} \leq \binom{|P_{n,i}^a| + |P_{n,i}^b|}{|P_{n,i}^a|} \leq \binom{\lfloor p_a n + \varepsilon n \rfloor + \lfloor p_b n + \varepsilon n \rfloor}{\lfloor p_a n + \varepsilon n \rfloor}. \quad (7.5.1)$$

Similarly, the inequalities of (7.5.1) hold when a and b are replaced by c and d , respectively.

To count the permutations in $|X_{n,i}(a, b) \cap X_{n,i}(c, d)|$, that is, the permutations that contain both $P_{n,i}^a$ followed by $P_{n,i}^b$ as well as $P_{n,i}^c$ followed by $P_{n,i}^d$, we choose $|P_{n,i}^a| + |P_{n,i}^b| + |P_{n,i}^c| + |P_{n,i}^d|$ positions among n positions for the elements of $P_{n,i}^a$, $P_{n,i}^b$, $P_{n,i}^c$, and $P_{n,i}^d$. From among these chosen positions, we choose $|P_{n,i}^a| + |P_{n,i}^b|$ positions for the elements of $P_{n,i}^a$ and $P_{n,i}^b$. There are $|P_{n,i}^a|!$ ways to arrange the elements of $P_{n,i}^a$ in the first of these positions and $|P_{n,i}^b|!$ ways to arrange the elements of $P_{n,i}^b$ in the remaining positions chosen for the elements of $P_{n,i}^a$ and $P_{n,i}^b$. In the remaining $|P_{n,i}^c| + |P_{n,i}^d|$ positions chosen from n , there are $|P_{n,i}^c|!$ ways to arrange the elements of $P_{n,i}^c$ in the first of these positions and there are $|P_{n,i}^d|!$ ways to arrange the elements of $P_{n,i}^d$ in the last of these positions. Finally, there are $(n - |P_{n,i}^a| - |P_{n,i}^b| - |P_{n,i}^c| - |P_{n,i}^d|)!$ ways to arrange the remaining elements of $[n]$. This total can be simplified as follows:

$$\begin{aligned} & |X_{n,i}(a, b) \cap X_{n,i}(c, d)| \\ &= \binom{n}{|P_{n,i}^a| + |P_{n,i}^b| + |P_{n,i}^c| + |P_{n,i}^d|} \binom{|P_{n,i}^a| + |P_{n,i}^b| + |P_{n,i}^c| + |P_{n,i}^d|}{|P_{n,i}^a| + |P_{n,i}^b|} |P_{n,i}^a|! |P_{n,i}^b|! |P_{n,i}^c|! |P_{n,i}^d|! (n - |P_{n,i}^a| - |P_{n,i}^b| - |P_{n,i}^c| - |P_{n,i}^d|)! \\ &= n! \binom{|P_{n,i}^a| + |P_{n,i}^b|}{|P_{n,i}^a|}^{-1} \binom{|P_{n,i}^c| + |P_{n,i}^d|}{|P_{n,i}^c|}^{-1}. \end{aligned} \quad (7.5.2)$$

Similarly,

$$|X_{n,j}(a, b)| = n! \binom{|P_{n,j}^a| + |P_{n,j}^b|}{|P_{n,j}^a|}^{-1}. \quad (7.5.3)$$

For convenience, let $A_{n,i,j}$ denote $\frac{|X_{n,i}(a,b) \cap X_{n,i}(c,d)|}{|X_{n,j}(a,b)|}$. Using the formulae in (7.5.2) and (7.5.3), and the bounds given in (7.5.1), for all $n \geq n_\varepsilon$ and for all $i, j \in \{1, \dots, m_n\}$, we have

$$A_{n,i,j} \leq \frac{\binom{\lfloor p_a n + \varepsilon n \rfloor + \lfloor p_b n + \varepsilon n \rfloor}{\lfloor p_a n + \varepsilon n \rfloor}}{\binom{\lceil p_a n - \varepsilon n \rceil + \lceil p_b n - \varepsilon n \rceil}{\lceil p_a n - \varepsilon n \rceil} \binom{\lceil p_c n - \varepsilon n \rceil + \lceil p_d n - \varepsilon n \rceil}{\lceil p_c n - \varepsilon n \rceil}}. \quad (7.5.4)$$

Define $\Delta_n = \lfloor p_a n + \varepsilon n \rfloor - \lceil p_a n - \varepsilon n \rceil$ and $\Theta_n = \lfloor p_b n + \varepsilon n \rfloor - \lceil p_b n - \varepsilon n \rceil$. By cancelling common factors, the upper bound given in (7.5.4) can be rewritten as follows:

$$A_{n,i,j} \leq \frac{(\lfloor p_a n + \varepsilon n \rfloor + \lfloor p_b n + \varepsilon n \rfloor)_{\Delta_n + \Theta_n}}{(\lfloor p_a n + \varepsilon n \rfloor)_{\Delta_n} (\lfloor p_b n + \varepsilon n \rfloor)_{\Theta_n}} \frac{[p_c n - \varepsilon n]!}{(\lceil p_c n - \varepsilon n \rceil + \lceil p_d n - \varepsilon n \rceil)_{\lceil p_c n - \varepsilon n \rceil}}. \quad (7.5.5)$$

The second factor of our upper bound given in (7.5.5) is bounded as follows:

$$\begin{aligned}
\frac{[p_c n - \varepsilon n]!}{([p_c n - \varepsilon n] + [p_d n - \varepsilon n])_{[p_c n - \varepsilon n]}} &\leq \left(\frac{[p_c n - \varepsilon n]}{[p_c n - \varepsilon n] + [p_d n - \varepsilon n]} \right)^{[p_c n - \varepsilon n]} \quad (\text{by Lemma 7.1.3}) \\
&\leq \left(\frac{p_c n - \varepsilon n + 1}{p_c n - \varepsilon n + p_d n - \varepsilon n} \right)^{p_c n - \varepsilon n} \\
&= \left(\frac{p_c - \varepsilon + \frac{1}{n}}{p_c + p_d - 2\varepsilon} \right)^{(p_c - \varepsilon)n}. \tag{7.5.6}
\end{aligned}$$

The first factor of our upper bound given in (7.5.5) can be rewritten as follows:

$$\frac{([p_a n + \varepsilon n] + [p_b n + \varepsilon n])_{\Delta_n + \Theta_n}}{[p_a n + \varepsilon n]_{\Delta_n} [p_b n + \varepsilon n]_{\Theta_n}} = \frac{([p_a n + \varepsilon n] + [p_b n + \varepsilon n])_{\Delta_n} ([p_a n + \varepsilon n] + [p_b n + \varepsilon n] - \Delta_n)_{\Theta_n}}{[p_a n + \varepsilon n]_{\Delta_n} [p_b n + \varepsilon n]_{\Theta_n}}. \tag{7.5.7}$$

Notice that $2\varepsilon n - 2 \leq \Delta_n \leq 2\varepsilon n$ for all n , and similarly, $2\varepsilon n - 2 \leq \Theta_n \leq 2\varepsilon n$. Like the bound given in (7.5.6), we can similarly bound (7.5.7) as follows:

$$\begin{aligned}
&\left(\frac{[p_a n + \varepsilon n] + [p_b n + \varepsilon n] - \Delta_n}{[p_a n + \varepsilon n] - \Delta_n} \right)^{\Delta_n} \left(\frac{[p_a n + \varepsilon n] + [p_b n + \varepsilon n] - \Delta_n - \Theta_n}{[p_b n + \varepsilon n] - \Theta_n} \right)^{\Theta_n} \\
&= \left(\frac{[p_a n - \varepsilon n] + [p_b n + \varepsilon n]}{[p_a n - \varepsilon n]} \right)^{\Delta_n} \left(\frac{[p_a n - \varepsilon n] + [p_b n - \varepsilon n]}{[p_b n - \varepsilon n]} \right)^{\Theta_n} \\
&\leq \left(\frac{p_a n - \varepsilon n + 1 + p_b n + \varepsilon n}{p_a n - \varepsilon n} \right)^{\Delta_n} \left(\frac{p_a n - \varepsilon n + 1 + p_b n - \varepsilon n + 1}{p_b n - \varepsilon n} \right)^{\Theta_n} \\
&\leq \left(\frac{p_a + p_b + \frac{1}{n}}{p_a - \varepsilon} \right)^{2\varepsilon n} \left(\frac{p_a + p_b - 2\varepsilon + \frac{2}{n}}{p_b - \varepsilon} \right)^{2\varepsilon n}. \tag{7.5.8}
\end{aligned}$$

From (7.5.6) and (7.5.8), for any $\varepsilon > 0$ and for all $n \geq n_\varepsilon$, we have the following bound:

$$A_{n,i,j} \leq \left(\frac{p_a + p_b + \frac{1}{n}}{p_a - \varepsilon} \right)^{2\varepsilon n} \left(\frac{p_a + p_b - 2\varepsilon + \frac{2}{n}}{p_b - \varepsilon} \right)^{2\varepsilon n} \left(\frac{p_c - \varepsilon + \frac{1}{n}}{p_c + p_d - 2\varepsilon} \right)^{(p_c - \varepsilon)n}. \tag{7.5.9}$$

We can choose δ such that $\varepsilon \geq \delta > 0$, and $n_\delta \geq n_\varepsilon$ such that for all $n \geq n_\delta$ we have

$$\left(\frac{p_a + p_b + \frac{1}{n}}{p_a - \delta} \right)^{\sqrt{\delta}} \leq \left(\frac{p_c + p_d - 2\delta}{p_c - \delta + \frac{1}{n}} \right) \text{ and } \left(\frac{p_a + p_b - 2\delta + \frac{2}{n}}{p_b - \delta} \right)^{\sqrt{\delta}} \leq \left(\frac{p_c + p_d - 2\delta}{p_c - \delta + \frac{1}{n}} \right).$$

Consequently, for all $n \geq n_\delta$ we have

$$\left(\frac{p_a + p_b + \frac{1}{n}}{p_a - \delta} \right)^{2\delta n} \leq \left(\frac{p_c - \delta + \frac{1}{n}}{p_c + p_d - 2\delta} \right)^{-2\sqrt{\delta}n} \quad (7.5.10)$$

and

$$\left(\frac{p_a + p_b - 2\delta + \frac{2}{n}}{p_b - \delta} \right)^{2\delta n} \leq \left(\frac{p_c - \delta + \frac{1}{n}}{p_c + p_d - 2\delta} \right)^{-2\sqrt{\delta}n}. \quad (7.5.11)$$

Finally, choose γ such that $\delta \geq \gamma > 0$ and $p_c > \gamma + 4\sqrt{\gamma}$. It now follows from (7.5.9), (7.5.10), and (7.5.11) that, for all $n \geq n_\gamma$, we have

$$\begin{aligned} A_{n,i,j} &\leq \left(\frac{p_c - \gamma + \frac{1}{n}}{p_c + p_d - 2\gamma} \right)^{-2\sqrt{\gamma}n} \left(\frac{p_c - \delta + \frac{1}{n}}{p_c + p_d - 2\delta} \right)^{-2\sqrt{\delta}n} \left(\frac{p_c - \gamma + \frac{1}{n}}{p_c + p_d - 2\gamma} \right)^{(p_c - \gamma)n} \\ &= \left(\frac{p_c - \gamma + \frac{1}{n}}{p_c + p_d - 2\gamma} \right)^{(p_c - \gamma - 4\sqrt{\gamma})n} \end{aligned} \quad (7.5.12)$$

From (7.5.12), it now follows that

$$\lim_{n \rightarrow \infty} \frac{|X_{n,i}(a, b) \cap X_{n,i}(c, d)|}{|X_{n,j}(a, b)|} \leq \lim_{n \rightarrow \infty} \left(\frac{p_c - \gamma + \frac{1}{n}}{p_c + p_d - 2\gamma} \right)^{(p_c - \gamma - 4\sqrt{\gamma})n} = 0. \quad \blacksquare$$

Lemma 7.5.4 Let $ab, ac \in E(F)$ with $b \neq c$. If Premise 7.5.2 holds, then

$$\lim_{n \rightarrow \infty} \frac{|X_{n,i}(a, b) \cap X_{n,i}(a, c)|}{|X_{n,j}(a, b)|} = 0,$$

where $i, j \in \{1, \dots, m_n\}$ for each n .

[proof] The proof is similar to that of Lemma 7.5.3.

First, we have

$$|X_{n,i}(a, b) \cap X_{n,i}(a, c)| = n! \binom{|P_{n,i}^a| + |P_{n,i}^b| + |P_{n,i}^c|}{|P_{n,i}^a|}^{-1}$$

and

$$|X_{n,j}(a, b)| = n! \binom{|P_{n,j}^a| + |P_{n,j}^b|}{|P_{n,j}^a|}^{-1}.$$

Therefore

$$\frac{|X_{n,i}(a, b) \cap X_{n,i}(a, c)|}{|X_{n,j}(a, b)|} = \frac{\binom{|P_{n,j}^a| + |P_{n,j}^b|}{|P_{n,j}^a|}}{\binom{|P_{n,i}^a| + |P_{n,i}^b| + |P_{n,i}^c|}{|P_{n,i}^a|}}. \quad (7.5.13)$$

We now work on bounding the expression in (7.5.13).

By Premise 7.5.2, for every $\varepsilon > 0$ there exists an n_ε such that for all $n \geq n_\varepsilon$ and for all $i, j \in \{1, \dots, m_n\}$, we have

$$\begin{aligned} \frac{|X_{n,i}(a, b) \cap X_{n,i}(a, c)|}{|X_{n,j}(a, b)|} &\leq \frac{\binom{\lfloor p_a n + \varepsilon n \rfloor + \lfloor p_b n + \varepsilon n \rfloor}{\lfloor p_a n + \varepsilon n \rfloor}}{\binom{\lceil p_a n - \varepsilon n \rceil + \lceil p_b n - \varepsilon n \rceil + \lceil p_c n - \varepsilon n \rceil}{\lceil p_a n - \varepsilon n \rceil}} \\ &= \frac{(\lfloor p_a n + \varepsilon n \rfloor + \lfloor p_b n + \varepsilon n \rfloor)_{\lfloor p_a n + \varepsilon n \rfloor}}{(\lfloor p_a n + \varepsilon n \rfloor)_{\lfloor p_a n + \varepsilon n \rfloor} (\lceil p_a n - \varepsilon n \rceil + \lceil p_b n - \varepsilon n \rceil + \lceil p_c n - \varepsilon n \rceil)_{\lceil p_a n - \varepsilon n \rceil}} \end{aligned} \quad (7.5.14)$$

To bound (7.5.14), define $\Delta_n = \lfloor p_a n + \varepsilon n \rfloor - \lceil p_a n - \varepsilon n \rceil$. Rewrite (7.5.14) as follows, and apply the bounds given by Lemma 7.1.3 as shown below:

$$\begin{aligned} &\frac{(\lfloor p_a n + \varepsilon n \rfloor + \lfloor p_b n + \varepsilon n \rfloor)_{\Delta_n + \lceil p_a n - \varepsilon n \rceil}}{(\lfloor p_a n + \varepsilon n \rfloor)_{\Delta_n} (\lceil p_a n - \varepsilon n \rceil + \lceil p_b n - \varepsilon n \rceil + \lceil p_c n - \varepsilon n \rceil)_{\lceil p_a n - \varepsilon n \rceil}} \\ &= \frac{(\lfloor p_a n + \varepsilon n \rfloor + \lfloor p_b n + \varepsilon n \rfloor)_{\Delta_n} (\lfloor p_a n + \varepsilon n \rfloor + \lfloor p_b n + \varepsilon n \rfloor - \Delta_n)_{\lceil p_a n - \varepsilon n \rceil}}{(\lfloor p_a n + \varepsilon n \rfloor)_{\Delta_n} (\lceil p_a n - \varepsilon n \rceil + \lceil p_b n - \varepsilon n \rceil + \lceil p_c n - \varepsilon n \rceil)_{\lceil p_a n - \varepsilon n \rceil}} \\ &\leq \left(\frac{\lfloor p_a n + \varepsilon n \rfloor + \lfloor p_b n + \varepsilon n \rfloor - \Delta_n}{\lfloor p_a n + \varepsilon n \rfloor - \Delta_n} \right)^{\Delta_n} \left(\frac{\lfloor p_a n + \varepsilon n \rfloor + \lfloor p_b n + \varepsilon n \rfloor - \Delta_n}{\lceil p_a n - \varepsilon n \rceil + \lceil p_b n - \varepsilon n \rceil + \lceil p_c n - \varepsilon n \rceil} \right)^{\lceil p_a n - \varepsilon n \rceil} \\ &\quad \text{(by Lemma 7.1.3)} \\ &= \left(\frac{\lceil p_a n - \varepsilon n \rceil + \lfloor p_b n + \varepsilon n \rfloor}{\lfloor p_a n - \varepsilon n \rceil} \right)^{\Delta_n} \left(\frac{\lceil p_a n - \varepsilon n \rceil + \lfloor p_b n + \varepsilon n \rfloor}{\lceil p_a n - \varepsilon n \rceil + \lceil p_b n - \varepsilon n \rceil + \lceil p_c n - \varepsilon n \rceil} \right)^{\lceil p_a n - \varepsilon n \rceil} \\ &\leq \left(\frac{p_a n - \varepsilon n + 1 + p_b n + \varepsilon n}{p_a n - \varepsilon n} \right)^{2\varepsilon n} \left(\frac{p_a n - \varepsilon n + 1 + p_b n + \varepsilon n}{p_a n - \varepsilon n + p_b n - \varepsilon n + p_c n - \varepsilon n} \right)^{(p_a - \varepsilon)n} \end{aligned}$$

$$= \left(\frac{p_a + p_b + \frac{1}{n}}{p_a - \varepsilon} \right)^{2\varepsilon n} \left(\frac{p_a + p_b + \frac{1}{n}}{p_a + p_b + p_c - 3\varepsilon} \right)^{(p_a - \varepsilon)n} \quad (7.5.15)$$

Choose $\delta > 0$ small enough and n_δ large enough that, for all $n \geq n_\delta$, we have

$$\left(\frac{p_a + p_b + \frac{1}{n}}{p_a - \delta} \right)^{\sqrt{\delta}} \leq \left(\frac{p_a + p_b + p_c - 3\delta}{p_a + p_b + \frac{1}{n}} \right).$$

Equivalently,

$$\left(\frac{p_a + p_b + \frac{1}{n}}{p_a - \delta} \right)^{2\delta n} \leq \left(\frac{p_a + p_b + \frac{1}{n}}{p_a + p_b + p_c - 3\delta} \right)^{-2\sqrt{\delta}n}. \quad (7.5.16)$$

Choose $\gamma > 0$ such that $\delta \geq \gamma > 0$ and $p_a > \gamma + 2\sqrt{\gamma}$. It now follows from (7.5.15) and (7.5.16) that, for all $n \geq n_\gamma$, we have

$$\begin{aligned} \frac{|X_{n,i}(a, b) \cap X_{n,i}(a, c)|}{|X_{n,j}(a, b)|} &\leq \left(\frac{p_a + p_b + \frac{1}{n}}{p_a - \gamma} \right)^{2\gamma n} \left(\frac{p_a + p_b + \frac{1}{n}}{p_a + p_b + p_c - 3\gamma} \right)^{(p_a - \gamma)n} \\ &\leq \left(\frac{p_a + p_b + \frac{1}{n}}{p_a + p_b + p_c - 3\gamma} \right)^{(p_a - \gamma - 2\sqrt{\gamma})n}. \end{aligned} \quad (7.5.17)$$

From (7.5.17), the desired limit now follows:

$$\lim_{n \rightarrow \infty} \frac{|X_{n,i}(a, b) \cap X_{n,i}(a, c)|}{|X_{n,j}(a, b)|} \leq \lim_{n \rightarrow \infty} \left(\frac{p_a + p_b + \frac{1}{n}}{p_a + p_b + p_c - 3\gamma} \right)^{(p_a - \gamma - 2\sqrt{\gamma})n} = 0. \quad \blacksquare$$

Lemma 7.5.5 Let S and T be subsets of $E(F)$. If $T \subseteq S$, then

$$\left| \bigcap_{ab \in S} X_{n,i}(a, b) \right| \leq \left| \bigcap_{ab \in T} X_{n,i}(a, b) \right|. \quad \blacksquare$$

We now have the means to prove the main theorem for this section. Let $\beta_{\geq 2}$ denote the sum of the terms of $\beta(F, \mathcal{P}_n, n)$ with two or more arcs, that is,

$$\beta_{\geq 2} = \sum_{i=1}^{m_n} \sum_{\substack{S \in \mathfrak{S} \\ |S| \geq 2}} (-1)^{|S|+1} \left| \bigcap_{ab \in S} X_{n,i}(a, b) \right|$$

where $\mathfrak{S}$ denotes the set of all nonempty subsets $S \subseteq E(F)$ such that S is acyclic and $S = S^t = \hat{S}$.

Theorem 7.5.6 Let F be a follow digraph, and let $\{\mathcal{P}_n\}_{n=1}^\infty$ be a sequence of maximum F -following collections of v -packings. If Premise 7.5.2 holds, then

$$\lim_{n \rightarrow \infty} \beta(F, \mathcal{P}_n, n) / \beta_1 = 1.$$

[proof] For each subset $S \in \mathfrak{S}$ such that $|S| \geq 2$, choose a subset $T_S \subseteq S$ with $|T_S| = 2$. By Lemma 7.5.5, we have

$$\beta(F, \mathcal{P}_n, n) \leq \beta_1 + |\beta_{\geq 2}| \leq \beta_1 + \sum_{i=1}^{m_n} \sum_{\substack{S \in \mathfrak{S} \\ |S| \geq 2}} \left| \bigcap_{ab \in T_S} X_{n,i}(a, b) \right|.$$

For each T_S and for a fixed n , define $i_{\max} = i_{\max}(T_S, n)$ to be the index in $\{1, \dots, m_n\}$ such that $|\bigcap_{ab \in T_S} X_{n,i_{\max}}(a, b)| \geq |\bigcap_{ab \in T_S} X_{n,i}(a, b)|$ for all $i \in \{1, \dots, m_n\}$. Similarly, for a fixed arc $ab \in E(F)$ and a fixed n , define $i_{\min} = i_{\min}(ab, n)$ to be the index such that $|X_{n,i_{\min}}(a, b)| \leq |X_{n,i}(a, b)|$ for all $i \in \{1, \dots, m_n\}$. Consequently,

$$\begin{aligned} \lim_{n \rightarrow \infty} \frac{|\beta_{\geq 2}|}{\beta_1} &= \lim_{n \rightarrow \infty} \frac{\sum_{\substack{S \in \mathfrak{S} \\ |S| \geq 2}} \sum_{i=1}^{m_n} \left| \bigcap_{ab \in S} X_{n,i}(a, b) \right|}{\sum_{ab \in E(F)} \sum_{i=1}^{m_n} |X_{n,i}(a, b)|} \\ &\leq \lim_{n \rightarrow \infty} \frac{\sum_{\substack{S \in \mathfrak{S} \\ |S| \geq 2}} \sum_{i=1}^{m_n} \left| \bigcap_{ab \in T_S} X_{n,i}(a, b) \right|}{\sum_{ab \in E(F)} \sum_{i=1}^{m_n} |X_{n,i}(a, b)|} \quad (\text{using } T_S \subseteq S \text{ and Lemma 7.5.5}) \\ &\leq \lim_{n \rightarrow \infty} \frac{\sum_{\substack{S \in \mathfrak{S} \\ |S| \geq 2}} m_n \left| \bigcap_{ab \in T_S} X_{n,i_{\max}}(a, b) \right|}{\sum_{ab \in E(F)} m_n |X_{n,i_{\min}}(a, b)|} \quad (\text{by definition of } i_{\max} \text{ and } i_{\min}) \end{aligned}$$

$$= \sum_{\substack{S \in \mathfrak{S} \\ |S| \geq 2}} \lim_{n \rightarrow \infty} \frac{\left| \bigcap_{ab \in T_S} X_{n, i_{\max}}(a, b) \right|}{\sum_{ab \in E(F)} |X_{n, i_{\min}}(a, b)|}. \quad (7.5.18)$$

Notice that the denominator in (7.5.18) satisfies $\sum_{ab \in E(F)} |X_{n, i_{\min}}(a, b)| \geq |X_{n, i_{\min}}(x, y)|$ for any choice of $xy \in E(F)$.

For each T_S , label its two arcs as $a_S b_S$ and $c_S d_S$ so that $|\bigcap_{ab \in T_S} X_{n, i_{\max}}(a, b)| = |X_{n, i_{\max}}(a_S, b_S) \cap X_{n, i_{\max}}(c_S, d_S)|$.

We can bound the expression given in (7.5.18) as follows:

$$\sum_{\substack{S \in \mathfrak{S} \\ |S| \geq 2}} \lim_{n \rightarrow \infty} \frac{\left| \bigcap_{ab \in T_S} X_{n, i_{\max}}(a, b) \right|}{\sum_{ab \in E(F)} |X_{n, i_{\min}}(a, b)|} \leq \sum_{\substack{S \in \mathfrak{S} \\ |S| \geq 2}} \lim_{n \rightarrow \infty} \frac{|X_{n, i_{\max}}(a_S, b_S) \cap X_{n, i_{\max}}(c_S, d_S)|}{|X_{n, i_{\min}}(a_S, b_S)|} \quad (7.5.19)$$

where we arbitrarily choose the arc $a_S b_S \in T_S$ to give the lower bound used in the denominator in (7.5.19).

Therefore, for each subset T_S , we may apply Lemma 7.5.3 or Lemma 7.5.4 to the limit in (7.5.19), as required. We sum over the number of two-arc subsets of $E(F)$, which is a constant at most $2^{|E(F)|} - |E(F)|$. Thus, we have a finite sum of limits that converge to zero. It now follows that,

$$\lim_{n \rightarrow \infty} |\beta_{\geq 2} / \beta_1| = 0.$$

Consequently,

$$\lim_{n \rightarrow \infty} \frac{\beta(F, \mathcal{P}_n, n)}{\beta_1} = \lim_{n \rightarrow \infty} \frac{\beta_1 + \beta_{\geq 2}}{\beta_1} = 1. \quad \blacksquare$$

The following observation regarding the non-single-arc terms of $\beta(F, \mathcal{P}_n, n)$, along with Theorem 7.5.6, allow us to give an asymptotic upper bound on $m(n, K_v^{\text{loop}})$ at the end of this section.

Corollary 7.5.7 If Premise 7.5.2 holds, then $\lim_{n \rightarrow \infty} \beta_{\geq 2} / n! = 0$.

[**proof**] Since $\mathcal{P}_n$ is an F -following collection, each permutation π of $[n]$ is an element of at most one of the unions $\bigcup_{ab \in E(F)} X_{n,i}(a, b)$ (for at most one $P_{n,i} \in \mathcal{P}_n$). Thus, in β_1 , a permutation π can be counted at most $|E(F)|$ times (π can be counted up to $|E(F)|$ times in $\sum_{ab \in E(F)} |X_{n,i}(a, b)|$ for at most one $i \in [m_n]$).

Thus, $0 \leq \beta_1 \leq |E(F)| n!$ and it follows that

$$-|E(F)| \left| \frac{\beta_{\geq 2}}{\beta_1} \right| \leq - \left| \frac{\beta_1 \beta_{\geq 2}}{n! \beta_1} \right| \leq \frac{\beta_{\geq 2}}{n!} \leq \left| \frac{\beta_1 \beta_{\geq 2}}{n! \beta_1} \right| \leq |E(F)| \left| \frac{\beta_{\geq 2}}{\beta_1} \right|$$

By Theorem 7.5.6, we have $\lim_{n \rightarrow \infty} \beta_{\geq 2}/\beta_1 = 0$, and the result follows. ■

If Premise 7.5.2 holds, then, for large n , Theorem 7.5.6 provides a basis for justifying the following single-arc estimate:

$$\beta(F, \mathcal{P}, n) \sim \beta_1.$$

Essentially, Theorem 7.5.6 says that $\beta_{\geq 2}$ is negligible for large n . Informally, using β_1 to estimate $\beta(F, \mathcal{P}, n)$ is desirable since, for larger follow digraphs, $\beta_{\geq 2}$ gets messy, while β_1 remains very simple.

7.6 Alignment decomposition balance for single-arc terms

Let H be a strong graph with $V(H) = [v]$, let (W, X, Y) be its alignment decomposition, and let $F = F^H$ be its maximal follow digraph. If $\mathcal{P}$ is an H -intersecting collection of v -packings of $[n]$, let β_1 denote the sum of the single-arc terms of $\beta(F, \mathcal{P}, n)$, that is,

$$\beta_1 = \sum_{i=1}^{|\mathcal{P}|} \sum_{ab \in E(F)} |X_i(a, b)|.$$

We have seen that single-arc terms are easy to count: for any given arc $ab \in E(F)$, we have

$$|X_i(a, b)| = n! \binom{|P_i^a| + |P_i^b|}{|P_i^a|}^{-1}.$$

Thus,

$$\beta_1 = \sum_{i=1}^{|\mathcal{P}|} \sum_{ab \in E(F)} n! \binom{|P_i^a| + |P_i^b|}{|P_i^a|}^{-1}. \quad (7.6.1)$$

If we use β_1 to approximate $\beta(F, \mathcal{P}, n)$, then, in order to approximate an upper bound on $m(n, H)$, we would like a lower bound for β_1 .

Define a function f on v variables as follows:

$$f(x_1, \dots, x_v) = \sum_{ab \in E(F)} \binom{x_a + x_b}{x_a}^{-1}.$$

Now, we can rewrite β_1 in terms of f :

$$\beta_1 = \sum_{i=1}^{|\mathcal{P}|} n! f(|P_i^1|, |P_i^2|, \dots, |P_i^v|).$$

To obtain a lower bound on β_1 , we are looking for the minimizing values of $x_1, \dots, x_v$ with respect to the value of f . This is the same general approach we used to obtain bounds on $\beta(F^{S_3}, \mathcal{P}, n)$ and $\beta(F^{K_3^{\text{loop}}}, \mathcal{P}, n)$. Now we apply this approach to a generic strong graph H , but restrict our attention to single-arc terms, that is, β_1 .

In Proposition 7.6.1, we will derive a lower bound for β_1 by showing that there exist integers $l_1, \dots, l_v$ such that $l_a \geq 1$, for all $a \in [v]$, $\sum_{a \in [v]} l_a = n$, and $f(l_1, \dots, l_v) \leq f(|P_i^1|, |P_i^2|, \dots, |P_i^v|)$ for all i . Moreover, the integers l_a , $a \in [v]$ will be **balanced with respect to the alignment decomposition of H** , meaning

1. for all $w, w' \in W$ we have $|l_w - l_{w'}| \leq 1$,
2. for all $x, x' \in X$ we have $|l_x - l_{x'}| \leq 1$, and
3. for all $y, y' \in Y$ we have $|l_y - l_{y'}| \leq 1$.

Proposition 7.6.1 Let H be a strong graph with $V(H) = [v]$ and maximal follow digraph F^H . If $\mathcal{P}$ is an H -intersecting collection of packings of $[n]$, then there exist positive integers $l_1, \dots, l_v$ such that

$$|\mathcal{P}| n! \sum_{ab \in E(F^H)} \binom{l_a + l_b}{l_a}^{-1} \leq \beta_1 = \sum_{i=1}^{|\mathcal{P}|} n! \sum_{ab \in E(F^H)} \binom{|P_i^a| + |P_i^b|}{|P_i^a|}^{-1},$$

and the integers $l_1, \dots, l_v$ are balanced with respect to the alignment decomposition of H .

[**proof**] Let (W, X, Y) be the alignment decomposition of H . Recall that in the maximal follow digraph F^H every two distinct vertices in W are symmetrically adjacent, each vertex in X is adjacent to all vertices in $W \cup Y$, and each vertex in W is adjacent to all vertices in Y .

Suppose there exist vertices b and c such that $|P_i^b|$ and $|P_i^c|$ are unbalanced and the vertices b and c both belong to the same part of the alignment decomposition of H . Assume without loss of generality that $|P_i^c| \geq |P_i^b| + 2$. We will consider all terms of β_1 involving $|P_i^b|$ or $|P_i^c|$ and show that the substitutions $|P_i^b| \leftarrow |P_i^b| + 1$ and $|P_i^c| \leftarrow |P_i^c| - 1$ can only reduce the value of β_1 .

If an arc of F^H involves both b and c , then b and c must both belong to W . In this case, β_1 contains the two terms

$$|X_i(b, c)| = n! \binom{|P_i^b| + |P_i^c|}{|P_i^b|}^{-1} \quad \text{and} \quad |X_i(c, b)| = n! \binom{|P_i^b| + |P_i^c|}{|P_i^b|}^{-1}.$$

Since $|P_i^b| + 2 \leq |P_i^c|$, we have $|P_i^b| + 1 \leq \frac{1}{2}(|P_i^b| + |P_i^c|)$. Thus,

$$\binom{|P_i^b| + 1 + |P_i^c| - 1}{|P_i^b| + 1}^{-1} \leq \binom{|P_i^b| + |P_i^c|}{|P_i^b|}^{-1}.$$

Consider the arcs of F^H involving b but not c (the argument for arcs involving c but not b is similar). If an arc of F^H involves b but not c , then its other end must be some vertex $a \in [v] - \{b, c\}$. If a is adjacent to b , then $a \in W \cup X$, and we can pair the arc ab with ac . If b is adjacent to a , then $a \in W \cup Y$ and we can pair the arc ba with bc . In either case, the terms of β_1 corresponding to these pairs of arcs yields the same contribution to β_1 , namely

$$n! \binom{|P_i^a| + |P_i^b|}{|P_i^b|}^{-1} \quad \text{and} \quad n! \binom{|P_i^a| + |P_i^c|}{|P_i^c|}^{-1}.$$

By Lemma 7.1.4, it follows that

$$\binom{|P_i^a| + |P_i^b| + 1}{|P_i^b| + 1}^{-1} + \binom{|P_i^a| + |P_i^c| - 1}{|P_i^c| - 1}^{-1} \leq \binom{|P_i^a| + |P_i^b|}{|P_i^b|}^{-1} + \binom{|P_i^a| + |P_i^c|}{|P_i^c|}^{-1}.$$

The terms of β_1 corresponding to arcs of F^H involving neither b nor c will not be affected by the substitutions $|P_i^b| \leftarrow |P_i^b| + 1$ and $|P_i^c| \leftarrow |P_i^c| - 1$. Thus, in all cases, the substitutions $|P_i^b| \leftarrow |P_i^b| + 1$ and $|P_i^c| \leftarrow |P_i^c| - 1$ help to reduce β_1 . We can iterate the above substitutions until we reach balanced cardinalities $||P_i^b| - |P_i^c|| \leq 1$.

Our procedure for making substitutions and applying Lemma 7.1.4 terminates when we have integers $l_i^1, \dots, l_i^v$ that are balanced with respect to the alignment decomposition of H . At this stage we have

$$\sum_{ab \in E(F^H)} \binom{l_i^a + l_i^b}{l_i^a}^{-1} \leq \sum_{ab \in E(F^H)} \binom{|P_i^a| + |P_i^b|}{|P_i^a|}^{-1}. \quad (\star)$$

Since there exist integers l_i^a , $a \in [v]$ for each i , we can choose $l_a, \dots, l_b$ to be the l_i^a with the smallest sum on the left side of $(\star)$, among all i . ■

7.6.1 The single-arc asymptotic upper bound on $m(n, K_v^{\text{loop}})$

Using the single-arc estimate and bound given by Proposition 7.6.1, we obtain the following upper bound on $m(n, K_v^{\text{loop}})$.

Theorem 7.6.2 If Premise 7.5.2 holds, then

$$m(n, K_v^{\text{loop}}) \leq \frac{1}{v^2 - v} \binom{2\lfloor n/v \rfloor + 2}{\lfloor n/v \rfloor + 1} (1 + o(1)).$$

[proof] Let $H = K_v^{\text{loop}}$, let $F = F^H$, and let $\mathcal{P}$ be a maximum H -intersecting collection of v -packings of $[n]$. By Proposition 7.6.1, a lower bound for β_1 is given by

$$\sum_{i=1}^{|\mathcal{P}|} n! \sum_{ab \in E(F)} \binom{l_a + l_b}{l_a}^{-1} \leq \beta_1 = \sum_{i=1}^{|\mathcal{P}|} n! \sum_{ab \in E(F^H)} \binom{|P_i^a| + |P_i^b|}{|P_i^a|}^{-1},$$

where the integers $l_1, \dots, l_v$ satisfy $l_a \geq 1$ for all $a \in [v]$, $\sum_{a \in [v]} l_a = n$, and the l_a , $a \in [v]$, are balanced with respect to the alignment decomposition of H . In this case, the entire alignment decomposition of $H = K_v^{\text{loop}}$ is simply W (as X and Y are empty). Thus, for all $a \in [v] = W$, the balanced integers l_a have two options: $l_a \in \{\leq \lfloor n/v \rfloor, \lceil n/v \rceil\}$. It now follows that, for all $a, b \in [v]$, we have

$$\binom{l_a + l_b}{l_a} \leq \binom{2\lfloor n/v \rfloor + 2}{\lfloor n/v \rfloor + 1}.$$

We get the following lower bound on β_1 :

$$|\mathcal{P}| \sum_{ab \in E(F)} n! \binom{2\lfloor n/v \rfloor + 2}{\lfloor n/v \rfloor + 1}^{-1} \leq \beta_1 \leq n! - \beta_{\geq 2}. \quad (7.6.2)$$

In F^H , there are $2\binom{v}{2} = v^2 - v$ arcs, thus, the expression in (7.6.2) is equivalent to the following upper bound on $|\mathcal{P}| = m(n, K_3^{\text{loop}})$:

$$m(n, K_3^{\text{loop}}) \leq \frac{1}{v^2 - v} \binom{2\lfloor n/v \rfloor + 2}{\lfloor n/v \rfloor + 1} \left(1 - \frac{\beta_{\geq 2}}{n!}\right).$$

By Corollary 7.5.7, the sum of the two-or-more-arc terms satisfies $\beta_{\geq 2}/n! = o(1)$. ■

If the upper bound of Theorem 7.6.2 does not hold, then Premise 7.5.2 must be false. In particular, the seemingly natural belief that there should always exist optimal covering arrays exhibiting a balanced occurrence of symbols would not hold for $v \geq 3$. Since Premise 7.5.2 is based on one particular sequence of F -following collections, if Premise 7.5.2 were false, then there would not even exist an infinite sequence of optimal covering arrays for which the frequency of symbols tended to any limiting distribution.

Chapter 8

FOR arrays

In this chapter, we define forbidden–optional–required arrays, abbreviated FOR arrays, which are generalizations of covering arrays that accommodate all three types of interactions and any combination of alphabet sizes and interaction-strengths. They are, by far, the most general version of covering arrays considered in this thesis.

In Section 8.1, we introduce FOR arrays and our model using hypergraphs. In Section 8.2, we examine some properties that can prevent FOR arrays from existing. In Section 8.3, we give bounds on the number of rows in FOR arrays, when they exist. In Section 8.4, we establish that several decision problems related to FOR arrays are NP-hard. In Section 8.5, we study compatibility hypergraphs which we define to encode sets of required interactions that can consistently be covered together in a row of a FOR array. In Section 8.6, we investigate critical FOR systems and the effects of deleting required or forbidden interactions. In Section 8.8, we model a particular class of FOR arrays using binary relational systems and homomorphisms. We show that a relevant binary relational system is a core.

8.1 The general FOR model

Suppose we have a testing problem with k factors, labelled $1, \dots, k$. Each factor $j \in [k]$ can have one of v_j possible values, labelled $1, \dots, v_j$. Based on the particulars of this problem, we are interested in generating a test suite that caters to all our whims: we want certain interactions covered by the test suite, we want to avoid

covering certain other interactions, and we do not care what happens with the rest. We have the freedom to classify every interaction (any strength t) of our testing problem as one of these three types.

We use a hypergraph to encode the required, forbidden and optional interactions of such a testing problem as follows:

A **FOR system** is a k -partite hypergraph X with vertices labelled by the factor-value pairs of a given testing problem: $V(X) = \{(j, a_j) : j \in [k], a_j \in [v_j]\}$. Each part of X corresponds to one factor: $P_j = \{(j, a) : a \in [v_j]\}$. The edge set of X is partitioned into three classes, denoted $F(X)$, $O(X)$, and $R(X)$. For all $t \in [k]$, each t -way interaction must belong to exactly one of the three classes $F(X)$, $O(X)$, or $R(X)$. Let $I = \{(j_1, a_1), \dots, (j_t, a_t)\}$ be a t -way interaction. If $I \in R(X)$, then I is called a **required interaction**. If $I \in F(X)$, then I is a **forbidden interaction**. If $I \in O(X)$, then I is called an **optional interaction**.

The **family of FOR systems** having k factors with alphabet sizes $v_1, \dots, v_k$ is denoted $\mathcal{X}_{(v_1, \dots, v_k)}$. If, for all $i \in [k]$, we have a constant v such that $v_i = v$, then we denote the family by $\mathcal{X}_{k,v}$ instead. If, for some $t \in [k]$, we have $|I| = t$ for all $I \in R(X)$, then X has **required strength** t . If, for some $t \in [k]$, we have $|I| = t$ for all $I \in F(X)$, then X has **forbidden strength** t . If X has required strength t and forbidden strength t , then X is a FOR system of **strength** t . If $X \in \mathcal{X}_{k,v}$ has a homogeneous alphabet $[v]$, then X is a **v -ary** FOR system. If $X \in \mathcal{X}_{k,2}$, then X is a **binary** FOR system.

FOR systems are generalizations of the forbidden edges graphs used to encode the forbidden interactions of CAFEs.

Remark 8.1.1 Much of the terminology we use in this chapter is based on the paper in which CAFEs were introduced, namely [19], and adapted as necessary to fit the FOR setting.

Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ be a FOR system and let $I = \{(j_1, a_1), \dots, (j_t, a_t)\}$ be a t -way interaction of X . Let T be a k -tuple, where $T = (x_1, \dots, x_k) \in [v_1] \times \dots \times [v_k]$. If $x_{j_i} = a_i$ for all $i \in [t]$, then T is said to **cover** I . If T does not cover I , then T is said to **avoid** I . If, for all $I \in F(X)$, T avoids I , then T is called a **k -tuple avoiding** $F(X)$, or T is said to be **consistent with** X .

Definition 8.1.2 Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ be a FOR system. A **FOR array** of X , denoted

$\text{FOR}(n, X)$, is an $n \times k$ array A with the following properties:

- For each $i \in [k]$, column i has symbols from the alphabet $[v_i]$.
- Every row of A forms a k -tuple avoiding $F(X)$.
- For each required edge $I \in R(X)$, there exists a row of A that covers I .

The **FOR array number** of X , denoted $\text{FORN}(X)$, is the smallest integer n for which there exists a $\text{FOR}(n, X)$, if there exists a FOR array of X ; if there does not exist a FOR array of X , then we write $\text{FORN}(X) = +\infty$.

Some remarks

We think of testing problems interchangeably with the corresponding FOR system $X \in \mathcal{X}_{(v_1, \dots, v_k)}$. Since, in terms of arrays, factors correspond to columns and values correspond to the respective alphabets of each column, we sometimes refer to factors as columns, or values as the alphabet.

When defining the relations of a particular FOR system $X \in \mathcal{X}_{(v_1, \dots, v_k)}$, we omit specifying the edges of the optional relation $O(X)$. A FOR array of X depends only on the relations $R(X)$ and $F(X)$; it is implied that all interactions that are not in $R(X) \cup F(X)$ are necessarily in $O(X)$.

Given $X \in \mathcal{X}_{(v_1, \dots, v_k)}$, if $I \in R(X)$ is a required interaction, then any k -tuple that covers I necessarily covers I' for all $I' \subset I$. By the same token, if $I \in F(X)$ is a forbidden interaction, then every row of a $\text{FOR}(n, X)$ must avoid I . Consequently, for all J such that $J \supseteq I$, each row of a $\text{FOR}(n, X)$ necessarily avoids J as well.

For the sake of illustrating an example of a FOR system, we only illustrate maximal (with respect to set inclusion) required edges, and minimal (with respect to set inclusion) forbidden edges; we do not illustrate optional edges. Our convention is to illustrate required edges using green and forbidden edges using red.

8.1.1 An example to motivate the use of FOR arrays

To illustrate the applicability of FOR arrays, we present a toy example of a testing problem; this example is extracted from [10] and can also be found in [19, 41].

Table 8.1 lists the five factors of a mobile phone product line and their possible values.

FACTORS	1. display	2. email viewer	3. camera	4. video camera	5. video ringtones
VALUES	1. 16 million colours 2. 8 million colours 3. b & w	1. graphical 2. text 3. none	1. 2 MP 2. 1 MP 3. none	1. yes 2. no	1. yes 2. no

Table 8.1: Mobile phone product line

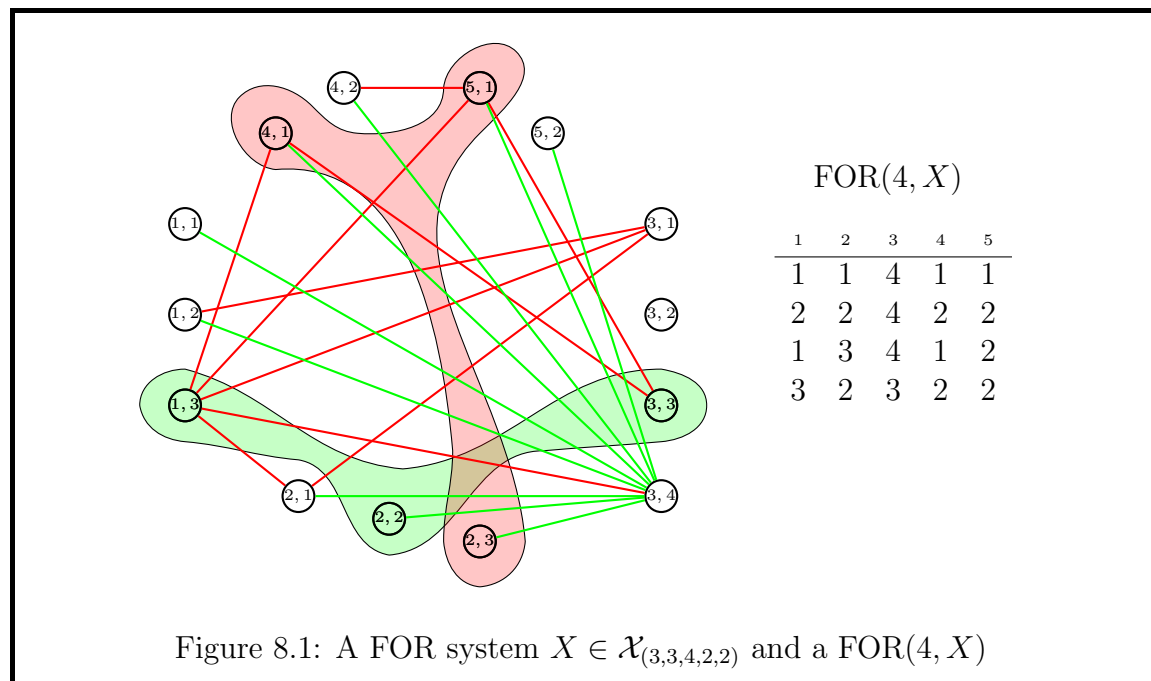
The mobile phone product line contains some inherent constraints. For example, video ringtones cannot be used without the presence of a video camera. Table 8.2 gives a list of constraints on the various options, as well as the resulting forbidden interactions.

CONSTRAINTS	FORBIDDEN INTERACTIONS
(C1) graphical email viewer requires a colour display	$\{(1, 3), (2, 1)\}$
(C2) 2 MP camera requires a colour display	$\{(1, 3), (3, 1)\}$
(C3) graphical email viewer is not supported with 2 MP camera	$\{(2, 1), (3, 1)\}$
(C4) 8 million colour display does not support a 2 MP camera	$\{(1, 2), (3, 1)\}$
(C5) video camera requires a camera and a colour display	$\{(3, 3), (4, 1)\}$ $\{(1, 3), (4, 1)\}$
(C6) video ringtones cannot occur without a video camera	$\{(4, 2), (5, 1)\}$

Table 8.2: Constraints on the mobile phone product line

Using a FOR system $X \in \mathcal{X}_{(3,3,3,2,2)}$, we encode the forbidden interactions given in Table 8.2 as edges in $F(X)$. In $R(X)$, we include all pairwise interactions other than those corresponding to the constraints of Table 8.2. Notice that X restricted to $F(X)$ is precisely the forbidden edges graph $G \in \mathcal{G}_{(3,3,3,2,2)}$ given in Figure 2.3. The avoidance closure $\hat{G}$ and a $\text{CAFE}(10, \hat{G})$ are also given in Figure 2.3.

Using the CAFE given in Figure 2.3, we run the ten tests on the mobile phone product line. From these tests, we discover a faulty 3-way interaction $\{(2, 3), (4, 1), (5, 1)\}$ corresponding to the options “no email viewer, video camera, and video ringtones.” Since running these tests, a new value for the camera factor has become available for testing: a 4 MP camera, corresponding to the new factor-value pair $(3, 4)$. Furthermore, the 4 MP camera **requires** a colour display, resulting in a new forbidden interaction $\{(1, 3), (3, 4)\}$. We also notice that the CAFE did not cover the 3-way interaction $\{(1, 3), (2, 2), (3, 3)\}$ corresponding to the options “b & w display, text email viewer, and no camera.” We would like to test this 3-way interaction since those three values are a likely grouping for a basic phone model.



We want to run tests to see how the 4 MP camera interacts with the other mobile phone product line options, but we do not want our previous tests to go to waste. We can accomplish this using a FOR array.

In Figure 8.1, we give a FOR system $X \in \mathcal{X}_{(3,3,4,2,2)}$ that encodes the resulting required and forbidden interactions. The green edges depict the required edges from the new factor-value pair (3, 4) to the other factors of the system. The green blob depicts the required 3-way interaction $\{(1, 3), (2, 2), (3, 3)\}$ which was not covered by the CAFE. The red edges are the forbidden interactions based on the constraints of the mobile phone product line and the avoidance closure of the corresponding forbidden edges graph. We also include the new forbidden edge $\{(1, 3), (3, 4)\}$ and the discovered forbidden 3-way interaction $\{(2, 3), (4, 1), (5, 1)\}$. The remaining interactions are optional—they have either been tested already, or go beyond the scope of our testing. In Figure 8.1, we also include an optimal FOR(4, X).

8.1.2 How FOR arrays generalize covering arrays and allies

To see that a covering array $CA(n; t, k, (v_1, \dots, v_k))$ is a particular FOR array, define a FOR system $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ as follows. For each t -subset $\{j_1, \dots, j_t\} \subseteq [k]$, let

$I = \{(j_1, a_1), \dots, (j_t, a_t)\} \in R(X)$ for all t -tuples $(a_1, \dots, a_t) \in [v_{j_1}] \times \dots \times [v_{j_t}]$. Let $F(X) = \emptyset$. Clearly, the required edges of X encode required coverage so that a $\text{FOR}(n, X)$ is a $\text{CA}(n; t, k, (v_1, \dots, v_l))$.

To see that CAFEs are special cases of FOR arrays, take a forbidden edges graph $G \in \mathcal{G}_{(v_1, \dots, v_k)}$ and define a FOR system $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ as follows. Let $I = \{(i, a), (j, b)\}$, where $i, j \in [k]$, $i \neq j$, $a \in [v_i]$, and $b \in [v_j]$. If $I \in E(G)$ is a forbidden edge, then we let $I \in F(X)$. Otherwise, we let $I \in R(X)$. It is easy to see that a $\text{FOR}(n, X)$ is simply a $\text{CAFE}(n, G)$.

To see that covering arrays on graphs are special cases of FOR arrays, take a simple graph G with $V(G) = [k]$ and an integer $v \geq 2$. Define a FOR system $X \in \mathcal{X}_{k,v}$ as follows. For each $i, j \in [k]$ such that $ij \in E(G)$, let $\{(i, a), (j, b)\} \in R(X)$ for all $(a, b) \in [v]^2$. Let $F(X) = \emptyset$. In this case, a $\text{FOR}(n, X)$ is a $\text{CA}(n; 2, G, v)$.

To see that covering arrays on column graphs with alphabet graphs are a special subfamily of FOR arrays, let G be a column graph with $V(G) = [k]$ and let H be an alphabet graph with $V(H) = [v]$. Define a FOR system $X \in \mathcal{X}_{k,v}$ with $F(X) = \emptyset$ and where $R(X)$ is given by the edges of the underlying graph of the categorical product $G \times H$; all other interactions are optional. It is easy to see that a $\text{FOR}(n, X)$ is a $\text{CA}(n; 2, G, H)$.

To see that variable strength covering arrays are special cases of FOR arrays, let Λ be a collection of nonempty subsets of $[k]$. For each $i \in [k]$, let v_i denote the number of values of factor i . Define a FOR system $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ as follows. For each set $\{j_1, \dots, j_t\} \in \Lambda$, let $\{(j_1, a_1), \dots, (j_t, a_t)\} \in R(X)$ for all $(a_1, \dots, a_t) \in [v_{j_1}] \times \dots \times [v_{j_t}]$. Let $F(X) = \emptyset$. Clearly, a $\text{FOR}(n, X)$ is a $\text{VCA}(n; \Lambda, (v_1, \dots, v_k))$.

8.2 Existence of FOR arrays

As with CAFEs, knowing whether a FOR array exists, for a given FOR system, is a nontrivial question which we explore in this section.

Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ be a FOR system. A required interaction $I \in R(X)$ is **consistent with** X if there exists a k -tuple avoiding $F(X)$ that covers I . If there is no k -tuple avoiding $F(X)$ that covers I , then I is **inconsistent** with X . If all edges $I \in R(X)$ are consistent with X , then X is a **consistent FOR system**.

Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ be a FOR system. The **downset of** $R(X)$, denoted $R^\downarrow(X)$, is the set of nonempty interactions

$$R^\downarrow(X) = \{I \subseteq V(X) : I \subseteq J \text{ for some } J \in R(X)\}.$$

The **upset of** $F(X)$, denoted $F_\uparrow(X)$, is the set of interactions

$$F_\uparrow(X) = \{I \subseteq V(X) : J \subseteq I \text{ for some } J \in F(X)\}.$$

The **downset-facets** of the downset $R^\downarrow(X)$ are the maximal (with respect to set inclusion) required edges in $R^\downarrow(X)$. Similarly, the **upset-facets** of the upset $F_\uparrow(X)$ are the minimal (with respect to set inclusion) forbidden edges in $F_\uparrow(X)$.

The following is an obvious necessary condition for a FOR array to exist.

Lemma 8.2.1 Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ be a FOR system. If a FOR array of X exists, then $R^\downarrow(X) \cap F_\uparrow(X) = \emptyset$.

[**proof**] If we had an interaction $I \in R^\downarrow(X) \cap F_\uparrow(X)$, then $I \subseteq J$ for some $J \in R(X)$ and $I \supseteq J'$ for some $J' \in F(X)$. Consequently, $J' \subseteq J$. In this case, a k -tuple that covers J cannot avoid J' , so J is inconsistent. ■

Given a FOR system $X \in \mathcal{X}_{(v_1, \dots, v_k)}$, consider the FOR system $X' \in \mathcal{X}_{(v_1, \dots, v_k)}$ with $R(X') = R^\downarrow(X)$ and $F(X') = F_\uparrow(X)$. It is clear that an array is a FOR array of X if and only if it is a FOR array of X' .

Two FOR systems X_1 and X_2 from the same family $\mathcal{X}_{(v_1, \dots, v_k)}$ are **equivalent** if $R^\downarrow(X_1) = R^\downarrow(X_2)$ and $F_\uparrow(X_1) = F_\uparrow(X_2)$. Among a set of equivalent FOR systems, we have two extreme systems: the **full system** X such that $R(X) = R^\downarrow(X)$ and $F(X) = F_\uparrow(X)$, and the **compact system** X' such that $R(X')$ and $F(X')$ are the downset-facets of $R^\downarrow(X)$ and upset-facets of $F_\uparrow(X)$, respectively. In the compact system X' , no required (or forbidden) interaction is a proper subset of another required (or forbidden) interaction.

Remark 8.2.2 From now on, we assume that FOR systems are compact unless stated otherwise. Given $X \in \mathcal{X}_{(v_1, \dots, v_k)}$, we also assume $R^\downarrow(X) \cap F_\uparrow(X) = \emptyset$.

Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ be a FOR system. If X is not consistent, then we can transform X into a consistent FOR system, denoted $\hat{X}$, called the **avoidance closure of** X , as follows. Let $I_1, \dots, I_s$ be the list of inconsistent interactions from the downset $R^\downarrow(X)$.

The avoidance closure $\hat{X}$ has $V(\hat{X}) = V(X)$. The required edge set $R(\hat{X})$ consists of the downset-facets of $R^\downarrow(X) - \{I_1, \dots, I_s\}$. The forbidden edge set $F(\hat{X})$ consists of the upset-facets of $F(X) \cup \{I_1, \dots, I_s\}$.

The avoidance closure $\hat{X}$ is a consistent FOR system and is uniquely determined by X . In the most extreme case, every required interaction of $R^\downarrow(X)$ is inconsistent and $\hat{X}$ has $R(\hat{X}) = \emptyset$.

To build a consistent system from X , it suffices to let $R(\hat{X})$ be the downset-facets of $R^\downarrow(X) - \{I_1, \dots, I_s\}$ and let $O(\hat{X}) = O(X) \cup \{I_1, \dots, I_s\}$. If we had chosen to let the inconsistent I_j 's be optional rather than forbidden, we still would not have any consistent k -tuples covering any of the I_j ; it is therefore superfluous to label inconsistent interactions as optional, which justifies the definition of avoidance closure given above.

Danziger, Mendelsohn, Moura, and Stevens [19] gave the following characterization of consistent binary forbidden edges graphs, which applies to binary FOR systems of strength 2, as follows.

Proposition 8.2.3 (Danziger, Mendelsohn, Moura & Stevens [19]) A binary forbidden edges graph $G \in \mathcal{G}_{k,2}$ is consistent if and only if

1. $\{(i, a), (j, b)\} \in E(G)$ whenever there exist vertices in the same part $(l, 0)$ and $(l, 1)$ such that $\{(i, a), (l, 0)\} \in E(G)$ and $\{(j, b), (l, 1)\} \in E(G)$;
2. for all $j \in [k]$, for all $b \in \{0, 1\}$, we have $\{(i, a), (j, b)\} \in E(G)$ whenever there exists a factor $l \in [k]$ such that $\{(i, a), (l, 0)\} \in E(G)$ and $\{(i, a), (l, 1)\} \in E(G)$. ■

Corollary 8.2.4 A binary FOR system $X \in \mathcal{X}_{k,2}$ of strength 2 is consistent if and only if

1. $\{(i, a), (j, b)\} \in O(X) \cup F(X)$ whenever there exist vertices in the same part $(l, 0)$ and $(l, 1)$ such that $\{(i, a), (l, 0)\} \in F(X)$ and $\{(j, b), (l, 1)\} \in F(X)$;
2. for all $j \in [k]$, for all $b \in \{0, 1\}$, we have $\{(i, a), (j, b)\} \in O(X) \cup F(X)$ whenever there exists a factor $l \in [k]$ such that $\{(i, a), (l, 0)\} \in F(X)$ and $\{(i, a), (l, 1)\} \in F(X)$. ■

For larger alphabets, we do not have such a characterization for consistent FOR systems, but we can say something about “forced factors” of binary FOR systems

regardless of the strength of the required interactions. We also show that the situation is more complicated for non-binary alphabets. To this end, we need some definitions and notation.

Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ be a FOR system and let $U = \{(j_1, a_1), \dots, (j_t, a_t)\}$ be an interaction. The **row set** of U , denoted $rs(U)$, is the set of k -tuples $R = (r_1, \dots, r_k) \in [v_1] \times \dots \times [v_k]$ that cover U and avoid $F(X)$. Clearly, U is consistent with X if and only if $rs(U) \neq \emptyset$. Assuming $rs(U) \neq \emptyset$, a factor $i \in [k]$ is **forced** by U , if, for all k -tuples $(r_1, \dots, r_k) \in rs(U)$, the i th entry r_i is a constant. The **forced factor set of U** , denoted $f(U)$, is the set of factors forced by U . In particular, all factors in U are forced by U . For each $i \in f(U)$, we denote by $f_U(i)$ the **value of i forced by U** . For example, for all $(j_i, a_i) \in U$, we have $f_U(j_i) = a_i$. If $i \in f(U)$ and $f_U(i) = a$, then sometimes we write $(i, a) \in f(U)$. We also write $f(i, a)$ to abbreviate $f(\{(i, a)\})$, and similarly, we write $rs(i, a)$ to abbreviate $rs(\{(i, a)\})$.

A maximal (with respect to set inclusion) interaction has the smallest row set and largest forced factor set among those interactions contained in it, as follows.

Lemma 8.2.5 Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ and let $V = \{(j_1, a_1), \dots, (j_t, a_t)\}$ be a set of factor-value pairs, where the factors j_i are all distinct. If $U \subseteq V$, then $rs(V) \subseteq rs(U)$ and $f(U) \subseteq f(V)$. Moreover, for all $j \in f(U)$ we have $f_U(j) = f_V(j)$.

[**proof**] Let $U \subseteq V$ and let $R \in rs(V)$. In particular, R is a k -tuple that covers U and avoids $F(X)$, thus $R \in rs(U)$. Therefore, $rs(V) \subseteq rs(U)$. If $j \in f(U)$, then the j th entry of each k -tuple $R \in rs(U)$ is fixed to the value $f_U(j)$. As $rs(V) \subseteq rs(U)$, the j th entry of every k -tuple in $rs(V)$ is equal to $f_U(j)$. Thus $j \in f(V)$ and clearly $f_V(j) = f_U(j)$. ■

Forced factors have a “transitive property”, as follows.

Lemma 8.2.6 Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$. Suppose $j_1, j_2, j_3 \in [k]$ and $a_i \in [v_i]$ for $i = 1, 2, 3$. Suppose $rs(j_1, a_1) \neq \emptyset$. If $(j_2, a_2) \in f(j_1, a_1)$ and $(j_3, a_3) \in f(j_2, a_2)$, then $(j_3, a_3) \in f(j_1, a_1)$.

[**proof**] For any k -tuple $R = (r_1, \dots, r_k) \in rs(j_1, a_1)$, we must have $r_{j_1} = a_1$. Since $(j_2, a_2) \in f(j_1, a_1)$, it follows that $r_{j_2} = a_2$. Hence $R \in rs(j_2, a_2)$. Since $(j_3, a_3) \in f(j_2, a_2)$, it follows that $r_{j_3} = a_3$. ■

The following lemma gives one structure that results in a “globally forced factor.” Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ and let (i, a) be a fixed factor-value pair. If, for each factor-value pair (j, a_j) such that $rs(j, a_j) \neq \emptyset$, we have $(i, a) \in f(j, a_j)$, then i is called a **globally forced factor**.

Lemma 8.2.7 Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$. If $(i, a) \in f(j, b)$ for all $b \in [v_j]$, then $(i, a) \in f(l, c_l)$ for all (l, c_l) such that $l \in [k]$, $c_l \in [v_l]$, and $rs(l, c_l) \neq \emptyset$.

[proof] Let $R = (r_1, \dots, r_k)$ be a consistent k -tuple. Since $(i, a) \in f(j, b)$ for all $b \in [v_j]$, it follows that $(i, a) \in f(j, r_j)$. Consequently, $r_i = a$. Therefore, every consistent k -tuple has $r_i = a$. ■

When we have a binary FOR system with forbidden strength 2, the following proposition says that the forced factors of an interaction are determined by the forced factors of the individual factor-value pairs within the interaction. For $a \in \{0, 1\}$, let $\bar{a} = 1 - a$.

Proposition 8.2.8 Let $X \in \mathcal{X}_{k,2}$ be a binary FOR system with forbidden strength 2, and let $U = \{(j_1, a_1), \dots, (j_t, a_t)\}$ be a set of factor-value pairs, where the factors j_i are all distinct. If $rs(U) \neq \emptyset$, then $f(U) = \bigcup_{(j_i, a_i) \in U} f(j_i, a_i)$.

[proof] Let $A = \bigcup_{(j, a_j) \in U} f(j, a_j)$, let $B = f(U) \setminus A$, and let $C = [k] \setminus f(U)$. By Lemma 8.2.5, we have $f(j, a_j) \subseteq f(U)$ for all $(j, a_j) \in U$. Therefore, $A \subseteq f(U)$. Clearly, $A \cup B = f(U)$. We now prove that it is impossible to have $A \subsetneq f(U)$ by showing that $B = \emptyset$.

If $B \neq \emptyset$, then there exists $(i, a) \in B$ with $f_U(i) = a$. By definition of B , we must have $(i, a) \notin f(j, a_j)$ for all $(j, a_j) \in U$. In particular, this means that $(i, a) \notin U$, and there can be no forbidden interactions of the form $\{(j, a_j), (i, \bar{a})\}$ where $(j, a_j) \in A$. Moreover, (i, a) cannot be a globally forced factor-value pair.

Since (i, a) is not globally forced, there must exist at least one consistent k -tuple $T = (t_1, \dots, t_k)$ such that $t_i = \bar{a}$. Similarly, since $rs(U) \neq \emptyset$, there is a consistent k -tuple $R = (r_1, \dots, r_k)$ that covers all factor-value pairs in U and, consequently, in $f(U)$. Define a new k -tuple, $S = (s_1, \dots, s_k)$, as follows. Let

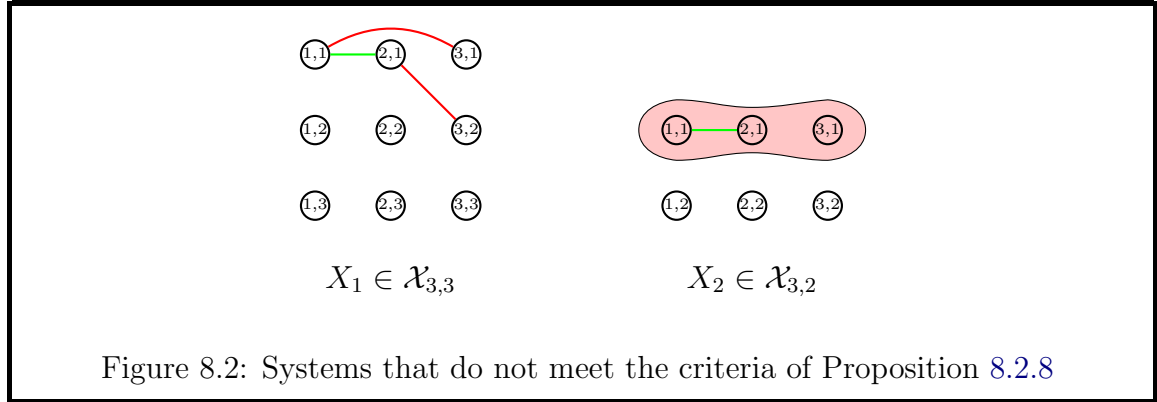
$$s_j = \begin{cases} r_j, & \text{if } j \in A; \\ t_j, & \text{if } j \in B \cup C. \end{cases}$$

Clearly, S covers all factor-value pairs in A but does not cover $(i, a) \in B \subseteq f(U)$. We claim that S is a consistent k -tuple (a contradiction).

For $x, y \in A$, the interaction $\{(x, s_x), (y, s_y)\}$ is not forbidden as R avoids $F(X)$. Similarly, for $x, y \in B \cup C$, the interaction $\{(x, s_x), (y, s_y)\}$ is not forbidden as T avoids $F(X)$. If there is no forbidden interaction of the form $\{(x, s_x), (y, s_y)\}$, where $x \in A$ and $y \in B \cup C$, then we will have shown that S is a k -tuple that covers U and avoids $F(X)$. Therefore, suppose $\{(x, s_x), (y, s_y)\}$ is forbidden for some x, y where $x \in A$ and $y \in B \cup C$.

Consequently, we have $(y, \bar{s}_y) \in f(x, s_x)$ where $(x, s_x) \in f(j, a_j)$ for some $(j, a_j) \in U$. By Lemma 8.2.6, this means that $(y, \bar{s}_y) \in f(j, a_j)$ for some $(j, a_j) \in U$, hence $y \in A$. This contradicts the fact that R is a consistent k -tuple.

Therefore, the interaction $\{(x, s_x), (y, s_y)\}$ cannot be forbidden. It now follows that S is a k -tuple that avoids $F(X)$ and covers U , but also covers $(i, \bar{a})$, contradicting the fact that $(i, a) \in B \subseteq f(U)$. Therefore, the set B must be empty, as claimed. ■



Proposition 8.2.8 does not hold for non-binary FOR systems, nor does it hold for binary FOR systems having forbidden interactions of strength $t \geq 3$. To see these claims are true, consider the two FOR systems given in Figure 8.2.

The system $X_1 \in \mathcal{X}_{3,3}$ has two forbidden pairwise interactions, $\{(1, 1), (3, 1)\}$ and $\{(2, 1), (3, 2)\}$ (represented by red edges), and one required pairwise interaction, $\{(1, 1), (2, 1)\}$ (represented by the green edge). Take $U = \{(1, 1), (2, 1)\}$. The forced factor set of U is $f(U) = \{1, 2, 3\}$. On the other hand, the union of the forced factor sets of the individual factor-value pairs in U is $f(1, 1) \cup f(2, 1) = \{1, 2\}$.

The system $X_2 \in \mathcal{X}_{3,2}$ has one forbidden 3-way interaction $\{(1,1), (2,1), (3,1)\} \in F(X_2)$ (represented by the red blob), and one required pairwise interaction, namely $\{(1,1), (2,1)\} \in R(X_2)$ (represented by the green edge). Take $U = \{(1,1), (2,1)\}$. The forced factor set of U is $f(U) = \{1,2,3\}$, while $f(1,1) \cup f(2,1) = \{1,2\}$.

Our next result says that for binary systems with forbidden strength 2, we can build a consistent k -tuple one factor-value pair at a time, given that the additional factor-value pair is compatible with each of the previously assigned factor-value pairs.

Corollary 8.2.9 Let $X \in \mathcal{X}_{k,2}$ be a binary FOR system with forbidden strength 2, let $U = \{(j_1, a_1), \dots, (j_m, a_m)\}$ be consistent with X , and let $(j_{m+1}, a_{m+1}) \in [k] \times [2]$ be a factor-value pair such that $j_{m+1} \notin \{j_1, \dots, j_m\}$. If, for each $i \in [m]$, the pairwise interaction $\{(j_i, a_i), (j_{m+1}, a_{m+1})\}$ is consistent, then $U \cup \{(j_{m+1}, a_{m+1})\}$ is also consistent.

[proof] Let $R = (r_1, \dots, r_k)$ be a consistent k -tuple that covers U , and let $T = (t_1, \dots, t_k)$ be a consistent k -tuple that covers (j_{m+1}, a_{m+1}) . Clearly, T also covers the forced factor set $f(j_{m+1}, a_{m+1})$. Define a new k -tuple $S = (s_1, \dots, s_k)$ as follows: Let

$$s_i = \begin{cases} t_i, & \text{if } i \in f(j_{m+1}, a_{m+1}) \\ r_i, & \text{otherwise.} \end{cases}$$

We claim that the k -tuple S is well-defined since any factor in $f(U) \cap f(j_{m+1}, a_{m+1})$ must have the same forced value. By Proposition 8.2.8, we know that $f(U) = \bigcup_{(j_x, a_x) \in U} f(j_x, a_x)$. Thus, if $i \in f(U) \cap f(j_{m+1}, a_{m+1})$, then $i \in f(j, b)$ for some $(j, b) \in U$. By assumption, $\{(j, b), (j_{m+1}, a_{m+1})\}$ is consistent, so we must have $f_{\{(j_{m+1}, a_{m+1})\}}(i) = f_{\{(j, b)\}}(i) = f_U(i)$, as claimed.

Furthermore, we claim that S is consistent. Since R is consistent with X , for all $x, y \in [k] \setminus f(j_{m+1}, a_{m+1})$, there are no forbidden interactions of the form $\{(x, s_x), (y, s_y)\}$. Similarly, since T is consistent with X , there are no forbidden interactions of the form $\{(x, s_x), (y, s_y)\}$ where $x, y \in f(j_{m+1}, a_{m+1})$. If $x \in f(j_{m+1}, a_{m+1})$ and $y \in f(U)$, then $\{(x, s_x), (y, s_y)\}$ cannot be forbidden. If it were, then we would have $(x, \bar{s}_x) \in f(y, s_y)$ and $(y, s_y) \in f(j_p, a_p)$ for some $(j_p, a_p) \in U$, and consequently, $(x, \bar{s}_x) \in f(U)$. This would mean that $f_{(j_{m+1}, a_{m+1})}(x) = s_x$, but $f_U(x) = \bar{s}_x$, contradicting the fact that S is well defined. Lastly, for all $x \in f(j_{m+1}, a_{m+1})$ and all $y \in [k] \setminus (f(U) \cup f(j_{m+1}, a_{m+1}))$, the interaction $\{(x, s_x), (y, s_y)\}$ is not forbidden, for if it were, this would contradict

the fact that $y \notin (f(U) \cup f(j_{m+1}, a_{m+1}))$. Therefore, S is indeed a consistent k -tuple and S covers $U \cup (j_{m+1}, a_{m+1})$. $\blacksquare$

We give one sufficient condition that guarantees the consistency of a FOR system. Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ be a FOR system, and let $i \in [k]$. If there exists a value $a_i \in [v_i]$ such that the factor-value pair (i, a_i) is not contained in any forbidden edge of X , then a_i is a **safe value** for factor i .

Lemma 8.2.10 Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$. If no forbidden edge of X is contained in a required edge of X , and if every factor $i \in [k]$ has a safe value, then X is consistent.

[proof] Let $I \in R(X)$, where $I = \{(j_1, b_1), \dots, (j_t, b_t)\}$. For each factor $i \in [k] \setminus \{j_1, \dots, j_t\}$, let a_i be a safe value for i . Define a k -tuple $T = (t_1, \dots, t_k)$ where, for each $i \in [k]$, we have $t_i = b_{j_l}$ if $i = j_l$ for some $l \in [t]$; otherwise, $t_i = a_i$ if $i \in [k] \setminus \{j_1, \dots, j_t\}$. We claim that T is consistent with X . If T were not consistent with X , then T would necessarily cover a forbidden edge of X , say $J \in F(X)$. We know that J is not contained in I , so some factors of J must belong to $[k] \setminus \{j_1, \dots, j_t\}$. This is not possible given that we used safe values for these factors. $\blacksquare$

8.3 Trivial bounds on the FOR array number

Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ be a FOR system. Let $A \subseteq [k]$, where $A = \{i_1, \dots, i_s\}$. For each s -tuple of values $\vec{a} = (a_1, \dots, a_s) \in [v_{i_1}] \times \dots \times [v_{i_s}]$, define $\rho_A(\vec{a})$ to be 1 if there exists a required edge $I \in R(X)$ such that $\{(i_1, a_1), \dots, (i_s, a_s)\} \subseteq I$, and 0 otherwise. Let S_A denote the sum
$$\sum_{\vec{a} \in [v_{i_1}] \times \dots \times [v_{i_s}]} \rho_A(\vec{a}).$$

Proposition 8.3.1 Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ be a compact FOR system. If X is consistent, then

$$\max_{A \subseteq [k]} S_A \leq \text{FORN}(X) \leq |R(X)|.$$

[proof] If X is consistent, consider an optimal $\text{FOR}(n, X)$. Let $A = \{i_1, \dots, i_s\}$ be an s -subset of $[k]$ and consider the columns $i_1, \dots, i_s$ of the $\text{FOR}(n, X)$. For every s -tuple of values $\vec{a} = (a_1, \dots, a_s) \in [v_{i_1}] \times \dots \times [v_{i_s}]$ such that $\rho_A(\vec{a}) = 1$, there must be a row that covers $\vec{a}$ in columns $i_1, \dots, i_s$; moreover, in that row, it is not possible

for these columns to cover another s -tuple of values distinct from $\vec{a}$. Consequently, for all subsets $A \subseteq [k]$, we have the lower bound $S_A \leq \text{FORN}(X)$.

The maximum number of rows needed in an optimal FOR array of X is $|R(X)|$, since one row per required edge is sufficient to cover all required edges. ■

The bounds of Proposition 8.3.1 are attained by consistent FOR systems $X \in \mathcal{X}_{(v_1, v_2)}$ with $k = 2$ factors and with required strength 2, since, in this case, the lower bound equals the upper bound: $S_{\{1,2\}} = R(X)$.

When $k \geq 3$, the upper bound is attained by any consistent FOR system $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ with required strength k . In this case, no two required interactions (being of strength k) can be covered simultaneously in one row.

8.4 Complexity results

As CAFEs are special cases of FOR systems, we get the following computational complexity results:

Proposition 8.4.1 Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$.

1. Determining whether there exists a k -tuple $T \in [v_1] \times \dots \times [v_k]$ that avoids $F(X)$ is NP-hard.
2. Determining whether X is a consistent FOR system is NP-hard.
3. For a given N , determining whether $\text{FORN}(X) \leq N$ is NP-hard.

[proof] Let $G \in \mathcal{G}_{k,v}$ be a forbidden edges graph. Danziger, Mendelsohn, Moura, and Stevens [19] showed that determining whether there exists a k -tuple avoiding $G \in \mathcal{G}_{k,v}$ is NP-complete for $v \geq 3$, and determining whether G is consistent is NP-complete for $v \geq 5$. Given N , we showed that determining whether $\text{CAFEN}(G) \leq N$ is NP-complete for $v \geq 2$ [39, 41]. Since G corresponds to a v -ary FOR system of strength 2, if we could solve these decision problems in polynomial time for FOR systems in general, then we could use these algorithms to solve the corresponding NP-complete CAFE problems in polynomial time. ■

8.5 Compatibility hypergraphs

In this section, we define compatibility hypergraphs to encode, for a given FOR system X , which sets of required interactions are consistent with X .

Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ be a FOR system. Let $u, v \in R(X)$ be required interactions of X . If there exists a consistent k -tuple that covers both u and v , then interactions u and v are **compatible** (with respect to X). Similarly, for any subset $W \subseteq R(X)$, if there exists a k -tuple $T = (t_1, \dots, t_k) \in [v_1] \times \dots \times [v_k]$ such that T is consistent with X and such that T covers w for all interactions $w \in W$, then W is a **compatible** set of interactions. Using the terminology of Section 8.2, W is a compatible set of interactions if and only if the row set, $rs(W)$, is nonempty.

From a FOR system X , we now define a hypergraph which encodes the compatibilities of required edges of X . The **compatibility hypergraph** of X , denoted H_X , is a hypergraph with vertex set $V(H_X) = R(X)$ and edge set $E(H_X) = \{W \subseteq V(H_X) : rs(W) \neq \emptyset\}$. In other words, a set of vertices form an edge of H_X if and only if the corresponding interaction set is compatible with respect to X .

It is clear from the definition of H_X that the FOR system X is consistent if and only if every vertex of its compatibility hypergraph H_X is contained in an edge (and therefore in an edge of rank 1). It is also straightforward to see that $\text{FORN}(X)$ is equal to the minimum number of edges needed to cover the vertices of the compatibility hypergraph H_X , as follows.

Proposition 8.5.1 Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$. If H_X is the compatibility hypergraph of X , then $\text{FORN}(X)$ is equal to the minimum number of edges required to cover the vertices of H_X .

[proof] Let $\mathcal{E}$ be a collection of edges of H_X such that $\bigcup \mathcal{E} = V(H_X)$. Suppose there is no collection $\mathcal{E}'$ with $|\mathcal{E}'| < |\mathcal{E}|$. For each edge $e \in \mathcal{E}$, there exists a consistent k -tuple that covers e . As $\bigcup \mathcal{E} = V(H_X) = R(X)$, the rows corresponding to the collection $\mathcal{E}$ cover all required interactions of X . Thus, $\text{FORN}(X) \leq |\mathcal{E}|$.

On the other hand, given an optimal $\text{FOR}(n, X)$, each row corresponds to a consistent k -tuple that covers a compatible subset of required interactions of X , hence an edge of H_X . Let $\mathcal{E}$ be the collection of edges corresponding to the rows of the array, and let $\mathcal{E}^*$ be an optimal collection of edges of H_X that cover all vertices of H_X . Since

the array $\text{FOR}(n, X)$ covers all required interactions, the union of the corresponding edges of H_X must cover all the vertices of H_X . Thus $|\mathcal{E}^*| \leq |\mathcal{E}| = \text{FORN}(X)$. $\blacksquare$

For a compatibility hypergraph H_X , if we consider an edge $W \in E(H_X)$, then every subset $U \subseteq W$ must also be an edge of H_X . Since $W \in E(H_X)$, there exists a k -tuple avoiding $F(X)$ that covers W ; clearly, such a k -tuple covers U for all $U \subseteq W$. Consequently, $U \in E(H_X)$. This means that the edge set of a compatibility hypergraph H_X forms a downset (or abstract simplicial complex) on the vertex set $V(H_X)$.

Since the edge set of a compatibility hypergraph corresponds to a downset, we know that each edge of H_X implies a clique in the sense of simple graphs. More precisely, if $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ is a FOR system with compatibility hypergraph H_X , then, for every $e \in E(H_X)$, the edge e corresponds to a compatible set of required interactions of X , say $e = \{U_1, \dots, U_m\}$, for which there exists a consistent k -tuple that covers e . Consequently, every pair of interactions $U_i, U_j \in e$ are pairwise compatible, thus correspond to a two-vertex edge of H_X . Since this is true for all such pairs in e , the edge e induces a clique of two-vertex edges in H_X .

Given a binary FOR system $X \in \mathcal{X}_{k,2}$ of forbidden strength 2, we now show that determining $\text{FORN}(X)$ is equivalent to determining the clique cover number of its compatibility hypergraph, where, for hypergraphs, we use the term “clique cover” as follows.

Given a hypergraph G , a **clique** of G is a subset of vertices $C \subseteq V(G)$, such that for all distinct pairs of vertices $u \neq v \in C$, the edge set of G contains the two-vertex edge uv , and, for all $u \in C$, the edge set of G contains the one-vertex edge u . A collection of cliques $\mathcal{C} = \{C_1, \dots, C_n\}$ is called a **clique cover** of G , if $\bigcup \mathcal{C} = V(G)$. If $\mathcal{C}^*$ is a clique cover of G and if $|\mathcal{C}^*| \leq |\mathcal{C}|$ for all clique covers $\mathcal{C}$ of G , then we say that $\mathcal{C}^*$ is an **optimal clique cover** of G . The cardinality of an optimal clique cover of G is called the **clique cover number** of G , and we denote it by $\theta(G)$.

Proposition 8.5.2 Let H_X be the compatibility hypergraph of a binary FOR system $X \in \mathcal{X}_{k,2}$ of forbidden strength 2. If C is a clique of H_X , then C is an edge of H_X .

[proof] Let $C = \{e_1, \dots, e_m\}$ be an m -clique of H_X . We prove that C forms an edge of H_X by induction on m . If $m \in \{1, 2\}$, then C is already an edge of H_X . For some $m \geq 2$, assume that C forms an edge of H_X whenever C is an m -clique of

H_X . Consider an $(m+1)$ -clique of H_X , $C = \{e_1, \dots, e_{m+1}\}$. Since $\{e_1, \dots, e_m\}$ is an m -clique of H_X , by our induction hypothesis, $\{e_1, \dots, e_m\}$ is an edge of H_X .

Let $U = \bigcup_{i \in [m]} e_i$ be the set of factor-value pairs corresponding to the m -clique $\{e_1, \dots, e_m\}$. For any $(i, a) \in U$ and any $(j, b) \in e_{m+1}$, it is clear that $\{(i, a), (j, b)\}$ is consistent with X . By Corollary 8.2.9, $U \cup \{(j, b)\}$ is also consistent with X . Write $e_{m+1} = \{(j_1, b_1), \dots, (j_l, b_l)\}$. Iteratively applying Corollary 8.2.9 for $i = 1, \dots, l$, we find that $U \cup e_{m+1}$ is consistent with X . Consequently, $\{e_1, \dots, e_{m+1}\}$ is compatible, hence an edge of H_X . $\blacksquare$

Corollary 8.5.3 Let $X \in \mathcal{X}_{k,2}$ be a consistent binary FOR system of forbidden strength 2. If H_X is the compatibility hypergraph of X , then $\text{FORN}(X) = \theta(H_X)$.

[proof] Let $\mathcal{C} = \{C_1, \dots, C_n\}$ be an optimal clique cover of H_X . By Proposition 8.5.2, each $C_i \in \mathcal{C}$ represents a compatible set of required interactions of X ; thus, for each $C_i \in \mathcal{C}$, there exists a consistent k -tuple that covers all interactions in C_i . Let these k -tuples be the rows of an $n \times k$ array. Since every required interaction of X is a vertex of H_X , it is covered by some clique $C_i \in \mathcal{C}$, hence covered by the corresponding row. Thus, $\text{FORN}(X) \leq n = \theta(H_X)$.

Consider an optimal $\text{FOR}(n; X)$. For each $i \in [n]$, the i th row is a consistent k -tuple that covers a set of required interactions of X ; let C_i denote the set of required interactions covered by the i th row, that is, C_i is the set of vertices of H_X covered by row i . Clearly, C_i is an edge of H_X , and any two vertices in C_i are pairwise compatible. Thus, C_i is a clique of H_X . Clearly, the collection $\mathcal{C} = \{C_1, \dots, C_n\}$ is a clique cover of H_X , thus, $\theta(H_X) \leq n = \text{FORN}(X)$. $\blacksquare$

Proposition 8.5.2 and Corollary 8.5.3 fail for non-binary FOR systems with forbidden strength 2. In Figure 8.3, we give an example of a FOR system $X \in \mathcal{X}_{7,3}$ with three required edges (e_1 , e_2 , and e_3 in green) and three forbidden edges (in red). Any two required edges of X are compatible, but the three required edges together are not compatible because the forbidden edges make it impossible to select a value for factor 7. The compatibility hypergraph H_X is also given in Figure 8.3. We only illustrate the facets of $E(H_X)$. In this case, $\text{FORN}(X) = 2$ while $\theta(H_X) = 1$.

Proposition 8.5.2 and Corollary 8.5.3 also fail for binary FOR systems with forbidden edges of higher strength. Suppose $X \in \mathcal{X}_{6,2}$ with $R(X) = \{e_1, e_2, e_3\}$, where $e_1 = \{(1, 0), (2, 0)\}$, $e_2 = \{(3, 0), (4, 0)\}$, and $e_3 = \{(5, 0), (6, 0)\}$, and $F(X)$ has one forbidden edge $f_1 = \{(1, 0), (3, 0), (5, 0)\}$. It is clear that any two required edges are

compatible, but the forbidden 3-way edge f_1 prevents the set $\{e_1, e_2, e_3\}$ from being compatible.

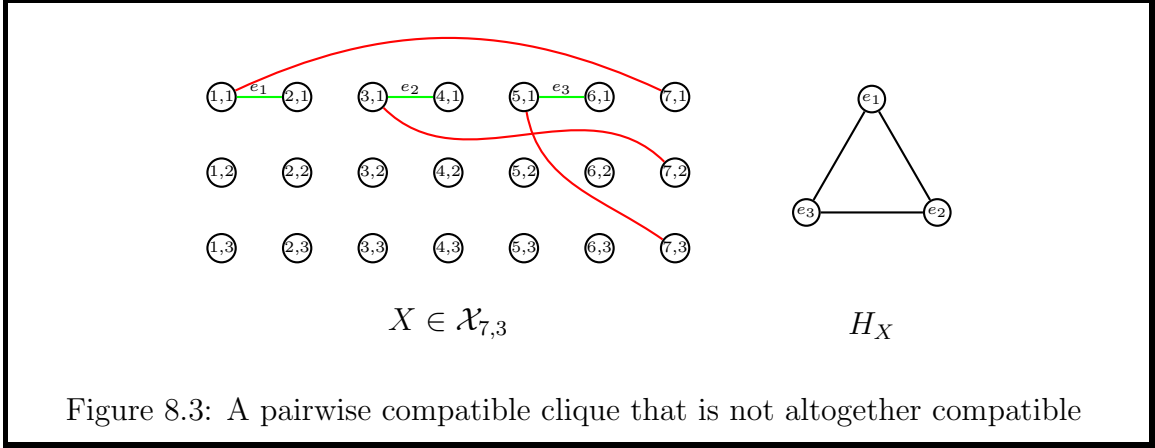


Figure 8.3: A pairwise compatible clique that is not altogether compatible

If $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ is a consistent FOR system whose compatibility hypergraph H_X is triangle-free, then $\text{FORN}(X) = \theta(H_X)$. Since no three vertices form a triangle and since $E(H_X)$ is a downset, it is impossible for H_X to have edges of rank greater than 2.

Lemma 8.5.4 Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ be a consistent FOR system. If the compatibility hypergraph H_X of X is triangle-free, then $\text{FORN}(X) = \theta(H_X)$. ■

In particular, for triangle-free graphs, we have the following result relating the clique cover number to the matching number. Recall that $\mu(G)$ denotes the number of edges in a maximum matching of a graph G , and $\text{def}(G)$ denotes the deficiency of G , that is, the number of vertices left uncovered by a maximum matching.

Proposition 8.5.5 Let G be a triangle-free graph. Then, $\theta(G) = \mu(G) + \text{def}(G)$. ■

Combining Lemma 8.5.4 with Proposition 8.5.5, we get the following corollary.

Corollary 8.5.6 Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ be a consistent FOR system. If the compatibility hypergraph H_X of X is triangle-free, then $\text{FORN}(X) = \mu(H_X) + \text{def}(H_X)$. ■

Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ be a FOR system with compatibility hypergraph H_X . The **compatibility graph** of X , denoted G_X , is the simple graph with $V(G_X) = V(H_X) =$

$R(X)$ and $E(G_X) = \{e \in E(H_X) : |e| = 2\}$, that is, G_X is the underlying graph of H_X .

For each consistent binary FOR system $X \in \mathcal{X}_{k,2}$ with forbidden strength 2, there is a graph, namely the compatibility graph of X , whose clique cover number is equal to the FOR array number of X . Conversely, every simple graph G is isomorphic to the compatibility graph of a consistent binary FOR system, as we now show.

Proposition 8.5.7 If G is a simple graph on n vertices, then there exists a consistent binary FOR system $X \in \mathcal{X}_{2n,2}$ such that G is isomorphic to the compatibility graph G_X of X and such that $\text{FORN}(X) = \theta(G)$.

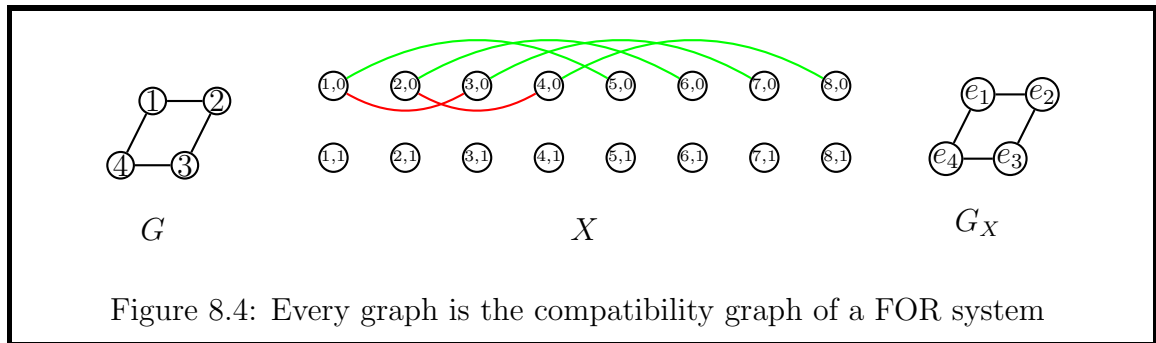
[proof] Label the vertices of G as $1, \dots, n$. Define a system $X \in \mathcal{X}_{2n,2}$ as follows. For each $i \in [n]$, let $e_i = \{(i, 0), (n + i, 0)\}$ be a required interaction of X . Let $\{(i, 0), (j, 0)\} \in F(X)$ if and only if $ij \notin E(G)$. All other interactions are optional.

Clearly, X is consistent because, for each factor, the value 1 is a safe value; for every $e_i \in R(X)$, the $(2n)$ -tuple given by $(x_1, \dots, x_{2n})$, where $x_r = 0$, if $r \in \{i, n + i\}$ and $x_r = 1$ otherwise, is a consistent $(2n)$ -tuple that covers e_i .

By Corollary 8.5.3, we have $\text{FORN}(X) = \theta(H_X)$ and, by restricting the compatibility hypergraph H_X to its edges of rank 2, we get G_X , the compatibility graph of X .

We claim that the map $f : V(G) \rightarrow V(G_X)$ given by $f(i) = e_i$ is an isomorphism. If $ij \in E(G)$, then the $(2n)$ -tuple $(x_1, \dots, x_{2n})$ given by $x_r = 0$ if $r \in \{i, j, n + i, n + j\}$ and $x_r = 1$ otherwise, is a consistent $(2n)$ -tuple that covers e_i and e_j . Thus, e_i and e_j are compatible, hence $e_i e_j \in E(G_X)$. If $ij \notin E(G)$, then $\{(i, 0), (j, 0)\}$ is forbidden; it then follows that e_i and e_j are not compatible, hence $e_i e_j \notin E(G_X)$.

Since G and G_X are isomorphic, we see that $\theta(G) = \theta(G_X) = \text{FORN}(X)$. ■



Example 8.5.8 Figure 8.4 shows an example of a graph G , the FOR system X given by Proposition 8.5.7, and the compatibility graph G_X . In X , green edges represent required edges while red edges represent forbidden edges.

8.6 Critical systems

Here we explore the notion of “critical” FOR systems.

Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ and let $I \in R(X)$ be a required interaction. Denote by $X - I$ the FOR system obtained from X by removing I from $R(X)$ and letting I be optional in $X - I$. Similarly, for a forbidden interaction $U \in F(X)$, let $X - U$ denote the FOR system obtained from X by removing U from $F(X)$ and letting U be optional in $X - U$.

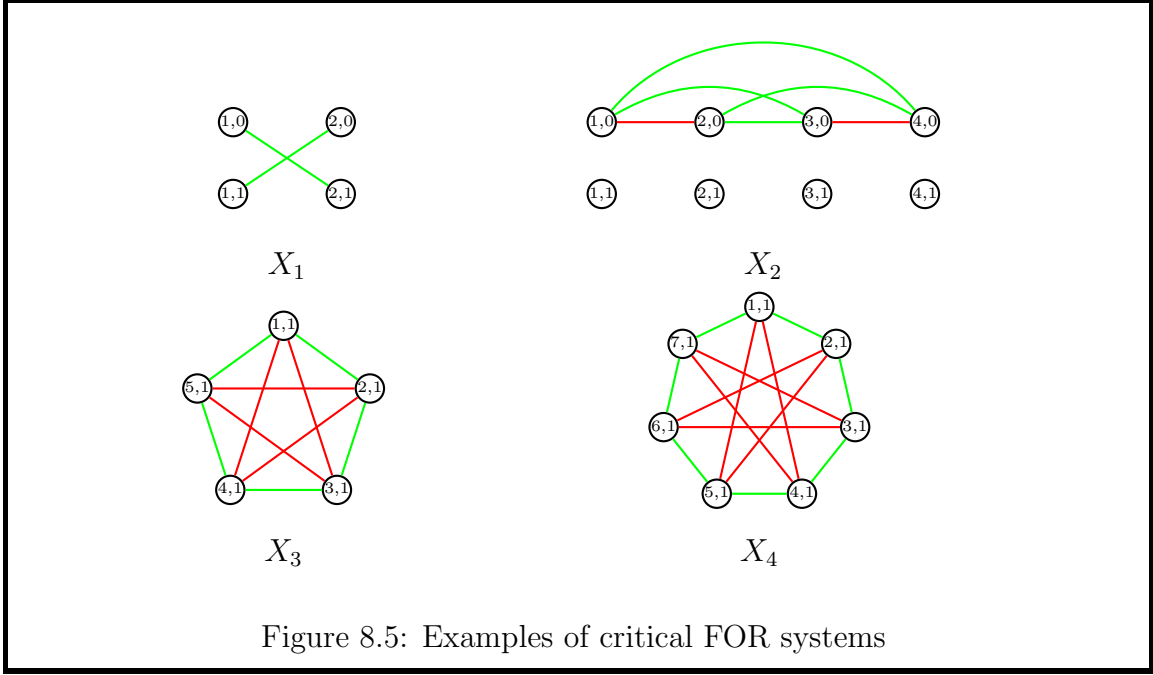
Definition 8.6.1 Let $n \geq 1$ and let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ be a consistent FOR system with $\text{FORN}(X) = n$ (thus $R(X) \neq \emptyset$). If $I \in R(X) \cup F(X)$ and $\text{FORN}(X - I) < n$, then I is a **critical element** of X . If, for all $I \in R(X)$, the required edge I is a critical element, then X is **n -required-critical**. If $F(X) \neq \emptyset$ and every forbidden edge $I \in F(X)$ is a critical element, then X is **n -forbidden-critical**. If every $I \in R(X) \cup F(X)$ is a critical element, then X is **n -critical**, or simply, a **critical** system.

Example 8.6.2 In Figure 8.5, the system $X_1 \in \mathcal{X}_{2,2}$ has two required interactions of strength 2 (green edges) and no forbidden interactions. Clearly, $\text{FORN}(X_1) = 2$ and X_1 is 2-required-critical. Since $R(X_1) \cup F(X_1) = R(X_1)$, the system X_1 is 2-critical.

Example 8.6.3 In Figure 8.5, the system $X_2 \in \mathcal{X}_{4,2}$ is 4-critical. Any 4-tuple consistent with X can cover at most one of the four required edges; thus, each edge is covered alone in a row using the value 1 as safe values to complete the row. Removing any required edge reduces the number of rows by one. Removing a forbidden edge allows two required edges to be covered by a single row, for a total of three rows.

Critical FOR systems similar to X_2 , consisting of two forbidden cliques completely joined by required edges, can be generated as follows.

Lemma 8.6.4 Let k and l be integers. If $k \geq 3$ and $2 \leq l \leq k - 1$, then there exists a $(kl - l^2)$ -critical FOR system $X \in \mathcal{X}_{k,2}$.



[proof] For all i, j such that $1 \leq i < j \leq l$, let $\{(i, 1), (j, 1)\} \in F(X)$. For all i, j such that $l + 1 \leq i < j \leq k$, let $\{(i, 1), (j, 1)\} \in F(X)$. For all i, j such that $1 \leq i \leq l$ and $l + 1 \leq j \leq k$, let $\{(i, 1), (j, 1)\} \in R(X)$. There are no forbidden or required interactions involving the value 0 which provides safe values, thus X is consistent. The forbidden edges prevent any two required edges from being compatible, thus $\text{FORN}(X) = |R(X)| = l \times (k - l)$, and clearly, X is required-critical. If we remove a forbidden edge $\{(i, 1), (j, 1)\} \in F(X)$, where $1 \leq i < j \leq l$, then, for all m with $l + 1 \leq m \leq k$, the required edges $\{(m, 1), (i, 1)\}$ and $\{(m, 1), (j, 1)\}$ become compatible. Similarly, if we remove a forbidden edge $\{(i, 1), (j, 1)\} \in F(X)$, where $l + 1 \leq i < j \leq k$, then, for all m with $1 \leq m \leq l$, the required edges $\{(m, 1), (i, 1)\}$ and $\{(m, 1), (j, 1)\}$ become compatible. Thus, X is forbidden-critical. $\blacksquare$

In Figure 8.5, the systems $X_3 \in \mathcal{X}_{5,2}$ and $X_4 \in \mathcal{X}_{7,2}$ are binary FOR systems of strength 2. Required edges are green and forbidden edges are red. These systems are constructed so that the value 0 provides safe values. Since no required or forbidden edges involve the value 0, we omit the isolated vertices corresponding to the value 0.

A FOR array of X_3 , shown in Figure 8.5, requires one row per required edge. The required edges form a 5-cycle on the vertices of value 1. If we remove a forbidden edge, then two required edges that are consecutive in the cycle become compatible.

So far, all examples of critical systems given need one row per required edge; however, there are examples of systems which optimally cover more than one required edge per row. For example, a FOR array of X_4 , shown in Figure 8.5, optimally covers two consecutive (in the cycle) required edges per row for three rows and a fourth row is needed to cover the remaining required interaction. Since each pair of consecutive (in the cycle) required edges can be covered by a single row, when we remove a required edge, we can cover the remaining six required edges with three rows. When we remove a forbidden edge, we can cover three consecutive required edges in a single row and the remaining four edges with two more rows.

In Lemma 8.6.5, we construct required-critical FOR systems having a similar structure to X_3 and X_4 . We build a cycle of required edges on one value and control the number of compatible required edges using forbidden chords.

Lemma 8.6.5 If x , a and k are positive integers such that $k = ax + 1$ and $a \geq 3$, then there exists an $(a + 1)$ -required-critical system $X \in \mathcal{X}_{k,2}$ such that X has k required interactions.

[proof] We build $X \in \mathcal{X}_{k,2}$ with required edges $\{(i, 1), (i + 1, 1)\} \in R(X)$, for all i such that $1 \leq i \leq k - 1$, and $\{(k, 1), (1, 1)\} \in R(X)$. These k required edges form a k -cycle on the vertices of value 1. The vertices of value 0 provide safe values. For all $i, j \in [k]$ such that the distance on the k -cycle between vertices $(i, 1)$ and $(j, 1)$ is greater than or equal to $x + 1$, we add a forbidden edge $\{(i, 1), (j, 1)\} \in F(X)$.

Every x required edges that are consecutive on the cycle are compatible. The forbidden interactions prevent any two required edges that have ends of distance $x + 1$ or greater from being compatible. Thus, covering x consecutive required edges together in one row is optimal. We can cover ax required edges using a rows. Since $k = ax + 1$, we need one more row to cover the k th required edge. Removing any required edge eliminates the need for this last row. ■

At this point we have provided very simple examples of critical systems, usually with safe values and a binary alphabet. The next results give properties of critical systems that hold more generally.

Lemma 8.6.6 If $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ is an n -required-critical system, then for every required interaction $I \in R(X)$, the set of factor-value pairs forced by I cannot contain all the factor-value pairs of any other required interaction $I' \neq I$.

[**proof**] If I and I' are two distinct required interactions of X , then a FOR array of $X - I'$ requires only $n - 1$ rows, and must cover I . If I' were forced by I , then the smaller array would necessarily cover I' and be a $\text{FOR}(n - 1, X)$. ■

Corollary 8.6.7 Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ be an n -required-critical system. For every required interaction $I \in R(X)$, there exists an optimal $\text{FOR}(n, X)$ such that there is exactly one row that covers I and every other required edge $I' \in R(X) - \{I\}$ is covered only within the other $n - 1$ rows.

[**proof**] If $I \in R(X)$, then a $\text{FOR}(n - 1, X - I)$ covers all required interactions of X except I . Since X is consistent, there exists a consistent row that covers I . If we append this row to the $\text{FOR}(n - 1, X - I)$, then we get a $\text{FOR}(n, X)$ with the desired property. ■

Lemma 8.6.8 Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ be an n -required-critical system. If $I \in R(X)$, then $\text{FORN}(X - I) = n - 1$.

[**proof**] If $\text{FORN}(X - I) < n - 1$, then we could build a $\text{FOR}(n - 1, X)$ by adding a row that covers I to an optimal FOR array of $X - I$. ■

While removing a required edge from a consistent FOR system can decrease the FOR array number by at most one, the effects of removing a forbidden edge from a FOR system can decrease the number of rows by a factor of t , where t is the rank of the removed forbidden edge.

Lemma 8.6.9 Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ be a FOR system with safe values for each factor. If $J \in F(X)$, then

$$\text{FORN}(X) \leq n_J + (t - 1)i_J,$$

where $n_J = \text{FORN}(X - J)$, t is the rank of J , and i_J is the number of rows that cover J in an (optimal) $\text{FOR}(n_J, X - J)$.

[**proof**] For each $j \in [k]$, let $s_j \in [v_j]$ denote a safe value for factor j . By relabelling factors if needed, we may assume that $J = \{(1, a_1), \dots, (t, a_t)\}$. Let $R = (a_1, a_2, \dots, a_t, a_{t+1}, \dots, a_k)$ be a row of a $\text{FOR}(n_J, X - J)$ that covers J . From R , we produce t new k -tuples that are consistent with X and that cover all the required interactions covered by R : for each $j \in [t]$ let R_j equal R except at position j where we replace a_j with the safe value s_j . Making t new rows for each of the i_J rows that

cover J in a $\text{FOR}(n_J, X - J)$, we can build a $\text{FOR}(n_J + (t - 1)i_J, X)$. We use the $n_J - i_J$ rows of the $\text{FOR}(n_J, X - J)$ that do not cover J , and we add to these rows the ti_J rows obtained by replacing each of the i_J rows that do cover J with t consistent rows using safe values. This yields a $\text{FOR}(n_J + (t - 1)i_J, X)$. $\blacksquare$

Corollary 8.6.10 Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ be a FOR system with safe values for each factor. If $J \in F(X)$, then

$$\text{FORN}(X - J) \geq \frac{1}{t} \text{FORN}(X),$$

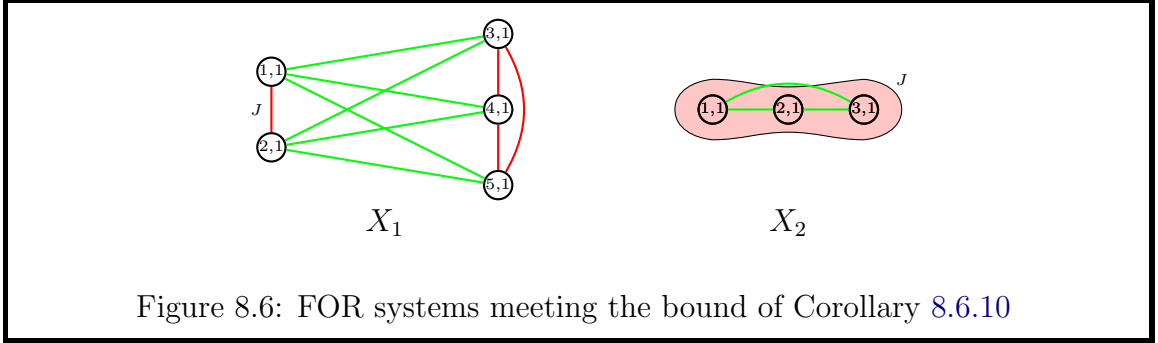
where t is the rank of J .

[**proof**] Let $n_J = \text{FORN}(X - J)$, let i_J be the number of rows that cover J in a $\text{FOR}(n_J, X - J)$, and let $t = |J|$. In an optimal $\text{FOR}(n_J, X - J)$, the edge J can be covered by at most n_J rows. By Lemma 8.6.9, $\text{FORN}(X) \leq n_J + (t - 1)i_J \leq n_J + (t - 1)n_J$. Therefore, $\text{FORN}(X) \leq t \text{FORN}(X - J)$. $\blacksquare$

With forbidden strength 2 and binary alphabet, we can construct FOR systems that attain the bound of Corollary 8.6.10 as follows. Let $X \in \mathcal{X}_{k,2}$, where $k \geq 3$. For all $i \geq 3$, let $\{(1, 1), (i, 1)\} \in R(X)$ and let $\{(2, 1), (i, 1)\} \in R(X)$. For all $i, j \in [k]$ such that $3 \leq i < j \leq k$, let $\{(i, 1), (j, 1)\} \in F(X)$. Finally, let $\{(1, 1), (2, 1)\} \in F(X)$. The system X has $2(k - 2)$ required edges, no pair of which are compatible. The vertices of value 0 provide safe values, so X is $(2k - 4)$ -required-critical. Removing a forbidden edge of the form $J = \{(i, 1), (j, 1)\}$ where $3 \leq i < j \leq k$ makes the required interactions $\{(i, 1), (1, 1)\}$ and $\{(j, 1), (1, 1)\}$ compatible. If we remove the particular forbidden edge $J = \{(1, 1), (2, 1)\}$, then, for all $i \in \{3, \dots, k\}$, the pairs of required edges $\{(i, 1), (1, 1)\}$ and $\{(i, 1), (2, 1)\}$ become compatible. Thus, the forbidden edge J meets the bound of Corollary 8.6.10.

In Figure 8.6, the system X_1 illustrates the above construction for $k = 5$. As usual, we omit the vertices of value 0 since these correspond to safe values. Required edges are green and forbidden edges are red.

For forbidden strength $t \geq 3$, we can also find critical FOR systems that meet the bound given by Corollary 8.6.10. For $t \geq 3$, let $k = t$. Build a system $X \in \mathcal{X}_{k,2}$ with one forbidden t -way edge $J = \{(1, 1), (2, 1), \dots, (t, 1)\} \in F(X)$. For every $r \in [t]$ let $I_r = J - \{(r, 1)\}$ be a required edge. No two required edges I_r and I_s are compatible since their union is the forbidden edge J . Thus, X is k -required-critical. When we



remove J from X , all required interactions can be covered simultaneously by a single row, that is, $\text{FORN}(X - J) = 1 = k/t = \frac{1}{t}\text{FORN}(X)$.

In Figure 8.6, the system X_2 illustrates the above construction for $t = 3$. Vertices corresponding to safe values are omitted, required edges of rank 2 are shown in green, and the forbidden edge J of rank 3 corresponds to the red blob.

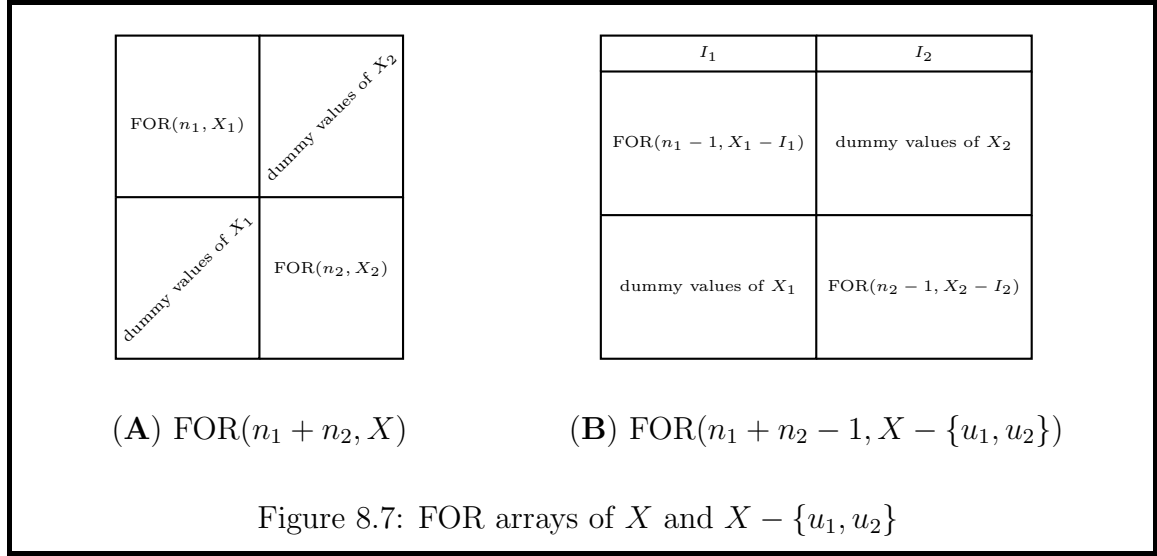
The following result allows us to build a larger critical system from two smaller critical systems, provided the systems have “dummy” values. Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ be a FOR system and let $i \in [k]$ be a factor. If, for factor i , there is a value $a_i \in [v_i]$ such that (i, a_i) is not contained in any required or forbidden edge of X , then a_i is a **dummy value** of factor i . If all factors $i \in [k]$ have dummy values, then the system X **has dummy values**.

Notice that dummy values are a particular instances of safe values, but with the stronger requirement that they are not contained in any required interactions.

Proposition 8.6.11 Let $X_1 \in \mathcal{X}_{(v_1, \dots, v_{k_1})}$ be an n_1 -critical system and let $X_2 \in \mathcal{X}_{(v'_1, \dots, v'_{k_2})}$ be an n_2 -critical system. If both X_1 and X_2 have dummy values, then there exists an $(n_1 + n_2)$ -critical system $X \in \mathcal{X}_{(v_1, \dots, v_{k_1}, v'_1, \dots, v'_{k_2})}$ such that X contains X_1 and X_2 as induced subsystems.

[proof] Let X be the disjoint union of X_1 and X_2 . Let C_1 be a minimal vertex cover of $R(X_1)$ and let C_2 be a minimal vertex cover of $R(X_2)$. Add to $F(X)$ all edges of the form $\{u_1, u_2\}$, where $u_1 \in C_1$ and $u_2 \in C_2$. We claim that X is $(n_1 + n_2)$ -critical.

Since every required edge of X_1 is incident with some $u_1 \in C_1$ and every required edge of X_2 is incident with some $u_2 \in C_2$, and since $\{u_1, u_2\} \in F(X)$ for all such u_1 and u_2 , no two required edges $I_1 \in R(X_1)$ and $I_2 \in R(X_2)$ are compatible. Consequently,



$$\text{FORN}(X) \geq n_1 + n_2.$$

Since X_1 and X_2 have dummy values, every k_1 -tuple that is consistent with X_1 can be extended into a $(k_1 + k_2)$ -tuple that is consistent with X by using the dummy values of X_2 to complete the tuple. Similarly, every k_2 -tuple that is consistent with X_2 can be extended using the dummy values of X_1 into a $(k_1 + k_2)$ -tuple that is consistent with X . We can thus build an optimal FOR($n_1 + n_2, X$) as follows. Below the rows of a FOR(n_1, X_1), we put an $n_2 \times k_1$ array of dummy values of X_1 . Above the rows of a FOR(n_2, X_2), we put an $n_1 \times k_2$ array of dummy values of X_2 . The columns of these two arrays form the columns of a FOR($n_1 + n_2, X$). This construction is depicted in Figure 8.7.A.

By the criticality of X_1 and X_2 , it is clear that X is $(n_1 + n_2)$ -required-critical. The forbidden edges of X are either completely contained in X_1 , completely contained in X_2 , or they are of the form (u_1, u_2) where $u_1 \in C_1 \subseteq V(X_1)$ and $u_2 \in C_2 \subseteq V(X_2)$. It is clear that those forbidden edges completely contained in one of X_1 or X_2 are critical elements of X . It remains to show that the forbidden edges bridged between the two systems are critical.

Let $\{u_1, u_2\} \in F(X)$ with $u_1 \in C_1$ and $u_2 \in C_2$. By minimality of the vertex cover C_1 , there exists a required edge $I_1 \in R(X_1)$ such that $C_1 - u_1$ does not cover I_1 . Similarly, there is a required edge $I_2 \in R(X_2)$ such that $C_2 - u_2$ does not cover I_2 . By Corollary 8.6.7, there exist optimal FOR arrays of X_1 and X_2 such that I_1 and

I_2 are each covered by exactly one row; moreover, using the dummy values, we can be certain that the row covering I_1 is compatible with the row that covers I_2 . The remaining required interactions of X can be covered in $(n_1 + n_2 - 2)$ rows producing a $\text{FOR}(n_1 + n_2 - 1, X - \{u_1, u_2\})$ as shown in Figure 8.7.B. ■

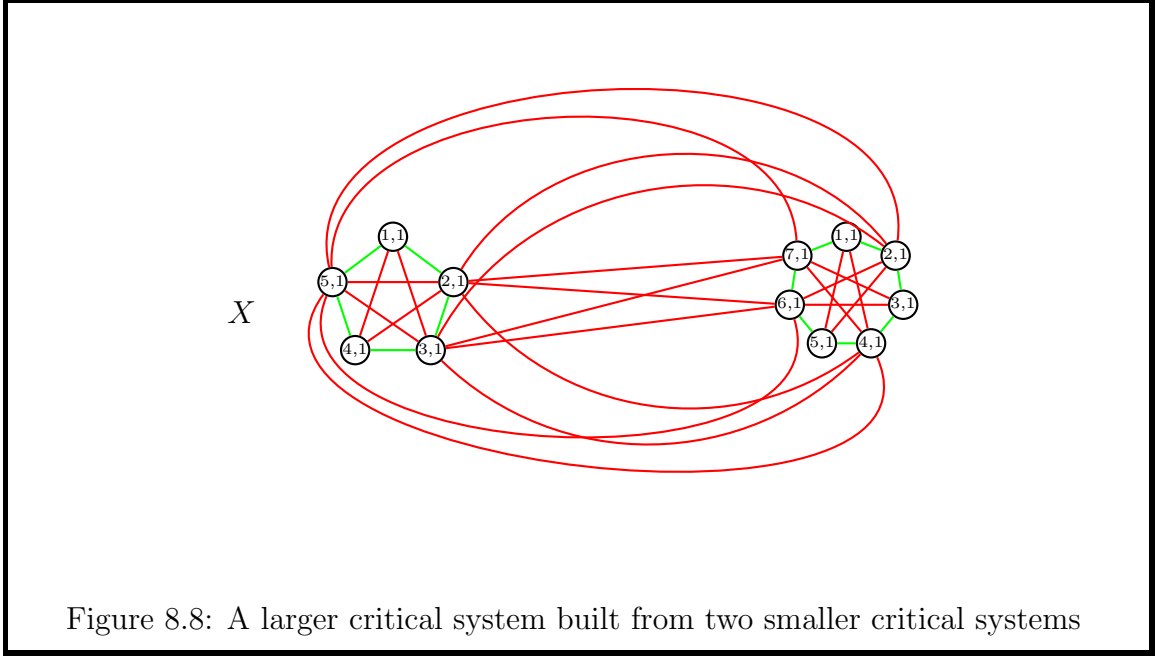


Figure 8.8: A larger critical system built from two smaller critical systems

Figure 8.8 depicts an example of the construction from Proposition 8.6.11 using the critical systems X_3 and X_4 given in Figure 8.5. In X_3 , the set of vertices $C_1 = \{(2, 1), (3, 1), (5, 1)\}$ is a minimal vertex cover of $R(X_3)$, and in X_4 , the set of vertices $C_2 = \{(2, 1), (4, 1), (6, 1), (7, 1)\}$ is a minimal vertex cover of $R(X_4)$. We add forbidden edges joining vertices in C_1 and C_2 to obtain the new critical system X , shown in Figure 8.8. Since the vertices of value 2 provide dummy values and are thus isolated from all required and forbidden edges, we omit these vertices from Figure 8.8.

We now prove that the construction of Proposition 8.6.11 is the only way to build an $(n_1 + n_2)$ -critical system from an n_1 -critical system and an n_2 -critical system, given that these systems have dummy values, and given that we only add forbidden edges bridged between the two systems as “repellent.”

Proposition 8.6.12 Let $X_1 \in \mathcal{X}_{(v_1, \dots, v_{k_1})}$ be an n_1 -critical system with dummy values, let $X_2 \in \mathcal{X}_{(v'_1, \dots, v'_{k_2})}$ be an n_2 -critical system with dummy values, and let $X \in \mathcal{X}_{(v_1, \dots, v_{k_1}, v'_1, \dots, v'_{k_2})}$ be obtained from X_1 and X_2 by adding to their disjoint union some

new forbidden edges of the form $\{u_1, u_2\}$, where $u_1 \in V(X_1)$ and $u_2 \in V(X_2)$. If X is $(n_1 + n_2)$ -critical, then for every pair of edges $I_1 \in R(X_1)$ and $I_2 \in R(X_2)$, one of the forbidden edges $\{u_1, u_2\}$ that we added to $F(X)$ must satisfy $u_1 \in I_1$ and $u_2 \in I_2$.

[proof] Since $\text{FORN}(X) = n_1 + n_2$, an optimal FOR array of X is given by optimal FOR arrays of X_1 and X_2 pasted together as in Figure 8.7.A. Let $I_1 \in R(X_1)$ and let $I_2 \in R(X_2)$. By Corollary 8.6.7, there exists a $\text{FOR}(n_1, X_1)$ that covers I_1 alone in a row, and similarly, there is a $\text{FOR}(n_2, X_2)$ that covers I_2 alone in a row. Using these arrays as in Figure 8.7.A yields an optimal $\text{FOR}(n_1 + n_2, X)$. If I_1 and I_2 were compatible, then we could build a FOR array of X with only $n_1 + n_2 - 1$ rows. Since the rows covering I_1 and I_2 cover only these required interactions and dummy values, it follows that there must be a forbidden edge adjacent to both I_1 and I_2 in X . ■

For the next result on critical systems, we make use of the following lemma; for a proof of Lemma 8.6.13, see Lemma 5.5 in [16].

Lemma 8.6.13 Let G be a graph and let $vw \in E(G)$. If v and w are both inessential, then G contains an odd cycle in which vw is an edge. ■

Proposition 8.6.14 Let $X_1 \in \mathcal{X}_{(v_1, \dots, v_{k_1})}$ and $X_2 \in \mathcal{X}_{(v'_1, \dots, v'_{k_2})}$ be critical FOR systems with dummy values. Let $X \in \mathcal{X}_{(v_1, \dots, v_{k_1}, v'_1, \dots, v'_{k_2})}$ be a critical system obtained from X_1 and X_2 by adding some forbidden edges of the form $\{(i, a_i), (j, b_j)\}$, where $(i, a_i) \in I$ for some $I \in R(X_1)$ and $(j, b_j) \in J$ for some $J \in R(X_2)$. If every two distinct required edges in X_1 are incompatible and if every two distinct required edges in X_2 are incompatible, then $\text{FORN}(X) = \text{FORN}(X_1) + \text{FORN}(X_2)$.

[proof] Let H_X be the compatibility hypergraph of X . The required edge set of X is $R(X) = R(X_1) \cup R(X_2)$, thus the vertices of H_X can be partitioned into two parts $R(X_1)$ and $R(X_2)$. Since no two required edges in $R(X_1)$ are compatible, the vertex set $R(X_1) \subset V(H_X)$ is an independent set. Similarly, the vertex set $R(X_2) \subset V(H_X)$ is an independent set. Consequently, H_X is bipartite.

It now follows that $\text{FORN}(X) = |R(X_1)| + |R(X_2)| - \mu(H_X)$ since an optimal FOR array of X covers as many compatible pairs of required edges as possible and such pairs correspond to a maximum matching of H_X .

By Corollary 8.6.7, for every required edge I of X , there exists an optimal FOR array in which I is covered by exactly one row; using dummy values, we can ensure that the

row covering I does not cover any required edges of X other than I itself. In terms of the compatibility hypergraph, this says that there exists a maximum matching M of H_X in which the vertex corresponding to I is M -exposed. This means that every vertex of H_X is inessential.

If $I_1 \in R(X_1)$ and $I_2 \in R(X_2)$ are compatible required edges of X , then $\{I_1, I_2\} \in E(H_X)$. Since both I_1 and I_2 are inessential vertices of H_X , by Lemma 8.6.13, it follows that the edge $\{I_1, I_2\} \in E(H_X)$ must belong to an odd cycle of H_X , contradicting the fact that H_X is bipartite.

Therefore, no two required edges of X are compatible, $\mu(H_X) = 0$, and $\text{FORN}(X) = \text{FORN}(X_1) + \text{FORN}(X_2)$ as required. $\blacksquare$

Lemma 8.6.15 Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ be an n -critical FOR system and let H_X be its compatibility hypergraph. If H_X is triangle-free, then every vertex of H_X is inessential and every edge of H_X belongs to an odd cycle of length at least 5.

[proof] Since H_X is triangle-free, it follows from Lemma 8.5.4 and Corollary 8.5.6 that $\text{FORN}(X) = \theta(H_X) = \mu(H_X) + \text{def}(H_X)$. By Corollary 8.6.7, for each $I \in R(X)$ there exists an optimal $\text{FOR}(n, X)$ in which I is covered by exactly one row, and all other required interactions are covered by the $n - 1$ remaining rows. In terms of H_X , this says that there is a maximum matching M of H_X for which the vertex I is M -exposed. Thus, I is an inessential vertex of H_X .

Since every vertex of H_X is inessential, it follows from Lemma 8.6.13 that any two adjacent vertices of H_X must belong to an odd cycle. Since H_X is triangle-free, such an odd cycle must have length at least 5. $\blacksquare$

8.7 Incompatibility graphs and chromatic numbers

For a simple graph G , it is easy to see that $\theta(G) = \chi(\bar{G})$, where $\bar{G}$ is the complement of G . In this section, we use this connection between clique cover numbers and chromatic numbers to establish a connection between critical FOR systems and colour-critical graphs.

Let $X \in \mathcal{X}_{(v_1, \dots, v_k)}$ and let H_X be its compatibility hypergraph. Recall that the underlying graph of H_X is the compatibility graph of X and it is denoted G_X .

Corollary 8.7.1 If $X \in \mathcal{X}_{k,2}$ is a consistent binary FOR system with forbidden strength 2, then $\text{FORN}(X) = \theta(G_X) = \chi(\bar{G}_X)$. ■

If G_X is the compatibility graph of a FOR system X , then its complement, denoted $\bar{G}_X$, is called the **incompatibility graph** of X . We now discuss the relationship between colour-critical incompatibility graphs and critical FOR systems.

Recall that a simple graph G is **k -critical** if $\chi(G) = k$ and $\chi(H) < \chi(G)$ for every proper subgraph $H \subset G$. If $\chi(G) = k$ and $\chi(G - v) < \chi(G)$ for every vertex $v \in V(G)$, then G is **k -vertex-critical**. If $\chi(G - v) < \chi(G)$ for some vertex $v \in V(G)$, then v is a **critical element** of G . Similarly, if $\chi(G - e) < \chi(G)$ for some edge $e \in E(G)$, then e is a **critical element** of G .

Proposition 8.7.2 If $X \in \mathcal{X}_{k,2}$ is an n -required-critical binary FOR system with forbidden strength 2, then its incompatibility graph $\bar{G}_X$ is n -vertex-critical.

[proof] Let $I \in R(X)$. It is easy to see that $G_X - I = G_{X-I}$. Since $\text{FORN}(X - I) = n - 1 = \chi(\bar{G}_{X-I}) = \chi(\bar{G}_X - I)$, we see that I is a critical vertex of $\bar{G}_X$. ■

Next we give some necessary conditions for a binary FOR system $X \in \mathcal{X}_{k,2}$ with forbidden strength 2 to be required-critical.

Corollary 8.7.3 If $X \in \mathcal{X}_{k,2}$ is an n -required-critical binary FOR system with forbidden strength 2, then the minimum degree of its incompatibility graph $\bar{G}_X$ satisfies $\delta(\bar{G}_X) \geq n - 1$. Moreover, $\bar{G}_X$ is connected.

[proof] By Proposition 8.7.2, $\bar{G}_X$ is an n -vertex-critical graph. It is easy to see that an n -vertex-critical graph must have minimum degree at least $n - 1$. It must also be connected. For proofs of these facts, see Theorems 8.1 and 8.2 in [6]. ■

8.8 Strength-2 FOR model and homomorphisms

In this section, we concentrate on v -ary FOR systems of strength 2; for these systems, we give an alternative model for the problem using a binary relational system. We also translate the problem of finding the FOR number into a homomorphism problem.

A **FOR BRS** (of strength 2) is a binary relational system S on the set $[k]$ of vertices, equipped with an “alphabet” parameter v , and $2 \binom{v}{2} + v$ binary relations on $[k]$.

The relations of the system S , denoted $R_{ab}(S)$ and $F_{ab}(S)$, where $1 \leq a \leq b \leq v$, encode (strength-2) required and forbidden interactions as follows: $ij \in R_{ab}(S)$ if and only if $\{(i, a), (j, b)\}$ is a required interaction; similarly, $ij \in F_{ab}(S)$ if and only if $\{(i, a), (j, b)\}$ is a forbidden interaction. The **family of FOR BRS** having k vertices and alphabet v is denoted $\mathcal{S}_{k,v}$.

For any $S \in \mathcal{S}_{k,v}$, there is a system $X \in \mathcal{X}_{k,v}$ that encodes the same set of required, forbidden, and optional interactions. Given $a, b \in [v]$ with $a \leq b$, we let $\{(i, a), (j, b)\} \in R(X)$ if and only if $ij \in R_{ab}(S)$, and we let $\{(i, a), (j, b)\} \in F(X)$ if and only if $ij \in F_{ab}(S)$. The remaining interactions are optional.

We introduce this notation because, for v -ary FOR systems of strength 2, the binary relational systems $S \in \mathcal{S}_{k,v}$ fit more naturally into the framework of homomorphisms. Using our new setup, we restate the definition of FOR arrays.

Definition 8.8.1 Let $S \in \mathcal{S}_{k,v}$. A **FOR array** of S , denoted $\text{FOR}(n, S)$, is an $n \times k$ array $A = A_{ij}$ with symbols from the alphabet $[v]$ such that

1. if $ij \in R_{ab}(S)$, then there exists a row index $r \in [n]$ such that $A_{ri} = a$ and $A_{rj} = b$;
2. if $ij \in F_{ab}(S)$, then, for all row indices $r \in [n]$, we have $A_{ri} \neq a$ or $A_{rj} \neq b$.

The **FOR array number** of S , denoted $\text{FORN}(S)$, is the smallest n for which a $\text{FOR}(n, S)$ exists, if a FOR array of S exists; if a FOR array of S does not exist, then $\text{FORN}(S) = +\infty$.

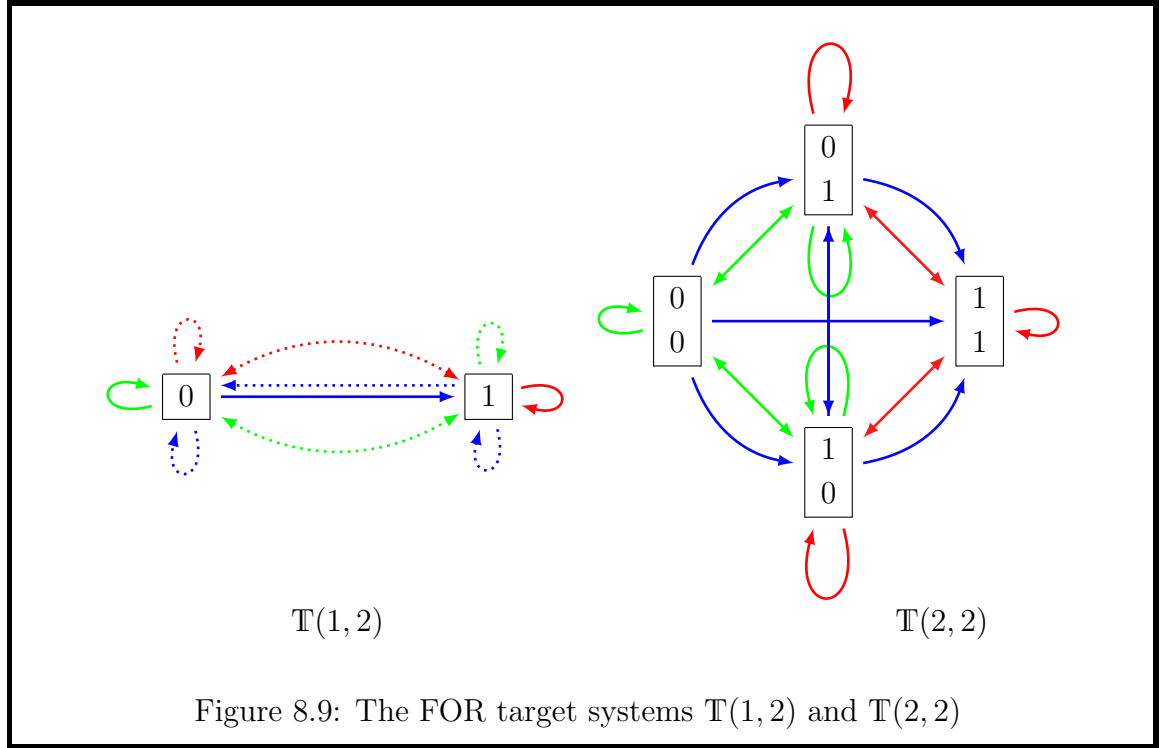
We now define a target BRS such that finding a FOR array of $S \in \mathcal{S}_{k,v}$ is equivalent to finding a homomorphism of S to the appropriate target. In the context of FOR arrays, these targets are analogues of H -dependence graphs.

Definition 8.8.2 Let n and v be positive integers. The **FOR target system**, denoted $\mathbb{T}(n, v)$, is the binary relational system with vertex set $[v]^n$, containing all v -ary n -tuples, and equipped with $v^2 + v$ binary relations R_{ab} and F_{ab} , where $1 \leq a \leq b \leq v$, such that the following property holds: for any two vertices $\vec{x} = (x_1, \dots, x_n)$ and $\vec{y} = (y_1, \dots, y_n)$ we have

1. $\vec{x}\vec{y} \in R_{ab}(\mathbb{T}(n, v))$ if and only if there exists an index $i \in [n]$ such that $x_i = a$ and $y_i = b$;
2. $\vec{x}\vec{y} \in F_{ab}(\mathbb{T}(n, v))$ if and only if, for all indices $i \in [n]$, we have $x_i \neq a$ or $y_i \neq b$.

The vertices of the FOR target system $\mathbb{T}(n, v)$ correspond to potential columns of a v -ary FOR array with n rows. The relations of $\mathbb{T}(n, v)$ encode which pairs of symbols are covered or avoided by any two columns. Using FOR target systems, FOR array optimization is now a generalized colouring problem, as follows.

Theorem 8.8.3 Let $S \in \mathcal{S}_{k,v}$. There exists a $\text{FOR}(n, S)$ if and only if $S \rightarrow \mathbb{T}(n, v)$, and $\text{FORN}(S) = \min\{n : S \rightarrow \mathbb{T}(n, v)\}$. ■



In Figure 8.9, we illustrate the two smallest binary FOR target systems, $\mathbb{T}(1, 2)$ and $\mathbb{T}(2, 2)$. These systems have three required relations and three forbidden relations. We use solid green arcs for the relation R_{00} . We use solid blue arcs for the relation R_{01} . We use solid red arcs for the relation R_{11} . We use dashed green arcs for the relation F_{00} . We use dashed blue arcs for the relation F_{01} . We use dashed red arcs for the relation F_{11} . The relations F_{ab} are the complements of the relations R_{ab} , for $0 \leq a \leq b \leq 1$, so we omit the dashed arcs in the picture of $\mathbb{T}(2, 2)$.

8.8.1 The core of $\mathbb{T}(n, v)$

Here, we show that FOR target systems are cores.

Proposition 8.8.4 For all $n \geq 1$, and for all $v \geq 1$, the binary relational system $\mathbb{T}(n, v)$ is a core.

[**proof**] If $v = 1$, then $\mathbb{T}(n, 1)$ is simply a vertex with a loop, which is indeed a core. Assume $v \geq 2$. Let $\vec{x} = (x_1, \dots, x_n)$ and $\vec{y} = (y_1, \dots, y_n)$ be two distinct vertices of $\mathbb{T}(n, v)$. There exists (at least) one index $i \in [n]$ such that $x_i \neq y_i$. Without loss of generality, suppose $x_i < y_i$. It follows that $(\vec{x}, \vec{y}) \in R_{x_i y_i}(\mathbb{T}(n, v))$. Consequently, no homomorphism of $\mathbb{T}(n, v) \rightarrow \mathbb{T}(n, v)$ can identify $\vec{x}$ and $\vec{y}$ because none of the relations $R_{ab}(\mathbb{T}(n, v))$ such that $a < b$ have loops. Thus, $\mathbb{T}(n, v)$ is not homomorphic to any proper subsystem of itself, and is therefore a core. $\blacksquare$

Let $\vec{x} = (x_1, \dots, x_n)$ be a v -ary n -tuple. For each $a \in [v]$, let

$$\vec{x}(a) = |\{i \in [n] : x_i = a\}|.$$

The **type** of $\vec{x}$ is the v -tuple $(\vec{x}(1), \dots, \vec{x}(v))$.

Lemma 8.8.5 Let $f : V(\mathbb{T}(n, v)) \rightarrow V(\mathbb{T}(n, v))$ be an automorphism of $\mathbb{T}(n, v)$. If $\vec{x} \in V(\mathbb{T}(n, v))$, then the type of $f(\vec{x})$ must be equal to the type of $\vec{x}$.

[**proof**] The case when $v = 1$ is trivial. Assume $v \geq 2$. Let $\vec{x} = (x_1, \dots, x_n)$ be a vertex of $\mathbb{T}(n, v)$. Choose a symbol $a \in [v]$ that occurs as an entry of $\vec{x}$. For any $b \in [v]$ such that $b > a$, consider the relation $R_{ab}(\mathbb{T}(n, v))$. Notice that the number of vertices $\vec{y} \in V(\mathbb{T}(n, v))$ such that $\vec{x}\vec{y} \in R_{ab}(\mathbb{T}(n, v))$ depends only on $\vec{x}(a)$. There are

$$\sum_{i=1}^{\vec{x}(a)} \binom{\vec{x}(a)}{i} v^{n-\vec{x}(a)} (v-1)^{\vec{x}(a)-i} = v^n - v^{n-\vec{x}(a)} (v-1)^{\vec{x}(a)}$$

such vertices $\vec{y}$. In other words, the outdegree of $\vec{x}$, with respect to the relation R_{ab} , is equal to $v^n - v^{n-\vec{x}(a)} (v-1)^{\vec{x}(a)}$.

Similarly, for any $c \in [v]$ such that $c < a$, the indegree of $\vec{x}$, with respect to the relation R_{ca} , is equal to $v^n - v^{n-\vec{x}(a)} (v-1)^{\vec{x}(a)}$. Given integers r and s , we have $v^n - v^{n-r} (v-1)^r = v^n - v^{n-s} (v-1)^s$ if and only if $r = s$.

Since automorphisms preserve adjacency for all relations, they must, in particular, preserve the indegree and outdegree of each vertex, with respect to each of the relations R_{ab} . For $\mathbb{T}(n, v)$, this can happen only if automorphisms preserve types. ■

Proposition 8.8.6 There are $n!$ automorphisms of $\mathbb{T}(n, v)$. They are given by the permutations of $[n]$.

[proof] For each permutation π of $[n]$, let $f_\pi : V(\mathbb{T}(n, v)) \rightarrow V(\mathbb{T}(n, v))$ be a map defined by $f_\pi(x_1, \dots, x_n) = (x_{\pi(1)}, \dots, x_{\pi(n)})$ for each $(x_1, \dots, x_n) \in V(\mathbb{T}(n, v))$. Clearly, f_π defines an automorphism of $\mathbb{T}(n, v)$.

Suppose $f : V(\mathbb{T}(n, v)) \rightarrow V(\mathbb{T}(n, v))$ is an automorphism. Consider the vertices of type $(1, n-1, 0, \dots, 0)$ having one occurrence of the symbol 1 and $(n-1)$ occurrences of the symbol 2. By Lemma 8.8.5, the automorphism f must map the vertices of type $(1, n-1, 0, \dots, 0)$ back onto vertices of the same type. There are n vertices of this type, one vertex for each position $i \in [n]$ where the symbol 1 is located. For convenience, denote the vertices as $\vec{e}_1, \dots, \vec{e}_n$, where $\vec{e}_i$ is the vertex of type $(1, n-1, 0, \dots, 0)$ with the symbol 1 in position i .

Define a permutation σ so that, for $i \in [n]$, we have $\sigma(i) = j$ if $f(\vec{e}_i) = \vec{e}_j$. We claim that $f = f_{\sigma^{-1}}$. If $f \neq f_{\sigma^{-1}}$, then there exists a vertex $\vec{x} = (x_1, \dots, x_n) \in V(\mathbb{T}(n, v))$ and an index $r \in [n]$ such that $f(\vec{x}) = (y_1, \dots, y_n)$ and $y_r \neq x_{\sigma^{-1}(r)}$. Let $s \in [n]$ be the index such that $\sigma(s) = r$ and consider $\vec{e}_s$. We have $\vec{e}_s \vec{x} \in R_{1x_s}(\mathbb{T}(n, v))$ and there is only one index, namely s , where the pair of symbols $(1, x_s)$ is covered; however, $f(\vec{e}_s)f(\vec{x}) \notin R_{1x_s}(\mathbb{T}(n, v))$ since the symbol 1 occurs only once in $f(\vec{e}_s) = \vec{e}_r$ at position r , and in $f(\vec{x}) = (y_1, \dots, y_n)$, we have $y_r \neq x_{\sigma^{-1}(r)} = x_s$. This contradicts the fact that f is an automorphism, hence f must equal $f_{\sigma^{-1}}$ as claimed. ■

Recall that in Question 3.2.5 we asked: for a given alphabet graph H , what is the core of the H -dependence graph $\text{QI}(n, H)$? Having proved, in Proposition 8.8.4, that the FOR target system $\mathbb{T}(n, v)$ is a core, we now observe that this result does not answer Question 3.2.5.

Let G be a column graph with $V(G) = [k]$ and let H be an alphabet graph with $V(H) = [v]$. Define a FOR BRS $S \in \mathcal{S}_{k,v}$ to encode the required interactions of $G \times H$ as follows. Let $F_{ab}(S) = \emptyset$, for all forbidden relations $F_{ab}(S)$. Pairs of columns in a $\text{CA}(n; 2, G, H)$ must be H -dependent whenever $ij \in E(G)$; so, for all $ij \in E(G)$, let $(i, j) \in R_{ab}(S)$ for all $ab \in E(H)$. Finding a $\text{CA}(n; 2, G, H)$ is equivalent to finding a $\text{FOR}(n, S)$. Finding a FOR array of S is equivalent to finding a homomorphism

of S to $\mathbb{T}(n, v)$ for some n ; however, the pattern of required edges encoded by S is uniform among all pairs (i, j) corresponding to an edge of G . We only need to consider pairs $\vec{xy}$ of vertices of $\mathbb{T}(n, v)$ in which $\vec{xy} \in R_{ab}(\mathbb{T}(n, v))$ for all $ab \in E(H)$, in other words, pairs which are H -dependent. In fact, every homomorphism of S to $\mathbb{T}(n, v)$ can be assumed to map to a subsystem of $\mathbb{T}(n, v)$ corresponding to the H -dependence graph, and the forbidden relations $F_{ab}(\mathbb{T}(n, v))$ do not come into play. The core of this subsystem (in which we do not use forbidden relations) is the subject of Question 3.2.5 and is certainly not equal to $\mathbb{T}(n, v)$.

8.8.2 Higher strength GRS model

It is also possible to model FOR systems of any mixed strength using general relational systems. For all $t \in [k]$, and for all t -tuples $(a_1, \dots, a_t) \in [v]^t$, we can encode the required interactions of strength t using t -ary relations $R_{(a_1, \dots, a_t)}$, and we can encode the forbidden interactions of strength t using t -ary relations $F_{(a_1, \dots, a_t)}$. Similarly, we can also define a general relational target system to convert the problem of finding FOR arrays into a homomorphism problem.

Although it is worthwhile to note these potential avenues of generalization, we do not endeavour to go beyond strength 2 here.

Chapter 9

Conclusion

To conclude, we highlight our main contributions, and we pose some of the many interesting open problems which have arisen as a result of this thesis.

LYM inequalities for alphabet graphs

By defining F -following collections, we were able to apply a permutation-counting technique to obtain infinitely many classes of LYM inequalities, each class corresponding to one follow digraph. We gave the simplified version of these LYM inequalities in Theorem 6.2.9.

We characterized the relationship between F -following collections and H -intersecting collections via alignment decompositions. In Corollary 6.3.2, we proved that the LYM inequality for F -following collections is applicable to H -intersecting collections for any follow digraph F such that $H \rightsquigarrow F$.

Using the alignment decomposition, we proved that strong graphs are the join of a complete graph with loops and a complete bipartite graph. We proved, in Corollary 6.4.6, that the maximal follow digraph F^H is the unique optimal follow digraph to use to get a direct bound for H -intersecting collections whenever H is a strong graph. In Theorem 6.4.8, we showed that if H is not a strong graph, then the best indirect bounds for H -intersecting collections are given by the maximal follow digraph of some strong subgraph of H .

We transformed the LYM inequality for the star S_3 into an upper bound on $m(n, S_3)$:

$$m(n, S_3) \leq \frac{1}{2 - \delta} \binom{a+b}{a} \approx \frac{1}{2} \binom{a+b}{a}$$

where $a + 2b = n$, $\delta = (2b)_b / (a + 2b)_b$, a is in an interval of at most three integers with $a \equiv n \pmod{2}$, and $\lim_{n \rightarrow \infty} a/b = \varphi$.

In Corollary 7.2.2, we improved a known construction for S_3 -intersecting collections, given in [35]. In Lemma 7.2.3, we showed that this construction is optimized when we have the golden ratio between the class cardinalities of the central vertex and the leaves.

We transformed the LYM inequality for K_3^{loop} into an upper bound on $\text{CAK}(n; 2, 3)$ using balancing lemmas. Our upper bound, given in Theorem 7.3.20, improves a known bound given in [48] for $v = 3$. For $v \geq 3$, we applied Theorem 7.3.20 to the three smallest classes of each v -packing in a qualitatively independent collection; this resulted in an improved bound on $m(n, v)$, for large enough v and n , which we give in Corollary 7.4.1.

In Theorem 7.5.6, we proved that the sum of the single-arc terms of β is asymptotically equal to β_1 if Premise 7.5.2 holds, that is, if there is an infinite sequence of F -following collections whose class cardinalities converge uniformly to some limiting distribution.

Using the single-arc terms of the LYM inequality for K_v^{loop} , we obtained the bound

$$m(n, K_v^{\text{loop}}) \leq \frac{1}{v^2 - v} \binom{2\lfloor n/v \rfloor + 2}{\lfloor n/v \rfloor + 1} (1 + o(1))$$

which, if Premise 7.5.2 holds, improves the bound we gave using K_3^{loop} .

Questions related to LYM inequalities

Q.9.1 (Stars)

Even though our upper bounds on $m(n, H)$ do not give us constructions, they do give us proportions of symbols (types) to consider. For example, our upper bound on $m(n, S_3)$ has the golden ratio between a and b (central vertex class cardinality and leaf class cardinality), and, for every n , a lies in a range of at most three integers.

Does there exist an infinite sequence of covering arrays, $\{\text{CA}(n_i; 2, k_i, S_3)\}_{i=1}^{\infty}$, such that $k_i = \text{CAK}(n_i; 2, S_3)$, the i th array has a_i ones, b_i twos, and c_i threes in every column, and $\lim_{i \rightarrow \infty} a_i/b_i = \lim_{i \rightarrow \infty} a_i/c_i = \varphi$?

For every n , does there exist a $\text{CA}(n; 2, k_n, S_3)$, where $k_n = \text{CAK}(n; 2, S_3)$, whose j th column has a_j ones and a_j is in the range given by Theorem 7.1.14, for all $j \in [k_n]$?

For S_3 , we also have a construction, given by Körner and Simonyi [35], that is asymptotically optimal with respect to its Sperner capacity. In this construction, given in Lemma 7.2.1, the symbols 2 and 3 always occur consecutively.

Question 1 For all n , does there exist a $\{\text{CA}(n; 2, \text{CAK}(n; 2, S_3), S_3)\}$ in which the symbols 2 and 3 always occur consecutively in every column?

Our upper bound on $m(n, S_3)$ is not tight (see Table 7.1 beginning with $n = 7$), and columns in optimal $\text{CA}(n; 2, k, S_3)$ do not necessarily have a common index-weight, as in the construction given in Lemma 7.2.1; nevertheless, the lower and upper bounds on $m(n, S_3)$ are relatively close and share the same golden proportions.

Problem 1 For all n , determine $\text{CAK}(n; 2, S_3)$.

Stars, in general, seem like good candidates for further work. The LYM inequality for star-intersecting collections (see Theorem 7.1.1) is relatively simple for all $v \geq 2$.

From the LYM inequality for S_4 , what is the corresponding upper bound on $m(n, S_4)$? Better yet, what is this upper bound on $m(n, S_v)$ for all $v \geq 4$?

Q.9.2 (Complete graphs with loops)

From our LYM inequality for K_4^{loop} -intersecting collections (see Appendix A), what is the corresponding upper bound on $m(n, K_4^{\text{loop}})$?

Is there a better approach for transforming the LYM inequality for K_3^{loop} -intersecting collections into an upper bound on $m(n, K_v^{\text{loop}})$? What is the best approach to transform the LYM inequality for K_v^{loop} into an upper bound on $m(n, K_v^{\text{loop}})$ for all $v \geq 3$?

For K_2^{loop} and K_3^{loop} , the upper bounds on $m(n, K_v^{\text{loop}})$ involve balanced class cardinalities in their formulas.

Conjecture 1 For all $v \geq 2$, the upper bound on $m(n, K_v^{\text{loop}})$, corresponding to the LYM inequality for K_v^{loop} -intersecting collections, is balanced.

Q.9.3 (Single-arc terms)

Assuming Premise 7.5.2 holds, we justified using the sum of the single-arc terms in $\beta(\mathcal{P}, F^H, n)$ as an estimate for $\beta(\mathcal{P}, F^H, n)$. Compare the actual upper bounds on $m(n, H)$ to the upper bound obtained from the single-arc estimate, where H is one of the alphabet graphs K_2 , K_2^{loop} , K_3^{loop} , or S_3 ; in these cases, both bounds exhibit the same type of balance.

Question 2 Does Premise 7.5.2 hold for complete graphs with loops? Does it hold for stars or complete bipartite graphs? Does it hold for strong graphs?

Q.9.4 (Sperner capacities)

There seems to be a parallel between Sperner capacities of alphabet graphs and the way we obtain our upper bounds from our LYM inequalities for H -intersecting collections: we balance occurrences of symbols to minimize β (this seems analogous to finding the maximizing probability distribution on $V(H)$) and we reciprocate and isolate a binomial coefficient corresponding to some single-arc term (this seems analogous to looking at the entropy of a single edge). It is also remarkable, that the upper bound we obtained on $m(n, S_3)$ has the golden proportion between a and b , while the maximizing distribution on $V(S_3)$, with respect to Sperner capacities, also has the golden ratio between the probability on the central vertex and the probability on the leaf vertices (see Table 5.1).

Given an alphabet graph H , how is our method for obtaining upper bounds on $m(n, H)$ using LYM inequalities connected to the Sperner capacity of H ?

Q.9.5 (Alphabet graphs that are not strong graphs)

If H is not a strong alphabet graph, then we get a finite list of LYM inequalities for H -intersecting collections—one inequality for each strong subgraph of H , given by the maximal follow digraph of the respective strong subgraph (recall that when H is a strong graph, there is only one LYM inequality for H worth considering: the LYM inequality of the maximal follow digraph F^H). The strong subgraph $K_2 \subset H$ always gives a LYM inequality for H -intersecting collections, but, intuitively, we prefer to use larger strong subgraphs, if possible, in order to capture more of the intersection properties encoded by H .

Among the list of LYM inequalities for a non-strong alphabet graph H , is there one that best captures H -intersecting collections? If, for each strong subgraph of H , we

transform the corresponding LYM inequality into an upper bound on $m(n, H)$, is there a particular strong subgraph that gives the tightest upper bound?

Covering arrays on column and alphabet graphs

We defined H -dependence graphs and showed that determining $\text{CAN}(2, G, H)$ is equivalent to finding the minimum n such that G is homomorphic to the H -dependence graph $\text{QI}(n, H)$.

We compared covering arrays on directed column graphs with the directed alphabet graph T_2 to undirected binary covering arrays. For any column graph G and any orientation G' of G , we established the bounds

$$\frac{1}{2}\text{CAN}(2, G, 2) - 1 \leq \text{CAN}(2, G', T_2) \leq \text{CAN}(2, G, 2) - 1$$

in Proposition 4.1.1, and we provided classes of column graphs achieving each of these bounds.

For a k -tournament column graph O , we gave the bounds

$$\lceil \log_2 k \rceil \leq \text{CAN}(2, O, T_2) \leq \min \left\{ n : k \leq 2 \binom{n-1}{\lfloor (n-1)/2 \rfloor} \right\}.$$

The lower bound followed from the fact that homomorphisms of tournaments into the T_2 dependence graph must be vertex-injective (see Lemma 4.4.2). The upper bound followed from a construction using the subsets of largest rank in the poset of subsets of $[n-1]$ (see Proposition 4.4.9). Both these bounds are asymptotically equal to $\log_2 k$.

In Theorem 4.4.3, we proved that $\text{CAN}(2, T_k, T_2) = \lceil \log_2 k \rceil$ for all k .

In Proposition 4.4.4, we gave a new construction for building binary covering arrays of strength 2 using covering arrays on transitive tournaments with alphabet graph T_2 as building blocks. Although this construction is not optimal, it demonstrates how covering arrays on directed column graphs might be useful as ingredients for building classical covering arrays.

Circular tournaments are an interesting family of column graphs that we considered. For small values of k , they have the largest covering array number among all k -tournament column graphs with alphabet graph T_2 .

In Proposition 4.5.6, we gave a construction for covering arrays on Ω_k with alphabet graph T_2 that makes use of the Kruskal–Katona Theorem. This construction implies

$$\text{CAN}(2, \Omega_k, T_2) \leq \min \left\{ n : k \leq \binom{n}{\lfloor n/2 \rfloor} + \binom{n-2}{\lfloor n/2 \rfloor + 1} \right\}.$$

In Proposition 4.5.11, we gave a recursive construction that implies

$$\text{CAN}(2, \Omega_k, T_2) = \lceil \log_2 k \rceil$$

for infinitely many values of k .

For a directed alphabet graph H , we defined the Sperner capacity of H with respect to transitive tournaments, and in Corollary 5.3.6, we showed that

$$\Sigma(H, \{T_L\}) = \max_P \min_{ab \in E(H)} (P_a + P_b) \cdot h \left(\frac{P_a}{P_a + P_b} \right)$$

where the maximum is taken over all probability distributions P on $V(H)$.

Questions related to $\text{CA}(n; 2, G, H)$

Q.9.6 (Tournament column graphs)

For circular tournament column graphs, determining $\text{CAN}(2, \Omega_k, T_2)$ would make a nice counterpart to Sperner’s Theorem.

Problem 2 For all k , determine $\text{CAN}(2, \Omega_k, T_2)$.

We conjectured that circular tournaments are the worst tournament column graphs in terms of having the largest covering array numbers among all tournament column graphs with alphabet graph T_2 (see Conjecture 4.5.1).

Is $\text{CAN}(2, O, T_2) \leq \text{CAN}(2, \Omega_k, T_2)$ for all k -tournaments O ?

Similar questions arise for covering arrays on tournament column graphs with directed alphabet graphs other than T_2 .

Given a directed alphabet graph H (other than T_2), and a k -tournament column graph O , is it true that $\text{CAN}(2, T_k, H) \leq \text{CAN}(2, O, H)$? If we sort all k -tournaments O according to $\text{CAN}(2, O, H)$, does this ordering change when we change the alphabet graph?

Q.9.7 (H -dependence graphs)

Given an alphabet graph H , what is the core of the H -dependence graph $\text{QI}(n, H)$? Do the vertices of the core of $\text{QI}(n, H)$ exhibit a specific proportion of symbols related to the structure of H ? What is the clique number $\omega(\text{QI}(n, H))$?

FOR arrays

In Proposition 8.5.1, we proved that determining $\text{FORN}(X)$ is equivalent to finding the minimum number of edges needed to cover the vertices of the compatibility hypergraph H_X .

When FOR systems are binary and have forbidden strength 2, we proved, in Proposition 8.5.1, that cliques in the compatibility hypergraph are edges; in other words, for the elements of a set of required interactions, being pairwise compatible implies being set-wise compatible. In this case (binary, forbidden strength 2), determining $\text{FORN}(X)$ is equivalent to determining the clique cover number $\theta(H_X)$. We proved that this is not the case if either the alphabet size is non-binary or if the forbidden strength goes beyond 2.

We determined the effects of removing (relabelling as optional) a required or forbidden interaction from a FOR system. Removing a required interaction can reduce FORN by at most one (see Lemma 8.6.8). Removing a forbidden interaction of strength t can reduce FORN by a factor of t (see Corollary 8.6.10).

We defined critical FOR systems, giving examples, direct constructions and recursive constructions. In Proposition 8.7.2, we showed that binary required-critical FOR systems of forbidden strength 2 have vertex-critical incompatibility graphs.

For testing problems of strength 2, we defined an alternative way to model FOR arrays using binary relational systems called FOR BRS. The vertices of a FOR BRS correspond to the factors of some testing problem and it has relations to encode every possible pair of symbols that could be required or forbidden. We defined FOR target systems; the vertices of $\text{T}(n, v)$ correspond to all possible columns of a FOR array with alphabet size v and n rows (all v -ary n -tuples), and the arc relations of $\text{T}(n, v)$ encode which pairs of columns cover or avoid a given pair of symbols. In Theorem 8.8.3, we proved that given a FOR BRS $S \in \mathcal{S}_{k,v}$, there exists $\text{FOR}(n, S)$ if and only if there is a homomorphism of S to the target FOR system $\text{T}(n, v)$.

In Proposition 8.8.4, we proved that the target FOR system $\mathbb{T}(n, v)$ is a core. Consequently, there is no smaller target system to consider that would suffice for every possible FOR BRS.

Questions related to FOR arrays

Q.9.8 (Compatibility hypergraphs)

In Proposition 8.5.2, we showed that a set of pairwise compatible required edges is compatible as a whole (that is, a clique of the compatibility graph is an edge) if the given FOR system X is binary and of forbidden strength 2. Let $X \in \mathcal{X}_{k,v}$ be a v -ary FOR system. If every v required interactions in a set $S \subset R(X)$ is compatible, then let us say that S is *v -wise compatible*.

Let $v \geq 3$. If $X \in \mathcal{X}_{k,v}$ has forbidden strength at most $v - 1$, does a set $S \subset R(X)$ being v -wise compatible guarantee that the entire set S is compatible?

Q.9.9 (Critical systems)

In Section 8.6, we explored the notion of critical FOR systems and gave a few simple constructions for binary systems of strength 2 with safe values or dummy values.

Problem 3 Find examples of critical FOR systems that do not have safe values. Find examples of critical systems with interactions of higher strength.

Appendix A

Inventory of LYM inequalities for H -intersecting collections

This appendix contains an inventory of LYM inequalities for H -intersecting collections. Each graph H is given with its maximal follow digraph F^H . The vertices of H are labelled with letters from $\{a, b, c, d\}$. We give the corresponding LYM inequality for an H -intersecting collection $\mathcal{P} = \{P_1, \dots, P_m\}$. To make the LYM inequalities more readable, for each $P_i \in \mathcal{P}$, and for each $\alpha \in V(H)$, the class cardinality $|P_i^\alpha|$ is denoted α_i , for the appropriate $\alpha \in \{a, b, c, d\}$.

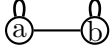


LYM inequality

$$\sum_{i=1}^m \frac{1}{\binom{a_i + b_i}{a_i}} \leq 1$$

Remarks

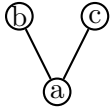
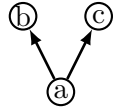
This is a well-known LYM-like inequality (see Theorem 2.1.3) and *the* LYM Inequality follows as a special case (see Theorem 2.1.2). Our proof using the given follow digraph corresponds to the proof techniques of Lubell [38], Katona [33], and Tarjan [59].

H  F^H **LYM inequality**

$$\sum_{i=1}^m \frac{2}{\binom{a_i + b_i}{a_i}} \leq 1$$

Remarks

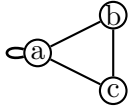
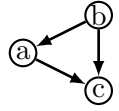
This is a known LYM-like inequality (see Theorem 6.1.5). In their proof of Theorem 2.3.4, Poljak and Tuza [48] applied the inequality of Theorem 2.1.3 to twice as many sets in the collection, which essentially yielded the above inequality. Stevens [55] proved this LYM inequality by counting permutations (our proof using the follow digraph F^H is essentially the same). The result also appeared in the paper by Stevens, Moura and Mendelsohn [57].

 H  F^H **LYM inequality**

$$\sum_{i=1}^m \frac{1}{\binom{a_i + b_i}{a_i}} + \frac{1}{\binom{a_i + c_i}{a_i}} - \frac{1}{\binom{a_i + b_i + c_i}{a_i}} \leq 1$$

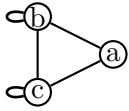
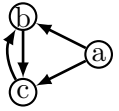
Remarks

This is a known LYM-like inequality. It was given without proof by Körner and Simonyi [35]. Ahlswede and Cai [1] determined the properties of those collections for which equality is achieved. In Theorem 7.1.14, we give the corresponding upper bound.

H  F^H 

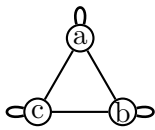
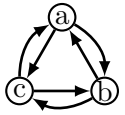
LYM inequality

$$\sum_{i=1}^m \frac{1}{\binom{a_i + b_i}{a_i}} + \frac{1}{\binom{b_i + c_i}{b_i}} + \frac{1}{\binom{a_i + c_i}{c_i}} - \frac{1}{\binom{a_i + b_i + c_i}{b_i}} - \frac{1}{\binom{a_i + b_i + c_i}{c_i}} \leq 1$$

 H  F^H 

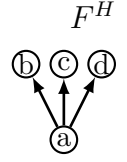
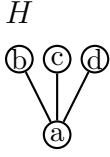
LYM inequality

$$\sum_{i=1}^m \frac{1}{\binom{a_i + b_i}{b_i}} + \frac{1}{\binom{a_i + c_i}{c_i}} + \frac{2}{\binom{b_i + c_i}{b_i}} - \frac{1}{\binom{a_i + b_i + c_i}{a_i}} - \frac{1}{\binom{a_i + b_i + c_i}{b_i}} - \frac{1}{\binom{a_i + b_i + c_i}{c_i}} \leq 1$$

 H  F^H 

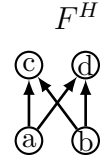
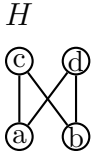
LYM inequality

$$\sum_{i=1}^m \frac{2}{\binom{a_i + b_i}{a_i}} + \frac{2}{\binom{b_i + c_i}{b_i}} + \frac{2}{\binom{a_i + c_i}{c_i}} - \frac{2}{\binom{a_i + b_i + c_i}{a_i}} - \frac{2}{\binom{a_i + b_i + c_i}{b_i}} - \frac{2}{\binom{a_i + b_i + c_i}{c_i}} \leq 1$$



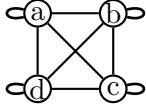
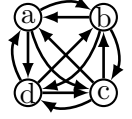
LYM inequality

$$\sum_{i=1}^m \frac{1}{\binom{a_i + b_i}{a_i}} + \frac{1}{\binom{a_i + c_i}{a_i}} + \frac{1}{\binom{a_i + d_i}{a_i}} - \frac{1}{\binom{a_i + b_i + c_i}{a_i}} - \frac{1}{\binom{a_i + b_i + d_i}{a_i}} - \frac{1}{\binom{a_i + c_i + d_i}{a_i}} + \frac{1}{\binom{a_i + b_i + c_i + d_i}{a_i}} \leq 1$$



LYM inequality

$$\begin{aligned} & \sum_{i=1}^m \frac{1}{\binom{a_i + c_i}{a_i}} + \frac{1}{\binom{a_i + d_i}{a_i}} + \frac{1}{\binom{b_i + c_i}{b_i}} + \frac{1}{\binom{b_i + d_i}{b_i}} - \frac{1}{\binom{a_i + c_i + d_i}{a_i}} - \frac{1}{\binom{a_i + b_i + c_i}{c_i}} \\ & - \frac{1}{\binom{a_i + d_i}{a_i} \binom{b_i + c_i}{b_i}} - \frac{1}{\binom{a_i + b_i + d_i}{d_i}} - \frac{1}{\binom{b_i + c_i + d_i}{b_i}} - \frac{1}{\binom{a_i + c_i}{a_i} \binom{b_i + d_i}{b_i}} \\ & + \frac{1}{\binom{a_i + b_i + c_i + d_i}{a_i, b_i, c_i, d_i}} \left[\sum_{j=0}^{d_i} \binom{c_i - 1 + j}{c_i - 1} \binom{a_i + b_i + d_i - j}{b_i} \right. \\ & \quad + \sum_{j=0}^{c_i} \binom{d_i - 1 + j}{d_i - 1} \binom{a_i + b_i + c_i - j}{b_i} + \sum_{j=0}^{d_i} \binom{c_i - 1 + j}{c_i - 1} \binom{a_i + b_i + d_i - j}{a_i} \\ & \quad \left. + \sum_{j=0}^{c_i} \binom{d_i - 1 + j}{d_i - 1} \binom{a_i + b_i + c_i - j}{a_i} \right] - \frac{1}{\binom{a_i + b_i + c_i + d_i}{a_i + b_i}} \leq 1 \end{aligned}$$

H  F^H **LYM inequality**

$$\begin{aligned}
& \sum_{i=1}^m \frac{2}{\binom{a_i+b_i}{a_i}} + \frac{2}{\binom{a_i+c_i}{a_i}} + \frac{2}{\binom{a_i+d_i}{a_i}} + \frac{2}{\binom{b_i+c_i}{b_i}} + \frac{2}{\binom{b_i+d_i}{b_i}} + \frac{2}{\binom{c_i+d_i}{c_i}} - \frac{2}{\binom{a_i+b_i+c_i}{a_i}} \\
& - \frac{2}{\binom{a_i+b_i+c_i}{b_i}} - \frac{2}{\binom{a_i+b_i+c_i}{c_i}} - \frac{2}{\binom{a_i+b_i+d_i}{a_i}} - \frac{2}{\binom{a_i+b_i+d_i}{b_i}} - \frac{2}{\binom{a_i+b_i+d_i}{d_i}} \\
& - \frac{2}{\binom{a_i+c_i+d_i}{a_i}} - \frac{2}{\binom{a_i+c_i+d_i}{c_i}} - \frac{2}{\binom{a_i+c_i+d_i}{d_i}} - \frac{2}{\binom{b_i+c_i+d_i}{b_i}} - \frac{2}{\binom{b_i+c_i+d_i}{c_i}} \\
& - \frac{2}{\binom{b_i+c_i+d_i}{d_i}} - \frac{2}{\binom{a_i+b_i}{a_i} \binom{c_i+d_i}{c_i}} - \frac{2}{\binom{a_i+c_i}{a_i} \binom{b_i+d_i}{b_i}} - \frac{2}{\binom{a_i+d_i}{a_i} \binom{b_i+c_i}{b_i}} \\
& + \frac{2}{\binom{a_i+b_i+c_i+d_i}{a_i}} + \frac{2}{\binom{a_i+b_i+c_i+d_i}{b_i}} + \frac{2}{\binom{a_i+b_i+c_i+d_i}{c_i}} + \frac{2}{\binom{a_i+b_i+c_i+d_i}{d_i}} \\
& + \frac{1}{\binom{a_i+b_i+c_i+d_i}{a_i, b_i, c_i, d_i}} \left[\sum_{j=0}^{c_i} \binom{d_i-1+j}{d_i-1} \binom{a_i+b_i+c_i-j}{b_i} + \sum_{j=0}^{d_i} \binom{c_i-1+j}{c_i-1} \binom{a_i+b_i+d_i-j}{a_i} \right. \\
& + \sum_{j=0}^{d_i} \binom{c_i-1+j}{c_i-1} \binom{a_i+b_i+d_i-j}{b_i} + \sum_{j=0}^{c_i} \binom{d_i-1+j}{d_i-1} \binom{a_i+b_i+c_i-j}{a_i} \\
& + \sum_{j=0}^{b_i} \binom{d_i-1+j}{d_i-1} \binom{a_i+b_i+c_i-j}{c_i} + \sum_{j=0}^{d_i} \binom{b_i-1+j}{b_i-1} \binom{a_i+c_i+d_i-j}{a_i} \\
& + \sum_{j=0}^{d_i} \binom{b_i-1+j}{b_i-1} \binom{a_i+c_i+d_i-j}{c_i} + \sum_{j=0}^{b_i} \binom{d_i-1+j}{d_i-1} \binom{a_i+b_i+c_i-j}{a_i} \\
& + \sum_{j=0}^{b_i} \binom{c_i-1+j}{c_i-1} \binom{a_i+b_i+d_i-j}{d_i} + \sum_{j=0}^{c_i} \binom{b_i-1+j}{b_i-1} \binom{a_i+c_i+d_i-j}{a_i} \\
& \left. + \sum_{j=0}^{c_i} \binom{b_i-1+j}{b_i-1} \binom{a_i+c_i+d_i-j}{d_i} + \sum_{j=0}^{b_i} \binom{c_i-1+j}{c_i-1} \binom{a_i+b_i+d_i-j}{a_i} \right]
\end{aligned}$$

(continues overleaf)

$$\begin{aligned}
& + \sum_{j=0}^{a_i} \binom{d_i-1+j}{d_i-1} \binom{a_i+b_i+c_i-j}{c_i} + \sum_{j=0}^{d_i} \binom{a_i-1+j}{a_i-1} \binom{b_i+c_i+d_i-j}{b_i} \\
& + \sum_{j=0}^{d_i} \binom{a_i-1+j}{a_i-1} \binom{b_i+c_i+d_i-j}{c_i} + \sum_{j=0}^{a_i} \binom{d_i-1+j}{d_i-1} \binom{a_i+b_i+c_i-j}{b_i} \\
& + \sum_{j=0}^{a_i} \binom{c_i-1+j}{c_i-1} \binom{a_i+b_i+d_i-j}{d_i} + \sum_{j=0}^{c_i} \binom{a_i-1+j}{a_i-1} \binom{b_i+c_i+d_i-j}{b_i} \\
& + \sum_{j=0}^{c_i} \binom{a_i-1+j}{a_i-1} \binom{b_i+c_i+d_i-j}{d_i} + \sum_{j=0}^{a_i} \binom{c_i-1+j}{c_i-1} \binom{a_i+b_i+d_i-j}{b_i} \\
& + \sum_{j=0}^{a_i} \binom{b_i-1+j}{b_i-1} \binom{a_i+c_i+d_i-j}{d_i} + \sum_{j=0}^{b_i} \binom{a_i-1+j}{a_i-1} \binom{b_i+c_i+d_i-j}{c_i} \\
& + \sum_{j=0}^{b_i} \binom{a_i-1+j}{a_i-1} \binom{b_i+c_i+d_i-j}{d_i} + \sum_{j=0}^{a_i} \binom{b_i-1+j}{b_i-1} \binom{a_i+c_i+d_i-j}{c_i} \Big] \\
& - \frac{2}{\binom{a_i+b_i+c_i+d_i}{a_i+b_i}} - \frac{2}{\binom{a_i+b_i+c_i+d_i}{a_i+c_i}} - \frac{2}{\binom{a_i+b_i+c_i+d_i}{a_i+d_i}} \leq 1
\end{aligned}$$

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