On Bounding the Probability of a Finite Union of Events using Partial Information

by

Jun Yang

A report submitted to the
Department of Mathematics and Statistics
in conformity with the requirements for
the degree of Master of Science

Queen's University
Kingston, Ontario, Canada
August 2014

Abstract

We consider bounding the probability of a finite union of events, $P\left(\bigcup_{i=1}^{N} A_i\right)$ where N is a finite integer, using partial information on the event probabilities, such as the individual event probabilities, $\{P(A_i)\}$, and the pairwise event probabilities, $\{P(A_i \cap A_j)\}$.

First, for bounds of $P\left(\bigcup_{i=1}^{N} A_i\right)$ that are established in terms of $\{P(A_i)\}$ and $\{\sum_j P(A_i \cap A_j)\}$, the optimal lower/upper bound are proposed by solving a linear programming (LP) problem, which has only $N^2 - N + 1$ variables. Furthermore, a new suboptimal analytical lower bound is derived by solving a relaxed LP problem, which is proven to be at least as good as the existing Kuai-Alajaji-Takahara (KAT) bound.

Second, for bounds of $P\left(\bigcup_{i=1}^{N} A_i\right)$ that are established in terms of $\{P(A_i)\}$ and $\{\sum_j c_j P(A_i \cap A_j)\}$ for a given weight or parameter vector $\boldsymbol{c} = (c_1, \ldots, c_N)^T$, a new class of lower bounds are established which has at most pseudo-polynomial computational complexity and can be sharper than the existing Gallot-Kounias (GK) bound under certain conditions.

Finally, for bounds of $P\left(\bigcup_{i=1}^{N} A_i\right)$ that fully exploit $\{P(A_i)\}$ and $\{P(A_i \cap A_j)\}$, a new numerical lower/upper bound is proposed by solving an LP problem with $\frac{(N-1)^3+N+3}{2}$ variables. This numerical lower/upper bound is proven to be an optimal

lower/upper bound when $N \leq 7$, and always sharper than the optimal lower/upper bound using $\{P(A_i)\}$ and $\{\sum_j P(A_i \cap A_j)\}$.

Acknowledgments

My work on this report could not have been possible without the support and guidance of many individuals. First, I am honored and deeply appreciative to my supervisor, Dr. Fady Alajaji, for admission to this program one year ago and his continuous support and guidance during the past year.

I also would like to extend my deepest appreciation to my co-supervisor, Dr. Glen Takahara, who provided me thorough, meaningful, and constructive comments and suggestions throughout the process.

Special thanks to my committee members, Dr. Tamás Linder and Dr. Serdar Yüksel, and my friends, Dr. Feng Qu and Dr. Chengpeng Hao, who devoted many hours of their time on this research project and provided valuable feedback.

Finally, I would like to thank and acknowledge all my friends around the world who have encouraged and inspired me during the past year, and my dad for his unconditional love and support.

This work is dedicated in memory of my mum, Li Zhang, on the 2nd anniversary of her death. I am grateful for all she taught me and hope that I am living in a way that makes her proud.

Contents

List of Tables

List of Figures

Chapter 1

Introduction

Consider a finite family of events $\{A_1, \ldots, A_N\}$ in a general probability space $(\Omega, \mathscr{F}, P)$, where N is a fixed positive integer. Note that there are only finitely many Boolean atoms[1] specified by the A_i's [8]. We are interested in bounding the probability of the finite union of events, i.e., $P\left(\bigcup_{i=1}^N A_i\right)$, in terms of partial probabilistic event information such as knowing the individual event probabilities, $\{P(A_1), \ldots, P(A_N)\}$, and the pairwise event probabilities $\{P(A_i \cap A_j), i \neq j\}$, or (linear) functions of the probabilities of individual and pairwise events.

For example, the well-known union upper bound and the Bonferroni inequality [12] are respectively given as follows:

$$P\left(\bigcup_{i=1}^N A_i\right) \leq \sum_{i=1}^N P(A_i), \tag{1.1}$$

$$P\left(\bigcup_{i=1}^N A_i\right) \geq \sum_{i=1}^N P(A_i) - \sum_{i<j} P(A_i \cap A_j). \tag{1.2}$$

[1]The problem can be directly reduced to the finite probability space case. Thus, through the numerical examples, as well as Chapters 4 and 5 of this work, we will consider finite probability spaces where $\omega \in \Omega$ denotes an elementary outcome instead of an atom.

We note that the union upper bound (1.1) is established in terms of only $\sum_{i=1}^{N} P(A_i)$ so that each of the individual event probability $P(A_i)$ is actually not needed. However, the Bonferroni lower bound (1.2) is established using two terms, $\sum_{i=1}^{N} P(A_i)$ and $\sum_{i<j} P(A_i \cap A_j)$. Therefore, the union upper bound (1.1) and the Bonferroni inequality (1.2) are established based on different partial information on the event probabilities.

In order to distinguish the use of different partial information, we assume that a vector $\theta = (\theta_1, \ldots, \theta_m) \in \mathbb{R}^m$ represents partial probabilistic information about the union $\bigcup_{i=1}^{N} A_i$. Specifically, we assume that for a given integer $m \geq 1$, Θ denotes the range of a function of $P(A_i)$'s and $P(A_i \cap A_j)$'s, $\eta_m : [0,1]^{N+\binom{N}{2}} \to \mathbb{R}^m$. Then θ equals to the value of the function η_m for given $A_1, \ldots, A_N$. For example,

$$\theta = (P(A_1), P(A_2), \ldots, P(A_N)), \tag{1.3}$$

or

$$\theta = \left(\sum_{i=1}^{N} P(A_i), \sum_{i<j} P(A_i \cap A_j) \right). \tag{1.4}$$

Then, we can define a lower bound (and similarly an upper bound) on $P\left(\bigcup_{i=1}^{N} A_i\right)$ that is established using the partial information represented by θ as follows.

Definition. *A lower bound of $P\left(\bigcup_{i=1}^{N} A_i\right)$ is a function of θ, $\ell(\theta)$, such that*

$$P\left(\bigcup_{i=1}^{N} A_i\right) \geq \ell(\theta), \tag{1.5}$$

for any set of events $\{A_i\}$ that the value of η_m for given $\{A_i\}$ equals to θ.

Note that, for given θ, such as $\theta = (P(A_1), \ldots, P(A_N))$, there are multiple functions of θ that are lower bounds, for example,

$$\begin{aligned} P\left(\bigcup_{i=1}^{N} A_i\right) &\geq \theta_1 = P(A_1), \\ P\left(\bigcup_{i=1}^{N} A_i\right) &\geq \frac{\sum_i \theta_i}{N} = \frac{\sum_i P(A_i)}{N}, \\ P\left(\bigcup_{i=1}^{N} A_i\right) &\geq \max_i \theta_i = \max_i P(A_i). \end{aligned} \tag{1.6}$$

Therefore, we need to define an *optimal* lower bound in a general class of lower bounds that are functions of θ.

Let $\mathscr{L}_\Theta$ denote the set of all lower bounds on $P\left(\bigcup_{i=1}^{N} A_i\right)$ that are functions of only θ.

Definition. *We say that a lower bound $\ell^\star \in \mathscr{L}_\Theta$ is optimal in $\mathscr{L}_\Theta$ if $\ell^\star(\theta) \geq \ell(\theta)$ for all $\theta \in \Theta$ and $\ell \in \mathscr{L}_\Theta$.*

Definition. *We say that a lower bound $\ell \in \mathscr{L}_\Theta$ is achievable if for every $\theta \in \Theta$,*

$$\inf_{A_1,\ldots,A_N} P\left(\bigcup_{i=1}^{N} A_i\right) = \ell(\theta), \tag{1.7}$$

where the infimum ranges over all collections $\{A_1, \ldots, A_N\}$, $A_i \in \mathscr{F}$, such that $\{A_1, \ldots, A_N\}$ is represented by θ.

For bounds in $\mathscr{L}_\Theta$, the following lemma shows that achievability is equivalent to optimality.

Lemma 1. *A lower bound $\ell^\star \in \mathscr{L}_\Theta$ is optimal in $\mathscr{L}_\Theta$ if and only if it is achievable.*

Proof. Suppose that $\ell^\star$ is achievable. Let $\theta \in \Theta$ and $\epsilon > 0$ be given, and let ℓ be any lower bound in $\mathscr{L}_\Theta$. By achievability there exist sets $A_1, \ldots, A_N$ in $\mathscr{F}$ represented by

θ such that

$$\ell^\star(\theta) > P\left(\bigcup_{i=1}^{N} A_i\right) - \epsilon \geq \ell(\theta) - \epsilon.$$

Since this holds for any ϵ we have $\ell^\star(\theta) \geq \ell(\theta)$. We prove the converse by the contrapositive. Suppose that $\ell^\star$ is not achievable. Then there exists $\theta' \in \Theta$ such that

$$\inf_{A_1,\ldots,A_N} P\left(\bigcup_{i=1}^{N} A_i\right) > \ell^\star(\theta'),$$

where the infimum ranges over all collections $\{A_1, \ldots, A_N\}$, $A_i \in \mathscr{F}$, such that $\{A_1, \ldots, A_N\}$ is represented by θ'. Define ℓ by

$$\ell(\theta) = \begin{cases} c & \text{if } \theta = \theta' \\ 0 & \text{if } \theta \neq \theta', \end{cases}$$

where c satisfies

$$\inf_{A_1,\ldots,A_N} P\left(\bigcup_{i=1}^{N} A_i\right) > c > \ell^\star(\theta').$$

Then $\ell \in \mathscr{L}_\Theta$ and is larger than $\ell^\star$ at θ'. Hence, $\ell^\star$ is not optimal. $\square$

Using Lemma 1, we can therefore prove that a lower bound $\ell(\theta)$ is optimal if for any value of $\theta \in \Theta$, one can construct a collection of events $\{A_i^*\}$ that is represented by θ and $P\left(\bigcup_{i=1}^{N} A_i^*\right) = \ell(\theta)$. The optimal upper bound can also be defined similarly (using a supremum in (1.7)) and proved by achievability. For example, one can easily verify the following by a construction proof of achievability.

- $P\left(\bigcup_{i=1}^{N} A_i\right) \geq \frac{\sum_i P(A_i)}{N}$ is the optimal lower bound in the class for $\theta = (\sum_i P(A_i))$.
- $P\left(\bigcup_{i=1}^{N} A_i\right) \geq \max_i P(A_i)$ is the optimal lower bound in the class for $\theta = (P(A_1), \ldots, P(A_N))$.

- $P\left(\bigcup_{i=1}^{N} A_i\right) \leq \min\{\sum_i P(A_i), 1\}$ is the optimal upper bound in the classes for both $\theta = (\sum_i P(A_i))$ and $\theta = (P(A_1), \ldots, P(A_N))$.

Furthermore, we can prove that a lower bound is not optimal by showing it is not achievable. For example, in order to show that the Bonferroni inequality (1.2) is not an optimal lower bound in the class of lower bounds that are functions of $\theta = \left(\sum_i P(A_i), \sum_{i<j} P(A_i \cap A_j)\right)$, we only need to show it is not achievable. Note that for $N > 3$, the lower bound (1.2) can have negative values. However, according to the definition of achievability, the LHS of (1.7) can never be negative, which means the lower bound (1.2) cannot be achievable. Therefore, the Bonferroni inequality (1.2) is not optimal.

In the rest of this work, we first give a review of existing work in Chapter 2. Then new bounds in terms of $\{P(A_i)\}$ and $\{\sum_j P(A_i \cap A_j)\}$ are derived in Chapter 3, and new bounds in terms of $\{P(A_i)\}$ and $\{\sum_j c_j P(A_i \cap A_j)\}$ for a given weight vector $\boldsymbol{c} = (c_1, \ldots, c_N)^T$ are established in Chapter 4. Finally, we investigate new bounds in terms of $\{P(A_i)\}$ and $\{P(A_i \cap A_j)\}$ in Chapter 5.

Thoughout the work, we mainly focus on lower bounds using different partial probabilistic information. Upper bounds are presented as remarks.

Chapter 2

Review of Existing Bounds

We start from the class of lower bounds in terms of $\sum_i P(A_i)$ and $\sum_{i<j} P(A_i \cap A_j)$, for which the Dawson-Sankoff (DS) lower bound [7] is known as optimal. Then we introduce some lower bounds in terms of $\{P(A_i)\}$ and $\{\sum_j P(A_i \cap A_j)\}$, including the D. de Caen (DC) bound [8] and the Kuai-Alajaji-Takahara (KAT) bound [19]. Next, a review of some lower bounds in terms of $\{P(A_i)\}$ and $\{P(A_i \cap A_j)\}$ is given, including the algorithmic stepwise lower bound [20] and the Gallot-Kounias (GK) bound [13, 17, 11]. Finally, some existing upper bounds are reviewed, including the Hunter upper bound and the algorithmic greedy upper bound [20].

We first define the degree of an atom (or outcome in finite probability space) $\omega \in \mathscr{F}$ as follows.

Definition. *For each atom $\omega \in \mathscr{F}$, let the degree of ω, denoted by* $\deg(\omega)$*, be the number of A_i's that contain ω.*

Therefore, the degree of any atom in $\bigcup_i A_i$ equals to an integer in $\{1, \ldots, N\}$.

2.1 Lower Bounds Using $\sum_i P(A_i)$ and $\sum_{i<j} P(A_i \cap A_j)$

Considering $\theta = \left(\sum_i P(A_i), \sum_{i<j} P(A_i \cap A_j)\right)$, we note that the Bonferroni inequality (1.2) is a lower bound in this class. However, we have shown that (1.2) is not optimal, which means there exists another function of only $\sum_i P(A_i)$ and $\sum_{i<j} P(A_i \cap A_j)$ that is a lower bound of $P\left(\bigcup_{i=1}^N A_i\right)$ and always sharper than the Bonferroni inequality.

Defining

$$a(k) := P\left(\left\{\omega \subseteq \bigcup_i A_i, \deg(\omega) = k\right\}\right), \tag{2.1}$$

one can easily verify the following identities:

$$P\left(\bigcup_{i=1}^N A_i\right) = \sum_{k=1}^N a(k), \tag{2.2}$$

$$\sum_{i=1}^N P(A_i) = \sum_{k=1}^N k a(k), \tag{2.3}$$

$$\sum_{i<j} P(A_i \cap A_j) = \sum_{k=2}^N \binom{k}{2} a(k), \tag{2.4}$$

$$\begin{aligned} \sum_{i,j} P(A_i \cap A_j) &= 2\sum_{i<j} P(A_i \cap A_j) + \sum_{i=1}^N P(A_i) \\ &= 2\sum_{k=2}^N \frac{k(k-1)}{2} a(k) + \sum_{k=1}^N k a(k) \\ &= \sum_{k=1}^N k^2 a(k). \end{aligned} \tag{2.5}$$

Note that using the above equalities, one can derive a lower bound simply via the

Cauchy-Schwarz inequality:

$$\left(\sum_k a(k)\right)\left(\sum_k k^2 a(k)\right) \geq \left(\sum_k ka(k)\right)^2, \tag{2.6}$$

where equality holds if and only if $a(k) > 0$ only for a particular k, i.e., all outcomes in the union has the same degree k. The resulting lower bound can be written as

$$P\left(\bigcup_{i=1}^N A_i\right) \geq \frac{\left(\sum_i P(A_i)\right)^2}{\sum_{i,j} P(A_i \cap A_j)}. \tag{2.7}$$

Since $\sum_{i,j} P(A_i \cap A_j) \leq \sum_{i,j} P(A_i) = N \sum_i P(A_i)$,

$$\frac{\left(\sum_i P(A_i)\right)^2}{\sum_{i,j} P(A_i \cap A_j)} \geq \frac{\sum_i P(A_i)}{N}; \tag{2.8}$$

hence the lower bound (2.7) is always sharper than $\frac{\sum_i P(A_i)}{N}$, which has been shown to be optimal in the class of $\theta = (\sum_i P(A_i))$. This is reasonable since the lower bound (2.7) is established using more information than $\frac{\sum_i P(A_i)}{N}$. However, it can be readily shown that the lower bound (2.7) is not always sharper than the Bonferroni inequality (1.2). Therefore, it cannot be the optimal lower bound in the class of $\theta = \left(\sum_i P(A_i), \sum_{i<j} P(A_i \cap A_j)\right)$.

2.1.1 Dawson-Sankoff (DS) Bound

The DS bound is known as the optimal lower bound in terms of only $\sum_i P(A_i)$ and $\sum_{i<j} P(A_i \cap A_j)$. Denoting $\theta_1 := \sum_i P(A_i)$ and $\theta_2 := \sum_{i<j} P(A_i \cap A_j)$, the DS bound

[7] can be written as

$$P\left(\bigcup_{i=1}^{N} A_i\right) \geq \frac{\kappa\theta_1^2}{(2-\kappa)\theta_1 + 2\theta_2} + \frac{(1-\kappa)\theta_1^2}{(1-\kappa)\theta_1 + 2\theta_2}, \tag{2.9}$$

where $\kappa = \frac{2\theta_2}{\theta_1} - \lfloor \frac{2\theta_2}{\theta_1} \rfloor$ and $\lfloor x \rfloor$ denotes the largest integer less than or equal to x.

We first show that the DS bound is the solution of a linear programming (LP) problem in the following lemma.

Lemma 2. *The DS bound is the solution of the following LP problem.*

$$\begin{aligned} \ell_{DS} :=& \min_{a(k)} \sum_k a(k), \\ s.t. \quad & \sum_k k a(k) = \sum_i P(A_i), \\ & \sum_k k^2 a(k) = \sum_{i,j} P(A_i \cap A_j), \\ & a(k) \geq 0, \quad k = 1, \ldots, N. \end{aligned} \tag{2.10}$$

Proof. For an LP problem, when a feasible solution exists and when the objective function (which is linear) is bounded, the optimal value of the objective function is always attained on the boundary of the optimal level-set and it is attained on at least one of the vertices of the polyhedron formed by the constraints (which is the set of feasible solutions) [3]. Then, the lemma can be readily verified using this fact that one of the optimal feasible points of the LP problem (2.10) is a vertex. To obtain a vertex, one need to make $N-2$ of the inequalities $a(k) \geq 0$ active, which means there are only two integers k_1 and k_2 that $1 \leq k_1 < k_2 \leq N$, satisfying

$$\begin{aligned} \min_{k_1,k_2} \quad & a(k_1) + a(k_2), \\ \text{s.t.} \quad & k_1 a(k_1) + k_2 a(k_2) = \sum_i P(A_i), \\ & k_1^2 a(k_1) + k_2^2 a(k_2) = \sum_{i,j} P(A_i \cap A_j), \\ & a(k_1) \geq 0, \quad a(k_2) \geq 0. \end{aligned} \tag{2.11}$$

It can be easily shown that the solution of the above problem is achieved at $k_1 = \lfloor \frac{\sum_{i,j} P(A_i \cap A_j)}{\sum_i P(A_i)} \rfloor$ and $k_2 = k_1 + 1$. Thus, the solution of (2.10) is the DS bound. $\square$

The existing proof of the optimality of the DS bound can be seen, e.g., in [12, p. 22]. We herein give an alternative and simpler proof by proving it is achievable.

Lemma 3. *The DS bound is optimal in the class of lower bounds in terms of* $\theta = \left(\sum_i P(A_i), \sum_{i<j} P(A_i \cap A_j)\right)$.

Proof. We have shown that the DS bound is the solution of (2.10) and can be written as $\ell_{\text{DS}} = a(k_1) + a(k_2)$, for some $a(k_1) \geq 0$, $a(k_2) \geq 0$, and $a(k) = 0, k \neq k_1, k \neq k_2$. Recalling the definition of $a(k)$, one can construct two outcomes ω_1 and ω_2 in a finite probability space such that

$$P(\omega_1) = a(k_1), \quad P(\omega_2) = a(k_2). \tag{2.12}$$

Then consider the following construction of collection of events $\{A_i^*\}$,

$$\begin{aligned} &A_i^* = \{\omega_1, \omega_2\}, \quad \text{if} \quad i \leq k_1, \\ &A_i^* = \{\omega_2\}, \quad \text{if} \quad k_1 < i \leq k_2, \\ &A_i^* = \emptyset, \quad \text{otherwise}. \end{aligned} \tag{2.13}$$

Then we always have $\ell_{\mathrm{DS}} = P\left(\bigcup_i A_i^*\right)$. Therefore, the DS bound is achievable, and hence optimal. □

Note that since the DS bound is optimal, it is always sharper than the lower bound in (2.7). Actually, this can be easily proved since the lower bound in (2.7) is a lower bound of the objective function of (2.10) by Cauchy-Schwarz inequality using the two constraints of (2.10).

2.2 Lower Bounds Using $\{P(A_i)\}$ and $\{\sum_{j\neq i} P(A_i \cap A_j)\}$

In this section, we review the lower bounds in terms of $\{P(A_i)\}$ and $\{\sum_{j\neq i} P(A_i \cap A_j)\}$, including the DC [8] and the KAT [19] bounds.

Similar to the definition of $a(k)$, define

$$a_i(k) := P\left(\{\omega \subseteq A_i : \deg(\omega) = k\}\right), \quad i = 1, \ldots, N, \quad k = 1, \ldots, N. \tag{2.14}$$

Then one can verify that $\sum_i a_i(k) = ka(k)$, i.e.,

$$a(k) = \frac{\sum_i a_i(k)}{k}. \tag{2.15}$$

For simplicity, we denote

$$\alpha_i := P(A_i), \quad \beta_i := \sum_{j\neq i} P(A_i \cap A_j), \quad \gamma_i := \alpha_i + \beta_i = \sum_j P(A_i \cap A_j). \tag{2.16}$$

We examine lower bounds that are functions of $\theta = (\alpha_1, \ldots, \alpha_N, \gamma_1, \ldots, \gamma_N)$.

One can verify that $P\left(\bigcup_{i=1}^N A_i\right)$, α_i and γ_i can all be written as linear functions of $\{a_i(k)\}$ as follows.

$$P\left(\bigcup_{i=1}^{N} A_i\right) = \sum_k a(k) = \sum_i \sum_k \frac{a_i(k)}{k}. \tag{2.17}$$

$$\alpha_i = P(A_i) = \sum_k a_i(k), \quad \gamma_i = \sum_j P(A_i \cap A_j) = \sum_k k a_i(k). \tag{2.18}$$

2.2.1 D. de Caen (DC) bound

Similar to the lower bound in (2.7), using the Cauchy-Schwarz inequality

$$\left(\sum_k \frac{a_i(k)}{k}\right)\left(\sum_k k a_i(k)\right) \geq \left(\sum_k a_i(k)\right)^2 \tag{2.19}$$

for $i = 1, \ldots, N$, and summing over i, one can get the DC bound as follows.

$$P\left(\bigcup_i A_i\right) = \sum_i \sum_k \frac{a_i(k)}{k} \geq \sum_i \left(\frac{\alpha_i^2}{\gamma_i}\right) = \sum_i \frac{P(A_i)^2}{\sum_j P(A_i \cap A_j)} =: \ell_{\mathrm{DC}}. \tag{2.20}$$

It is noted by D. de Caen [8] that the above lower bound can be (but is not always) sharper than the DS bound.

2.2.2 The Kuai-Alajaji-Takahara (KAT) bound

Now, we introduce the KAT bound

$$\ell_{\mathrm{KAT}} := \sum_{i=1}^{N} \left\{ \left[\frac{1}{\lfloor \frac{\gamma_i}{\alpha_i} \rfloor} - \frac{\frac{\gamma_i}{\alpha_i} - \lfloor \frac{\gamma_i}{\alpha_i} \rfloor}{(1+\lfloor \frac{\gamma_i}{\alpha_i} \rfloor)(\lfloor \frac{\gamma_i}{\alpha_i} \rfloor)} \right] \alpha_i \right\}, \tag{2.21}$$

as the solution of an LP problem, which is given in the following Lemma.

Lemma 4. *The KAT bound is the solution of the following LP problem*

$$\begin{aligned} \min_{\{a_i(k), i=1,\dots,N, k=1,\dots,N\}} \quad & \sum_{i=1}^{N}\sum_{k=1}^{N} \frac{a_i(k)}{k} \\ s.t. \quad & \sum_{k=1}^{N} a_i(k) = \alpha_i, \quad \sum_{k=1}^{N} k a_i(k) = \gamma_i, \quad i = 1,\dots,N, \\ & a_i(k) \geq 0, \quad i=1,\dots,N, \quad k=1,\dots,N, \end{aligned} \tag{2.22}$$

Proof. One can separate each i in the problem (2.22) and solve N sub-optimization problems separately for each i:

$$\begin{aligned} \min_{\{a_i(k), k=1,\dots,N\}} \quad & \sum_{k=1}^{N} \frac{a_i(k)}{k} \\ \text{s.t.} \quad & \sum_{k=1}^{N} a_i(k) = \alpha_i, \quad \sum_{k=1}^{N} k a_i(k) = \gamma_i, \\ & a_i(k) \geq 0, \quad k=1,\dots,N. \end{aligned} \tag{2.23}$$

Each of the sub-problems can be solved using the same method as solving the LP problem (2.10) for the DS bound. One can see [19] for details. An alternative proof is given in [18] by solving the dual LP problem of (2.23). □

It has been shown that the KAT bound is always sharper than both the DC bound and the DS bound [19]. Furthermore, Dembo has shown [9] that the KAT bound improves the DC bound by a factor of at most $\frac{9}{8}$. In the following lemma, we give alterative and simpler proofs of the above results.

Lemma 5. *Comparing with the DC and DS bounds, the KAT bound satisfies*

$$\max\{\ell_{DC}, \ell_{DS}\} \leq \ell_{KAT} \leq \frac{9}{8}\ell_{DC}. \tag{2.24}$$

Proof. First, substituting (2.15) in (2.10), one can get that the DS bound is the solution of the following LP problem of $\{a_i(k)\}$

$$\begin{aligned} \ell_{\text{DS}} = \min_{\{a_i(k), i=1,\ldots,N, k=1,\ldots,N\}} \quad & \sum_{i=1}^{N}\sum_{k=1}^{N} \frac{a_i(k)}{k} \\ \text{s.t.} \quad & \sum_{i=1}^{N}\sum_{k=1}^{N} a_i(k) = \sum_i \alpha_i, \quad \sum_{i=1}^{N}\sum_{k=1}^{N} k a_i(k) = \sum_i \gamma_i, \\ & \sum_i a_i(k) \geq 0, \quad k = 1, \ldots, N. \end{aligned} \tag{2.25}$$

Since every feasible point of (2.22) is also a feasible point of (2.25). The LP problem (2.25) is a relaxed problem of (2.22). Therefore, $\ell_{\text{KAT}} \geq \ell_{\text{DS}}$.

Next, it is easy to show that $\ell_{\text{KAT}} \geq \ell_{\text{DC}}$ since based on the constraints of (2.22), one can get the DC bound as a lower bound of the objective function of (2.22) using the Cauchy-Schwarz inequality. Therefore, ℓ_{KAT} is lower bounded by ℓ_{DC}.

Finally, we prove that $\ell_{\text{KAT}} \leq \frac{9}{8}\ell_{\text{DC}}$. Note that the DC bound (2.20) is given by $\ell_{\text{DC}} = \sum_i \frac{\alpha_i^2}{\gamma_i}$ and that the solution of (2.23) can be written as $\frac{a_i(k_1)}{k_1} + \frac{a_i(k_2)}{k_2}$ where $k_2 = k_1 + 1$. It then suffices to prove for any $i = 1, \ldots, N$ and integer $k = 1, \ldots, N-1$

$$\frac{a_i(k)}{k} + \frac{a_i(k+1)}{k+1} \leq \frac{9}{8}\frac{\alpha_i^2}{\gamma_i}, \tag{2.26}$$

where $a_i(k) + a_i(k+1) = \alpha_i$ and $ka_i(k) + (k+1)a_i(k+1) = \gamma_i$.

Denoting $x := a_i(k)$ and $y := a_i(k+1)$, one can get

$$\begin{aligned}\left(\frac{a_i(k)}{k} + \frac{a_i(k+1)}{k+1}\right) \Big/ \frac{\alpha_i^2}{\gamma_i} &= \frac{\left(\frac{x}{k} + \frac{y}{k+1}\right)[kx + (k+1)y]}{\alpha_i^2} \\ &= \frac{x^2 + \frac{k}{k+1}xy + \frac{k+1}{k}xy + y^2}{(x+y)^2} \\ &= 1 + \frac{1}{k(k+1)}\frac{xy}{(x+y)^2} \leq 1 + \frac{1}{4}\frac{1}{k(k+1)} \leq 1 + \frac{1}{8} = \frac{9}{8}.\end{aligned} \tag{2.27}$$

The first equality holds when $x = y = \frac{\alpha_i}{2}$ and the second equality holds when $k = 1$. Therefore, the inequality $\ell_{\mathrm{KAT}} \leq \frac{9}{8}\ell_{\mathrm{DC}}$ can be active. □

Remark 1. *Finally, we can derive an upper bound for $P\left(\bigcup_{i=1}^N A_i\right)$ using $\{P(A_i)\}$ and $\{\sum_j P(A_i \cap A_j)\}$ by maximizing the LP problem for the KAT bound.*

The following LP problem

$$\begin{aligned}\max_{\{a_i(k), i=1,\ldots,N, k=1,\ldots,N\}} \quad & \sum_{i=1}^N \sum_{k=1}^N \frac{a_i(k)}{k} \\ s.t. \quad & \sum_{k=1}^N a_i(k) = \alpha_i, \quad \sum_{k=1}^N k a_i(k) = \gamma_i, \quad i = 1, \ldots, N, \\ & a_i(k) \geq 0, \quad i = 1, \ldots, N, \quad k = 1, \ldots, N,\end{aligned} \tag{2.28}$$

gives the upper bound

$$\begin{aligned}P\left(\bigcup_i A_i\right) &\leq \sum_i \alpha_i - \frac{1}{N}\sum_i \beta_i \\ &= \sum_i P(A_i) - \frac{1}{N}\sum_{j\neq i} P(A_i \cap A_j) =: \hbar_{\textit{NEW-1}}.\end{aligned} \tag{2.29}$$

2.3 Lower Bounds Using $\{P(A_i)\}$ and $\{P(A_i \cap A_j)\}$

Lower and upper bounds on $P\left(\bigcup_{i=1}^{N} A_i\right)$ in terms of the individual event probabilities $P(A_i)$'s and the pairwise event probabilities $P(A_i \cap A_j)$'s can be seen as special cases of the Boolean probability bounding problem [4, 25], which can be solved numerically via a linear programming (LP) problem involving 2^N variables. Unfortunately, the number of variables for Boolean probability bounding problems increases exponentially with the number of events, N, which makes finding the solution impractical. Therefore, some suboptimal numerical bounds are proposed [4, 25, 23, 12] in order to reduce the complexity of the LP problem, for example, by using the dual basic feasible solutions.

On the other hand, analytical/algorithmic bounds are particularly important. One can apply an existing bound using $\{P(A_i), i \in \mathcal{I}\}$ and $\{\sum_{j\in\mathcal{I}} P(A_i \cap A_j)\}$ as a base bound, and then optimize the bound by choosing the optimal subset $\mathcal{I}$ of $\{1, \ldots, N\}$ algorithmically. Note that the bound by optimization via a subset exploits the full information of $\{P(A_i)\}$ and $\{P(A_i \cap A_j)\}$. Examples of bounds in this class includes the stepwise algorithmic implementation of the Kounias lower bound [20], the greedy algorithmic implementation of the Hunter upper bound [20]. Other analytical bounds, like the KAT bound, are also investigated in other works (e.g., see [5, 14, 15, 20, 1, 2, 22]).

The other class of bounds is established by $\{P(A_i)\}$ and $\{\sum_j c_j P(A_i \cap A_j)\}$, where $\{c_j\}$ can be arbitrarily chosen from a continuous set for $\boldsymbol{c} = (c_1, \ldots, c_N)^T$ or computed using $\{P(A_i)\}$ and $\{P(A_i \cap A_j)\}$. Then the resulting bound also exploits the full information of $\{P(A_i)\}$ and $\{P(A_i \cap A_j)\}$. Typical example of the bounds in this class is the Gallot-Kounias (GK) bound [13, 17] (see also [11, 22]).

2.3.1 Kounias Lower Bound and Algorithmic Implementation

The Kounias lower bound, which is a Bonferroni-type bound, can be written as

$$P\left(\bigcup_{i=1}^{N} A_i\right) \geq \max_{\mathcal{I}} \left\{ \sum_{i \in \mathcal{I}} P(A_i) - \sum_{i,j \in \mathcal{I}, i<j} P(A_i \cap A_j) \right\}, \tag{2.30}$$

where $\mathcal{I}$ is a subset of the set of indices $\{1, \ldots, N\}$. However, the computational complexity of the Kounias lower bound is exponential since there are exponential number of subsets of $\{1, \ldots, N\}$.

In order to reduce the computational complexity, an algorithmic algorithm is proposed in [20] using a stepwise algorithm to find a sub-optimal index set that maximizes the RHS of (2.30). We will refer to this algorithmic implementation of Kounias lower bound as the stepwise lower bound.

2.3.2 Gallot-Kounias (GK) Bound

Let $\boldsymbol{\alpha} = (P(A_1), P(A_2), \cdots, P(A_N))^T \in \mathbb{R}^{N \times 1}$ and

$$\boldsymbol{\Sigma} = \begin{pmatrix} P(A_1 \cap A_1) & P(A_1 \cap A_2) & \ldots & P(A_1 \cap A_N) \\ P(A_2 \cap A_1) & P(A_2 \cap A_2) & \ldots & P(A_2 \cap A_N) \\ \vdots & \vdots & \ldots & \vdots \\ P(A_N \cap A_1) & P(A_N \cap A_2) & \ldots & P(A_N \cap A_N) \end{pmatrix} \in \mathbb{R}^{N \times N}, \tag{2.31}$$

the GK bound [13, 17] is given as

$$P\left(\bigcup_{i-1}^{N} A_i\right) \geq \boldsymbol{c}^T \boldsymbol{\Sigma} \boldsymbol{c}, \tag{2.32}$$

where $\mathbf{\Sigma c} = \boldsymbol{\alpha}$. Kounias has shown in [17, Lemma 1.1] that the vector $\boldsymbol{\alpha}$ is in the range of $\mathbf{\Sigma}$, i.e., $\boldsymbol{\alpha}$ is orthogonal to the null space of $\mathbf{\Sigma}$. As a result, if $\mathbf{\Sigma}$ is singular, one can choose subsets of $\{A_1, \ldots, A_N\}$ to compute the corresponding GK bound, which results in the same bound if the rank of the corresponding $\mathbf{\Sigma}$ is the same.

Therefore, without loss of generality (WLOG), we assume herein $\mathbf{\Sigma}$ is non-singular, then the solution of $\mathbf{\Sigma c} = \boldsymbol{\alpha}$ is unique

$$\tilde{\boldsymbol{c}} = \mathbf{\Sigma}^{-1}\boldsymbol{\alpha}. \tag{2.33}$$

and the GK bound can be written as

$$P\left(\bigcup_{i-1}^{N} A_i\right) \geq \tilde{\boldsymbol{c}}^T \mathbf{\Sigma} \tilde{\boldsymbol{c}} = \boldsymbol{\alpha}^T \left(\mathbf{\Sigma}^T\right)^{-1} \boldsymbol{\alpha} = \boldsymbol{\alpha}^T \mathbf{\Sigma}^{-1} \boldsymbol{\alpha} =: \ell_{\mathrm{GK}}, \tag{2.34}$$

where $\left(\mathbf{\Sigma}^T\right)^{-1} = \mathbf{\Sigma}^{-1}$ as $\mathbf{\Sigma}$ is symmetric. Furthermore, the GK bound was recently revisited by [11]. The authors in [11] have shown that the GK bound can be reformulated as

$$\ell_{\mathrm{GK}} = \max_{\boldsymbol{c} \in \mathbb{R}^N} \frac{\left[\sum_i c_i P(A_i)\right]^2}{\sum_i \sum_k c_i c_k P(A_i \cap A_k)}. \tag{2.35}$$

2.4 Upper Bounds

There are only a few analytical/algorithmic upper bounds in the literature. In the following, we introduce the Hunter bound and its algorithmic implementation by a greedy algorithm.

2.4.1 Hunter Upper Bound and Algorithmic Implementation

The Hunter upper bound, which is a Bonferroni-type bound, can be written as

$$P\left(\bigcup_{i=1}^{N} A_i\right) \leq \sum_{i=1}^{N} P(A_i) - \max_{T_0 \in \mathcal{T}} \sum_{(i,j) \in T_0} P(A_i \cap A_j), \tag{2.36}$$

where $\mathcal{T}$ is the set of all trees spanning the N indices, i.e., the trees that include all indices as nodes.

However, the computational complexity of finding the optimal spanning tree is exponential via an exhaustive search. In order to reduce the complexity, one algorithmic algorithm is proposed in [20] using Kruskal's greedy algorithm for finding a sub-optimal spanning tree for a weighted graph. We will refer to this algorithmic implementation of the Hunter upper bound as the greedy upper bound, $\hbar_{\text{Greedy}}$.

Chapter 3

New Bounds using $\{P(A_i)\}$ and $\{\sum_j P(A_i \cap A_j)\}$

In this chapter, we consider lower bounds on $P\left(\bigcup_{i=1}^{N} A_i\right)$, in terms of the individual event probabilities $\{P(A_i), i = 1, \ldots, N\}$ and the *sums* of the pairwise event probabilities, *i.e.*, $\{\sum_{j:j\neq i} P(A_i \cap A_j), i = 1, \ldots, N\}$. We use the notations $\alpha_i = P(A_i)$, $\beta_i = \sum_{j\neq i} P(A_i \cap A_j)$ and $\gamma_i = \alpha_i + \beta_i = \sum_j P(A_i \cap A_j)$ as first defined in Chapter 2. Then the lower bounds considered in this chapter are established in terms of $\theta = (\alpha_1, \ldots, \alpha_N, \gamma_1, \ldots, \gamma_N)$. Let $\mathscr{L}$ denote the set of all lower bounds that are established in terms of only θ, then clearly, $\ell_{\mathrm{DC}} \in \mathscr{L}$ and $\ell_{\mathrm{KAT}} \in \mathscr{L}$.

Our contributions in this chapter are the following. First, the *optimal* lower bound in $\mathscr{L}$ is proposed numerically by solving an LP problem, which has only $N^2 - N + 1$ variables. This is proven by showing that the proposed optimal lower bound is achievable. The computational complexity of the optimal lower bound is low since the number of variables are not exponentially increasing in N. Next, a suboptimal analytical lower bound is established by solving a relaxed LP problem. The new analytical bound is proven to be at least as good as the KAT bound [19]. Finally, we analyze the performance of the new bounds by comparing them with the KAT bound and other existing bounds. In particular, numerical results show that the

GK bound [13, 17], which was recently revisited in [11, 22], is not necessarily sharper than the proposed lower bounds as well as the KAT bound (see also [10] for another example), even though it exploits full information of all $P(A_i \cap A_j)$'s and $P(A_i)$'s.

3.1 Optimal Numerical Lower/Upper Bounds

3.1.1 Non-optimality of the KAT bound

Since we have shown that $\ell_{\mathrm{KAT}} \geq \ell_{\mathrm{DC}}$, we first show that the KAT bound is not optimal in $\mathscr{L}$. Recall the definition of $a_i(k)$ in (2.14), one should note that for a given family of events, $\{A_i, i = 1, \ldots, N\}$, the $a_i(k)$'s can be obtained from their definition in (2.14). However, this does not mean that for each feasible point $\{a_i(k)\}$ of the LP problem (2.22), there exists a corresponding family of events $\{A_i, i = 1, \ldots, N\}$. In particular, for the solution of (2.22), it is possible that a family of events $\{A_i, i = 1, \ldots, N\}$ can never be constructed.

Example 1. *Considering a finite probability space (where atoms ω are reduced to elementary outcomes), shown as System V in Table 3.1, we have*

$$N = 3, \alpha_1 = 0.1, \alpha_2 = \alpha_3 = 0.2, \gamma_1 = 0.21, \gamma_2 = \gamma_3 = 0.265.$$

The KAT solution $\{a_i(k)\}$ for $\ell_{KAT} = 0.3833$ is obtained only at the following optimal feasible point of (2.22):

$$a_1(1) = 0, a_1(2) = 0.09, a_1(3) = 0.01, a_2(1) = a_3(1) = 0.135,$$
$$a_2(2) = a_3(2) = 0.065, a_2(3) = a_3(3) = 0.$$

However, $a_1(3) := P(\{\omega \in A_1 : \deg(\omega) = 3\}) = 0.01$ implies $P(A_1 \cap A_2 \cap A_3) \geq 0.01$, *since* $\deg(\omega) = 3$ *means that the corresponding outcome* ω *must be contained in all* $A_i, i = 1, \ldots, 3$. *However,* $a_2(3) := P(\{\omega \in A_2 : \deg(\omega) = 3\}) = 0$ *implies such* ω *is not in* A_2*, which is a contradiction. Therefore, there is no family of events* $\{A_1, A_2, A_3\}$ *that can be constructed for this system such that* $P(A_1 \cup A_2 \cup A_3) = 0.3833$. *In other words, for any sets* $\{A_1, A_2, A_3\}$ *with given value of* $\{\alpha_i\}$*'s and* $\{\gamma_i\}$*'s, we must have* $P(A_1 \cup A_2 \cup A_3) > 0.3833$.

Remark 2. *It can be shown that the LP problem (2.22) has a unique optimal feasible point (see Appendix A.1). Therefore, the KAT bound is achievable if and only if the optimal feasible point of the LP problem (2.22) has a corresponding family of events* $\{A_i, i = 1, \cdots, N\}$ *that satisfies the information represented by*

$$\theta = (\alpha_1, \cdots, \alpha_N, \gamma_1, \cdots, \gamma_N).$$

From Example 1, we see that ℓ_{KAT} *is not optimal in* $\mathscr{L}$.

3.1.2 Optimal Numerical Bound $\boldsymbol{\ell}_{\textbf{NEW-1}}$

In order to get a better lower bound than the KAT bound, we herein introduce more constraints on the $a_i(k)$'s in (2.22) so that the feasible set of $a_i(k)$'s becomes smaller, thus resulting in a sharper lower bound. By Lemma 1, if a family of events $\{A_i\}$ can always be constructed for any feasible point of the resulting LP problem, then the solution must be the optimal lower bound. We establish the numerically computable optimal lower bound in the following theorem.

Theorem 1 (**Optimal Numerical Lower Bound**)**.** *The* optimal *lower bound,* *denoted by $\ell_{NEW\text{-}1}$, is given by solving the following LP problem:*

$$\begin{aligned}
\min_{\{a_i(k), i=1,\ldots,N, k=1,\ldots,N\}} \quad & \sum_{i=1}^{N}\sum_{k=1}^{N}\frac{a_i(k)}{k} \\
s.t. \quad & \sum_{k=1}^{N} a_i(k) = \alpha_i, \quad \sum_{k=1}^{N} k a_i(k) = \gamma_i, \quad i = 1, \ldots, N, \\
& \sum_{i=1}^{N} a_i(k) \geq k a_j(k), \quad j = 1, \ldots, N, \quad k = 1, \ldots, N, \\
& a_i(k) \geq 0, \quad i = 1, \ldots, N, \quad k = 1, \ldots, N.
\end{aligned} \tag{3.1}$$

Proof. Denote the optimal lower bound in $\mathscr{L}$ by $\ell_{\text{NEW-1}}$ then $\ell_{\text{NEW-1}} \in \mathscr{L}$ satisfies $\ell_{\text{NEW-1}} \geq \ell$ for all $\ell \in \mathscr{L}$. Let the solution of (3.1) be $\ell'_{\text{NEW-1}}$, we will show that $\ell'_{\text{NEW-1}} = \ell_{\text{NEW-1}}$. First, it is easy to prove that for any $\{a_i(k)\}$ obtained by (2.14) from a family of events $\{A_i\}$, the additional constraints $\sum_{i=1}^{N} a_i(k) \geq k a_j(k)$ must hold for each $j = 1, \ldots, N$ and $k = 1, \ldots, N$. Therefore, $\ell'_{\text{NEW-1}}$ is a lower bound on $P\left(\bigcup_{i=1}^{N} A_i\right)$. Furthermore, since $\ell'_{\text{NEW-1}}$ is established in terms of only $\{\alpha_i\}$'s and $\{\gamma_i\}$'s, we have $\ell'_{\text{NEW-1}} \in \mathscr{L}$. Thus, we only need to prove $\ell'_{\text{NEW-1}} \geq \ell'$ for all $\ell' \in \mathscr{L}$. Also, note that for the solution of (3.1), since $\ell'_{\text{NEW-1}} \leq P\left(\bigcup_{i=1}^{N} A_i\right) \leq 1$, the objective value must be no larger than 1, i.e., $\sum_{i=1}^{N}\sum_{k=1}^{N}\frac{a_i(k)}{k} \leq 1$. Thus, the optimal feasible point of (3.1) must fall into the subset of the feasible set of (3.1), which is determined by the additional constraint $\sum_{i=1}^{N}\sum_{k=1}^{N}\frac{a_i(k)}{k} \leq 1$. In the following, we prove that $\ell'_{\text{NEW-1}}$ is achievable, i.e., a family of events $\{A_i\}$ can always be constructed from the solution of (3.1). Then, the optimality of $\ell'_{\text{NEW-1}}$ follows by Lemma 1.

Achievability: We prove that for any $\{a_i(k)\}$ that satisfies the constraints of (3.1) and the additional constraint $\sum_{i=1}^{N}\sum_{k=1}^{N}\frac{a_i(k)}{k} \leq 1$, it is always possible to construct a family of events $\{A_i\}$ such that $P(\{\omega \subseteq A_i : \deg(\omega) = k\}) = a_i(k)$ holds. The construction method is given as follows:

- The set Ω' is composed of $N \times N$ atoms, denoted as $\{\omega_i^{(k)}, i = 1, \ldots, N, k = 1, \ldots, N\}$. In the following, $\{\omega_i^{(k)}, i = 1, \ldots, N\}$ are constructed separately for each k.

- Consider N circles such that the k-th circle has a perimeter equals to $\sum_{i=1}^N \frac{a_i(k)}{k}$, $k = 1, \ldots, N$. Then for the k-th circle, $\sum_{i=1}^N a_i(k)$ equals k times its perimeter. Furthermore, since $a_j(k) \leq \sum_{i=1}^N \frac{a_i(k)}{k}$ for all j, $a_j(k)$ is no larger than the perimeter of the k-th circle.

- For $j = 1, \ldots, N$, we map the points on the arc of length $a_j(k)$ on the k-th circle from $2\pi \frac{k \sum_{l=1}^{j-1} a_l(k)}{\sum_{i=1}^N a_i(k)}$ to $2\pi \frac{k \sum_{l=1}^{j} a_l(k)}{\sum_{i=1}^N a_i(k)}$ to a set $B_j^{(k)}$. Then since for the k-th circle, $\sum_{i=1}^N a_i(k)$ equals to k times its perimeter and $a_j(k)$ is no larger than its perimeter, it follows that every point on the k-th circle is mapped to exactly k distinct sets in $\{B_1^{(k)}, \ldots, B_N^{(k)}\}$.

- On the k-th circle, the points at the following N angles,

$$2\pi \left(\frac{k \sum_{l=1}^{j} a_l(k)}{\sum_{i=1}^N a_i(k)} - \left\lfloor \frac{k \sum_{l=1}^{j} a_l(k)}{\sum_{i=1}^N a_i(k)} \right\rfloor \right), \quad j = 1, \ldots, N$$

divide the circle into (at most) N arcs, and the points on each arc are mapped to the same k sets in $\{B_1^{(k)}, \ldots, B_N^{(k)}\}$. Let $\{\theta_j^{(k)}, j = 1, \ldots, N\}$ be the ordered tuple of

$$\left\{ 2\pi \left(\frac{k \sum_{l=1}^{j} a_l(k)}{\sum_{i=1}^N a_i(k)} - \left\lfloor \frac{k \sum_{l=1}^{j} a_l(k)}{\sum_{i=1}^N a_i(k)} \right\rfloor \right), j = 1, \ldots, N \right\},$$

then $0 = \theta_1^{(k)} \leq \theta_2^{(k)} \leq \ldots \leq \theta_N^{(k)} \leq 2\pi$. Construct the atom $\omega_j^{(k)}$ such that its probability $p(\omega_j^{(k)})$ equals to the length of the j-th arc of the k-th circle, i.e.,

$$p(\omega_j^{(k)}) = \begin{cases} (\theta_{j+1}^{(k)} - \theta_j^{(k)}) \frac{\sum_{i=1}^N a_i(k)}{2\pi k} & \text{for } j < N, \\ (2\pi - \theta_N^{(k)}) \frac{\sum_{i=1}^N a_i(k)}{2\pi k} & \text{for } j = N. \end{cases} \tag{3.2}$$

- Since the points on the j-th arc are mapped to $\{B_{i_{1j}}^{(k)}, \ldots, B_{i_{kj}}^{(k)}\}$ where $\{i_{1j}, \ldots, i_{kj}\} \in \{1, \ldots, N\}$ that contains k different numbers, we let the atom $\omega_j^{(k)}$ is a subset of $A_{i_{1j}}, \ldots, A_{i_{kj}}$, respectively, i.e., $\omega_j^{(k)} \subseteq A_{i_{1j}} \cap \ldots \cap A_{i_{kj}}$.
- For each k, the total probability of all constructed atoms equals to the perimeter of the circle, $\sum_{i=1}^N \frac{a_i(k)}{k}$. Also, each atom $\omega_j^{(k)}$ is contains in exactly k events of $A_1, \ldots, A_N$. Finally, since there are in total $N \times N$ atoms $\{\omega_j^{(k)}, j = 1, \ldots, N, k = 1, \ldots, N\}$, each constructed A_i contains a finite number of atoms.

With the construction described above, it can be readily checked that the constructed $\{A_i\}$ satisfy $P(\{\omega \subseteq A_i : \deg(\omega) = k\}) = a_i(k)$ for all $i = 1, \ldots, N$. Since $\ell'_{\text{NEW-1}}$ is achieved at one feasible point of (3.1), by the proposed construction method a family of events, say $\{A_i^*\}$, can be constructed so that $P\left(\bigcup_{i=1}^N A_i^*\right) = \ell'_{\text{NEW-1}}$. Since the first two constraints of (3.1) are also satisfied, we have $P(A_i^*) = \alpha_i$ and $\sum_j P(A_i^* \cap A_j^*) = \gamma_i$ for all i.

Finally, the optimality of $\ell'_{\text{NEW-1}}$ directly follows by Lemma 1. $\square$

Example 2. *We give an example in a finite probability space to illustrate the construction provided in the achievability part of the above proof for $N = 4$ and $k = 2$. Assume that $a_1(k) = 0.1$, $a_2(k) = 0.2$, $a_3(k) = 0.3$, and $a_4(k) = 0.4$ for $k = 2$. Since $a_j(k) \le \sum_{i=1}^4 \frac{a_i(k)}{k} = 0.5$ hold for $j = 1, \ldots, 4$, the given $a_j(k)$'s satisfy the constraints in (3.1) for $k = 2$.*

- *In order to construct the outcomes, we assume there is a circle with perimeter equals to* $\sum_{i=1}^{4}\frac{a_i(k)}{k} = 0.5$. *Then we map the arc* $(0, 0.4\pi)$ *to* $B_1^{(2)}$, $(0.4\pi, 1.2\pi)$ *to* $B_2^{(2)}$, $(1.2\pi, 2.4\pi)$ *to* $B_3^{(2)}$, *and* $(2.4\pi, 4\pi)$ *to* $B_4^{(2)}$, *as shown in Fig. 3.1. Then every arc generates an angle less than* 2π *and every point on the circle is mapped to exactly two sets in* $\{B_1^{(2)}, B_2^{(2)}, B_3^{(2)}, B_4^{(2)}\}$. *That is: the arc* $(0, 0.4\pi)$ *is mapped to* $B_1^{(2)}$ *and* $B_3^{(2)}$*; the arc* $(0.4\pi, 1.2\pi)$ *is mapped to* $B_2^{(2)}$ *and* $B_4^{(2)}$*; the arc* $(1.2\pi, 2\pi)$ *is mapped to* $B_3^{(2)}$ *and* $B_4^{(2)}$.

- *Since the ordered tuple of the angles* $\{0.4\pi, 1.2\pi, 2\pi(1.2-1), 2\pi(2-2)\}$ *is* $\{0, 0.4\pi, 0.4\pi, 1.2\pi\}$, *the circle is divided by* $N = 4$ *arcs with lengths equal to* $\{0.1, 0, 0.2, 0.2\}$, *respectively.*

- *The outcomes* $\omega_1^{(2)}$, $\omega_2^{(2)}$, $\omega_3^{(2)}$ *and* $\omega_4^{(2)}$ *are constructed with probabilities equal to the length of the arcs, i.e.,* $p(\omega_1^{(2)}) = 0.1$, $p(\omega_2^{(2)}) = 0$, $p(\omega_3^{(2)}) = 0.2$, $p(\omega_3^{(2)}) = 0.2$. *Finally, we set the outcomes belonging to events* A_i*'s as follows:* $\omega_1^{(2)} \in A_1 \cap A_3$, $\omega_3^{(2)} \in A_2 \cap A_4$ *and* $\omega_4^{(2)} \in A_3 \cap A_4$. *After the construction for* $k = 2$ *only, the events of* $\{A_i\}$ *become:* $A_1 = \{\omega_1^{(2)}\}$, $A_2 = \{\omega_3^{(2)}\}$, $A_3 = \{\omega_1^{(2)}, \omega_4^{(2)}\}$, $A_4 = \{\omega_3^{(2)}, \omega_4^{(2)}\}$. *Thus,* $P(\{\omega \in A_i : \deg(\omega) = k\}) = a_i(k)$ *is satisfied for* $i = 1, \ldots, 4$ *and* $k = 2$.

Remark 3. *Though the number of variables in the optimal lower bound (3.1) is* N^2, *one can further reduce it to* $N^2 - N + 1$ *by observing that for* $k = N$ *the constraint* $\sum_{i=1}^{N} a_i(k) \geq k a_j(k)$ *is equivalent to* $a_1(N) = a_2(N) = \ldots = a_N(N)$. *Thus, the* N *variables* $a_i(N), i = 1, \ldots, N$ *can be replaced by only one. The number variables of the optimal lower bound (3.1) is then* $N^2 - N + 1$.

Remark 4 (Optimal Numerical Upper Bound). *Since we have proved any point* *in the subset of the feasible set of (3.1), determined by* $\sum_{i=1}^{N}\sum_{k=1}^{N}\frac{a_i(k)}{k} \leq 1$*, is achievable, maximizing the objective function in (3.1), instead of minimizing it, with the same constraints in (3.1) as well as the additional constraint* $\sum_{i=1}^{N}\sum_{k=1}^{N}\frac{a_i(k)}{k} \leq 1$*, we can obtain an* optimal upper bound *in the class of all upper bounds that are expressed in terms of only the* $P(A_i)$*'s and the* $\sum_j P(A_i \cap A_j)$*'s. For the maximization problem, the additional constraint* $\sum_{i=1}^{N}\sum_{k=1}^{N}\frac{a_i(k)}{k} \leq 1$ *is to ensure that the obtained upper bound is no larger than* 1*. We denote this upper bound by* $\hbar_{NEW\text{-}2}$*.*

Remark 5. *Note that in the proof of achievability of Theorem 1, only the last two constraints of (3.1) with the additional constraint* $\sum_{i=1}^{N}\sum_{k=1}^{N}\frac{a_i(k)}{k} \leq 1$ *are required. Therefore, in other cases where different information is available, optimal lower/upper bounds can be obtained using the same methodology of Theorem 1. For example, in the classes of lower and upper bounds which are established in terms of only* $P(A_i) = \alpha_i, i = 1, \ldots, N$*, the optimal lower and upper bounds in these classes can be obtained by the following problems:*

$$\begin{aligned}
\min_{\{a_i(k)\}} / \max_{\{a_i(k)\}} \quad & \sum_{i=1}^{N}\sum_{k=1}^{N}\frac{a_i(k)}{k} \\
s.t. \quad & \sum_{k=1}^{N} a_i(k) = \alpha_i, \quad i = 1, \ldots, N, \\
& \sum_{i=1}^{N} a_i(k) \geq k a_j(k), \quad j = 1, \ldots, N, \quad k = 1, \ldots, N, \\
& a_i(k) \geq 0, \quad i = 1, \ldots, N, \quad k = 1, \ldots, N, \\
& \sum_{i=1}^{N}\sum_{k=1}^{N}\frac{a_i(k)}{k} \leq 1.
\end{aligned} \tag{3.3}$$

Note that the additional constraint $\sum_{i=1}^{N}\sum_{k=1}^{N}\frac{a_i(k)}{k} \leq 1$ *can be relaxed for the minimization* *problem, since it is redundant. For the maximization problem, however, it can be active, in which case the obtained upper bound is equal to* 1*. Solving the LP problems of (3.3), we get that the optimal lower bound* $P\left(\bigcup_{i=1}^N A_i\right) \geq \max_i \alpha_i$*, and that the optimal upper bound* $P\left(\bigcup_{i=1}^N A_i\right) \leq \min\{\sum_i P(A_i), 1\}$*, i.e., the minimum of* 1 *and the union upper bound. The optimality of these bounds can be proved using similar arguments as the proof of Theorem 1.*

Remark 6 (**Optimality of the DS Bound**)**.** *The existing DS bound [7] is known to be optimal in the class of lower bounds with the information* $\theta = (\theta_1 = \sum_{i=1}^N P(A_i), \theta_2 = \sum_{i,j} P(A_i \cap A_j))$ *(e.g., see [12, p.22]). Using Lemma 1, we herein provide a different proof of the optimality of the DS bound [7]. Specifically, we only need to show that the DS bound is the solution of the following LP problem:*

$$
\begin{aligned}
\min_{\{a_i(k)\}} \quad & \sum_{i=1}^N \sum_{k=1}^N \frac{a_i(k)}{k} \\
s.t. \quad & \sum_{i=1}^N \sum_{k=1}^N a_i(k) = \theta_1, \quad \sum_{i=1}^N \sum_{k=1}^N k a_i(k) = \theta_2, \\
& \sum_{i=1}^N a_i(k) \geq k a_j(k), \quad j = 1, \ldots, N, \quad k = 1, \ldots, N, \\
& a_i(k) \geq 0, \quad i = 1, \ldots, N, \quad k = 1, \ldots, N.
\end{aligned}
\tag{3.4}
$$

The last two constraints in (3.4) together with $\sum_{i=1}^N \sum_{k=1}^N \frac{a_i(k)}{k} \leq 1$ *guarantee the achievability of the solution of (3.4). Thus, by Lemma 1, the solution of (3.4) is the optimal lower bound.*

Defining $a(k) = \sum_{i=1}^N a_i(k)$*, we show that the problem (3.4) has the same objective* *value as the following relaxed LP problem:*

$$\begin{aligned}
\min_{\{a(k)\}} \quad & \sum_{k=1}^{N} \frac{a(k)}{k} \\
s.t. \quad & \sum_{k=1}^{N} a(k) = \theta_1, \quad \sum_{k=1}^{N} k a(k) = \theta_2, \\
& a(k) \geq 0, \quad i = 1, \ldots, N, \quad k = 1, \ldots, N.
\end{aligned} \tag{3.5}$$

Since (3.5) is a relaxed problem of (3.4), it suffices to show that from the solution of (3.5), we can find a feasible point of (3.4) that gives the same objective value. This is done by setting $a_j(k) = a(k)/N$ *for all* $j = 1, \ldots, N$*, since all the relaxed constraints* $a(k) = \sum_{i=1}^{N} a_i(k) \geq k a_j(k)$ *and* $a_i(k) \geq 0$ *must be satisfied. Finally, note that the problem (3.5) is the same as the problem solved in [7]. Therefore, the solution of (3.5) is the DS bound.*

3.2 New Analytical Lower Bound

3.2.1 New Analytical Lower Bound $\ell_{\textbf{NEW-2}}$

In this section, we derive a new analytical lower bound, which is given in the following theorem.

Theorem 2 (**New Analytical Bound**)**.** *The lower bound is given by*

$$P\left(\bigcup_{i=1}^{N} A_i\right) \geq \ell_{NEW\text{-}2} := \delta + \sum_{i=1}^{N} \left\{ \left[\frac{1}{\chi(\frac{\gamma_i'}{\alpha_i'})} - \frac{\frac{\gamma_i'}{\alpha_i'} - \chi(\frac{\gamma_i'}{\alpha_i'})}{[1 + \chi(\frac{\gamma_i'}{\alpha_i'})][\chi(\frac{\gamma_i'}{\alpha_i'})]} \right] \alpha_i' \right\}, \tag{3.6}$$

where the function $\chi(\cdot)$ *is defined by*

$$\chi(x) = \begin{cases} n-1 & \text{if } x = n \text{ where } n \geq 2 \text{ is a integer} \\ \lfloor x \rfloor & \text{otherwise} \end{cases} \tag{3.7}$$

and

$$\delta := \left\{ \max_i \left[\gamma_i - (N-1)\alpha_i \right] \right\}^+ \geq 0, \quad \alpha'_i := \alpha_i - \delta, \quad \gamma'_i := \gamma_i - N\delta. \tag{3.8}$$

Proof. The new lower bound is the solution of the following relaxed LP:

$$\begin{aligned} \min_{\{a_i(k), i=1,\ldots,N, k=1,\ldots,N\}} \quad & \sum_{i=1}^{N} \sum_{k=1}^{N} \frac{a_i(k)}{k} \\ \text{s.t.} \quad & \sum_{k=1}^{N} a_i(k) = \alpha_i, \quad \sum_{k=1}^{N} k a_i(k) = \gamma_i, \quad i = 1, \ldots, N, \\ & \sum_{i=1}^{N} a_i(N) \geq N a_j(N), \quad j = 1, \ldots, N \\ & a_i(k) \geq 0, \quad i = 1, \ldots, N, \quad k = 1, \ldots, N. \end{aligned} \tag{3.9}$$

Note that the above problem is a relaxed problem of (3.1) because the constraints $\sum_{i=1}^{N} a_i(k) \geq k a_j(k), j = 1, \ldots, N$ for all $k \neq N$ in (3.1) are relaxed. Comparing with the LP problem of (2.22) that corresponds to the KAT bound, the additional constraints are only $\sum_{i=1}^{N} a_i(N) \geq N a_j(N), j = 1, \ldots, N$, which can be easily proved to be equivalent to requiring that $a_1(N) = a_2(N) = \ldots = a_N(N)$. We first introduce a new non-negative variable $x := a_1(N) = \ldots = a_N(N)$, and solve the problem (3.9) by assuming that x is known. Then the objective function in (3.9) becomes a function of x. Finally, we minimize the objective function to yield a solution of (3.9).

Replacing $a_i(N), i = 1, \ldots, N$ in (3.9) by x and assuming that x is given implies that (3.9) can be solved separately for each $i, i = 1, \ldots, N$, by solving the following N problems:

$$\begin{aligned} f_i(x) := \min_{a_i(k), k=1,\ldots,N-1} \quad & \sum_{k=1}^{N-1} \frac{a_i(k)}{k} + \frac{x}{N} \\ \text{s.t.} \quad & \sum_{k=1}^{N-1} a_i(k) = \alpha_i - x \\ & \sum_{k=1}^{N-1} k a_i(k) = \gamma_i - Nx \\ & a_i(k) \geq 0, k = 1, \ldots, N-1. \end{aligned} \tag{3.10}$$

Note that when x is given the above problem is equivalent to (2.22), the solution of which was derived in different ways in [19, 18]. However, since x is a variable which is assumed to be fixed at the current stage, the solution of problem (3.10) may not exist for any given x. Thus, one needs to investigate the condition for the existence of a solution for (3.10) when solving it. To this end, we solve the problem (3.10) by taking into account the feasible set for x.

Since the LP problem (3.10) has $N-1$ variables and the LP optimum must be achieved at one of vertices of the polyhedron formed by the constraints [3], the $N-3$ of the $N-1$ constraints $a_i(k) \geq 0, k = 1, \ldots, N-1$ must be active. Assume that the other two constraints $a_i(k) \geq 0$ that are not active are given for $k = k_1$ and $k = k_2$ and $1 \leq k_1 < k_2 \leq N-1$, then we obtain

$$a_i(k_1) + a_i(k_2) = \alpha_i - x, \quad k_1 a_i(k_1) + k_2 a_i(k_2) = \gamma_i - Nx, \tag{3.11}$$

which yields

$$a_i(k_1) = \frac{k_2(\alpha_i - x) - (\gamma_i - Nx)}{k_2 - k_1} \geq 0, \quad a_i(k_2) = \frac{(\gamma_i - Nx) - k_1(\alpha_i - x)}{k_2 - k_1} \geq 0. \tag{3.12}$$

Using the condition $1 \leq k_1 < k_2 \leq N - 1$, the solution exists when

$$[\gamma_i - (N-1)\alpha_i]^+ \leq x \leq \frac{\beta_i}{N-1}, \tag{3.13}$$

and k_2 and k_1 satisfy $k_1 \leq \frac{\gamma_i - Nx}{\alpha_i - x} \leq k_2$.

Since it is easy to prove that $\frac{a_i(k_1)}{k_1} + \frac{a_i(k_2)}{k_2}$ is non-decreasing with k_2 and non-increasing with k_1 (see Appendix A.2), the optimal k_2 and k_1 when $\frac{\gamma_i - Nx}{\alpha_i - x}$ is not an integer are

$$k_1 = \left\lfloor \frac{\gamma_i - Nx}{\alpha_i - x} \right\rfloor, \quad k_2 = k_1 + 1. \tag{3.14}$$

When $\frac{\gamma_i - Nx}{\alpha_i - x}$ is an integer, one can choose either $k_1 = \frac{\gamma_i - Nx}{\alpha_i - x}, k_2 = k_1 + 1$ or $k_1 = \frac{\gamma_i - Nx}{\alpha_i - x} - 1, k_2 = k_1 + 1$, since for both cases the values of $\frac{a_i(k_1)}{k_1} + \frac{a_i(k_2)}{k_2}$ are indeed identical. Note that the condition for the existence of the solution to (3.9) implies that $1 \leq k_1 < k_2 \leq N - 1$, thus, the optimal k_1 and k_2 that give the largest feasible set of x are

$$k_1 = \chi(\frac{\gamma_i - Nx}{\alpha_i - x}), \quad k_2 = k_1 + 1. \tag{3.15}$$

Then the solution of (3.10) which is a function of x can be written as

$$\begin{aligned} f_i(x) =& \frac{2\chi(\frac{\gamma_i - Nx}{\alpha_i - x}) + 1}{\chi(\frac{\gamma_i - Nx}{\alpha_i - x}) \left[\chi(\frac{\gamma_i - Nx}{\alpha_i - x}) + 1\right]}(\alpha_i - x) \\ &- \frac{1}{\chi(\frac{\gamma_i - Nx}{\alpha_i - x}) \left[\chi(\frac{\gamma_i - Nx}{\alpha_i - x}) + 1\right]}(\gamma_i - Nx) + \frac{x}{N}, \end{aligned} \tag{3.16}$$

where $[\gamma_i - (N-1)\alpha_i]^+ \le x \le \frac{\beta_i}{N-1}$.

Next, we prove that $f_i(x)$ is a non-decreasing function of x. First, we prove that the function $f_i(x)$ is continuous. Note that $\frac{\gamma_i - Nx}{\alpha_i - x}$ is strictly decreasing with x if $\frac{\gamma_i}{\alpha_i} < N$ (see Appendix A.3). When $\frac{\gamma_i - Nx}{\alpha_i - x}$ is an integer, say $\frac{\gamma_i - Nx}{\alpha_i - x} = n \le N-1$, choose $h > 0$ satisfies $n - 1 < \frac{\gamma_i - N(x+h)}{\alpha_i - (x+h)} < n$ and $n < \frac{\gamma_i - N(x-h)}{\alpha_i - (x-h)} < n+1$. Then we have $\chi(\frac{\gamma_i - Nx}{\alpha_i - x}) = n-1$, $\chi(\frac{\gamma_i - N(x+h)}{\alpha_i - (x+h)}) = n-1$ and $\chi(\frac{\gamma_i - N(x-h)}{\alpha_i - (x-h)}) = n$. Then $f_i(x+h) - f_i(x) = \left(\frac{1}{n-1} - \frac{1}{N}\right)\frac{N-n}{n} h > 0$ and $f_i(x) - f_i(x-h) = \left(\frac{1}{n+1} - \frac{1}{N}\right)\frac{N-n}{n} h \ge 0$ (see Appendix A.4). Both $f_i(x+h) - f_i(x)$ and $f_i(x) - f_i(x-h)$ tend to zero when $h \to 0$. Thus, the function $f_i(x)$ is continuous when $\frac{\gamma_i - Nx}{\alpha_i - x}$ is an integer.

When $\frac{\gamma_i - Nx}{\alpha_i - x}$ is not an integer, $\chi(\frac{\gamma_i - Nx}{\alpha_i - x}) \le N-1$ and the function $f_i(x)$ is continuous and differentiable. The derivative of $f_i(x)$ satisfies

$$\begin{aligned} f_i'(x) &= \frac{1}{N} - \frac{1}{\chi(\frac{\gamma_i - Nx}{\alpha_i - x})} - \frac{1}{\chi(\frac{\gamma_i - Nx}{\alpha_i - x}) + 1} + \frac{N}{\chi(\frac{\gamma_i - Nx}{\alpha_i - x})\left[\chi(\frac{\gamma_i - Nx}{\alpha_i - x}) + 1\right]} \\ &= \frac{\left[N - \chi(\frac{\gamma_i - Nx}{\alpha_i - x})\right]\left[N - \chi(\frac{\gamma_i - Nx}{\alpha_i - x}) - 1\right]}{N\chi(\frac{\gamma_i - Nx}{\alpha_i - x})\left[\chi(\frac{\gamma_i - Nx}{\alpha_i - x}) + 1\right]} \ge 0, \end{aligned} \tag{3.17}$$

which means that $f_i(x)$ is a non-decreasing function of x. Then we can finally solve the problem (3.9) to get the new lower bound

$$\ell_{\text{NEW-2}} = \min_x \left[\sum_{i=1}^{N} f_i(x)\right] \quad \text{s.t.} \quad \left\{\max_i[\gamma_i - (N-1)\alpha_i]\right\}^+ \le x \le \min_i \frac{\beta_i}{N-1}, \tag{3.18}$$

where $\ell_{\text{NEW-2}}$ denotes the new analytical bound. Since $\sum_{i=1}^{N} f_i(x)$ is non-decreasing in x, defining $\delta = \{\max_i[\gamma_i - (N-1)\alpha_i]\}^+$, the objective value is thus obtained at $x = \delta$ so that $\ell_{\text{NEW-2}} = \sum_{i=1}^{N} f_i(\delta)$. □

Remark 7. *We can also prove that the LP problem (3.9) has a unique optimal feasible point. Note that for a given* x*, the problem (3.9) reduces to the LP problem (2.22) for the KAT bound, which has a unique optimal feasible point by Remark 2. Therefore, it suffices to show that there does not exist* $\delta < \delta^* \leq \min_i \frac{\beta_i}{N-1}$ *such that* $\sum_{i=1}^N f_i(\delta^*) = \sum_{i=1}^N f_i(\delta)$*. Since* $f_i(x)$ *is non-negative and non-decreasing with* x*, it suffices to show that there does not exist* $\delta < \delta^* \leq \min_i \frac{\beta_i}{N-1}$ *such that* $f_i'(\delta^*) = 0$ *for all* i*. From (3.17), we know that* $f_i'(\delta^*) = 0$ *if and only if* $\chi(\frac{\gamma_i - N\delta^*}{\alpha_i - \delta^*}) = N-1$*, which is equivalent to* $N-1 < \frac{\gamma_i - N\delta^*}{\alpha_i - \delta^*} \leq N$*. In the following, we prove the nonexistence of* δ^* *by considering three cases: (i) If* $\delta = 0$ *for some* i*, which means* $\frac{\gamma_i}{\alpha_i} \leq N-1$*, then* $\frac{\gamma_i - N\delta^*}{\alpha_i - \delta^*} \leq \frac{\gamma_i}{\alpha_i} \leq N-1$*, which is a contradiction with* $N-1 < \frac{\gamma_i - N\delta^*}{\alpha_i - \delta^*} \leq N$*; (ii) If* $\delta > 0$ *and* $\frac{\gamma_i}{\alpha_i} = N$ *for some* i*, then* $x = \alpha_i = \delta$ *is the only point in the feasible set of (3.18), thus* $\delta^* > \delta$ *does not exist; (iii) If* $\delta > 0$ *and* $\frac{\gamma_i}{\alpha_i} < N$ *for all* i*, then* $\delta = \max_i[\gamma_i - (N-1)\alpha_i] = \gamma_k - (N-1)\alpha_k$ *for some* $k \in \{1, \cdots, N\}$*. Since* $\frac{\gamma_k - Nx}{\alpha_k - x}$ *strictly decreases with* x*, we have* $\frac{\gamma_k - N\delta^*}{\alpha_k - \delta^*} < \frac{\gamma_k - N\delta}{\alpha_k - \delta} = \frac{\gamma_k - N[\gamma_k - (N-1)\alpha_k]}{\alpha_k - [\gamma_k - (N-1)\alpha_k]} = \frac{(N-1)(N\alpha_k - \gamma_k)}{N\alpha_k - \gamma_k} = N-1$*, which contradicts with* $\frac{\gamma_k - N\delta^*}{\alpha_k - \delta^*} > N-1$*. Thus, the optimal feasible point of (3.18) is unique so that the optimal feasible point of (3.9) is unique. Therefore, the new analytical bound is achievable if and only if the optimal feasible point of the LP problem (3.9) has a corresponding family of events* $\{A_i, i = 1, \cdots, N\}$ *that satisfies the information represented by* $\theta = (\alpha_1, \cdots, \alpha_N, \gamma_1, \cdots, \gamma_N)$*.*

Remark 8. *It can be easily seen by comparing the LP problems of (2.22) and (3.9) that the new analytical bound* $\ell_{NEW\text{-}2}$ *is at least as good as the KAT bound* ℓ_{KAT}*. This is because the feasible set of (2.22) contains the feasible set of (3.9), and both problems (2.22) and (3.9) share the same objective function. Furthermore, setting* $\delta = 0$ *directly yields* $\ell_{NEW\text{-}2} = \ell_{KAT}$*. A more extensive comparison of* $\ell_{NEW\text{-}2}$ *with*

ℓ_{KAT} is undertaken in Section 3.2.2.

Remark 9 (**New Analytical Upper Bound**). *Finally, we can also get an upper bound of $P\left(\bigcup_{i=1}^N A_i\right)$ by maximizing instead of minimizing the objective function in the LP problem (3.9).*

The following LP problem

$$\begin{aligned} \max_{\{a_i(k), i=1,\dots,N, k=1,\dots,N\}} \quad & \sum_{i=1}^N \sum_{k=1}^N \frac{a_i(k)}{k} \\ s.t. \quad & \sum_{k=1}^N a_i(k) = \alpha_i, \quad \sum_{k=1}^N k a_i(k) = \gamma_i, \quad i = 1, \dots, N, \\ & a_1(N) = a_2(N) = \cdots = a_N(N), \\ & a_i(k) \geq 0, \quad i = 1, \dots, N, \quad k = 1, \dots, N, \end{aligned} \tag{3.19}$$

gives the upper bound

$$\begin{aligned} P\left(\bigcup_i A_i\right) &\leq \sum_i \alpha_i - \frac{1}{N-1} \sum_i \beta_i + \frac{1}{N-1} \min_i \beta_i \\ &= \sum_i P(A_i) - \frac{1}{N-1} \sum_{j \neq i} P(A_i \cap A_j) + \frac{1}{N-1} \min_i \{\sum_{j \neq i} P(A_i \cap A_j)\}, \\ &=: \hbar_{NEW\text{-}3}. \end{aligned} \tag{3.20}$$

It can be easily shown that the upper bound (3.20) is sharper than (2.29), i.e., $\hbar_{NEW\text{-}3} \leq \hbar_{NEW\text{-}1}$.

3.2.2 Comparison of $\ell_{\text{NEW-2}}$ with ℓ_{KAT}

In this subsection, we give a lower bound on $\ell_{\text{NEW-2}} - \ell_{\text{KAT}}$ which is given in the following lemma.

Lemma 6. *A lower bound on $\ell_{\textit{NEW-2}} - \ell_{\textit{KAT}}$ is given as follows:*

$$\ell_{\textit{NEW-2}} - \ell_{\textit{KAT}} \geq \left\{ \sum_{i=1}^{N} \frac{\left[N - \chi(\frac{\gamma_i}{\alpha_i})\right]\left[N - \chi(\frac{\gamma_i}{\alpha_i}) - 1\right]}{\chi(\frac{\gamma_i}{\alpha_i})\left[\chi(\frac{\gamma_i}{\alpha_i}) + 1\right]} \right\} \frac{\delta}{N}, \tag{3.21}$$

where the strict inequality holds if and only if there exists $0 < \delta' < \delta$ that $\frac{\gamma_i - N\delta'}{\alpha_i - \delta'}$ is an integer for some $i \in \{1, \dots, N\}$.

Proof. We first prove that $f_i(x)$ is convex in x. Note that $f_i(x)$ is a continuous and piecewise differentiable function. However, it is not differentiable when $\frac{\gamma_i - Nx}{\alpha_i - x}$ is an integer. In each interval of x where $\frac{\gamma_i - Nx}{\alpha_i - x}$ is between two successive integers, the derivative of $f_i(x)$ is given by (3.17) which is positive and only a function of $\chi(\frac{\gamma_i - Nx}{\alpha_i - x})$. Since $\chi(\frac{\gamma_i - Nx}{\alpha_i - x})$ is an integer that does not change in each interval where $\frac{\gamma_i - Nx}{\alpha_i - x}$ is between two successive integers, we only need to show that the derivative of $f_i(x)$ given by (3.17) is a non-decreasing function of x. By denoting $n(x) := \chi(\frac{\gamma_i - Nx}{\alpha_i - x})$, we can write $f_i'(x) = g_i(n)$ where

$$g_i(n) := \frac{(N-n)(N-n-1)}{N(n+1)n}. \tag{3.22}$$

Noting that $\gamma_i \leq N\alpha_i$, one can verify that $\frac{\gamma_i - Nx}{\alpha_i - x}$ decreases with x and by the definition of $\chi(\cdot)$, $n \leq N - 1$ and $n = \chi(\frac{\gamma_i - Nx}{\alpha_i - x})$ is a non-increasing function of x. Thus, we have

$g_i(n) > 0$ and $g_i(n)$ is a decreasing function of n for $1 < n \leq N-1$, since

$$g_i(n) - g_i(n-1) = \frac{(N-n)(N-n-1)}{N(n+1)n} - \frac{(N-n+1)(N-n)}{Nn(n-1)} < 0, \tag{3.23}$$

which implies $f_i'(x)$ is a non-decreasing function of x. Therefore $f_i(x)$ is a convex function of x. Finally, by the property of a convex function, we have

$$f_i(x) - f_i(0) \geq f_i'(0)(x-0). \tag{3.24}$$

Since $\ell_{\text{NEW-2}} - \ell_{\text{KAT}} = \sum_i [f_i(\delta) - f_i(0)]$, by substituting $x = \delta$ into (3.24) and summing over i, the inequality of (3.21) is obtained.

Note that if for all $i = 1, \ldots, N$ there does not exist $0 < \delta' < \delta$ such that $\frac{\gamma_i - N\delta'}{\alpha_i - \delta'}$ is an integer, the derivative $f_i'(x) = f_i'(0)$ for all $0 < x < \delta$ and $i = 1, \ldots, N$. Then equality in (3.24) holds for all i, and equality holds in (3.21). If there exists $0 < \delta' < \delta$ such that $\frac{\gamma_i - N\delta'}{\alpha_i - \delta'}$ is an integer for some i, then according to (3.23) and the definition of $\chi(\cdot)$, we have $f_i'(\delta') > f_i'(0)$. Then, it can be shown that for those i the strict inequality in (3.24) holds when $x = \delta$. This is because

$$\begin{aligned} f_i(\delta) - f_i(0) &= [f_i(\delta) - f_i(\delta')] + [f_i(\delta') - f_i(0)] \\ &\geq f_i'(\delta')(\delta - \delta') + f_i'(0)(\delta' - 0) \\ &> f_i'(0)(\delta - \delta') + f_i'(0)(\delta' - 0) \\ &= f_i'(0)(\delta - 0). \end{aligned} \tag{3.25}$$

Therefore, the strictly inequality in (3.21) holds. $\square$

Remark 10. *Lemma 6 readily yields another analytical lower bound, which is sharper* *than the KAT bound but looser than the new analytical bound:*

$$P\left(\bigcup_{i=1}^{N} A_i\right) \geq \ell_{KAT} + \left\{\sum_{i=1}^{N} \frac{\left[N - \chi(\frac{\gamma_i}{\alpha_i})\right]\left[N - \chi(\frac{\gamma_i}{\alpha_i}) - 1\right]}{\chi(\frac{\gamma_i}{\alpha_i})\left[\chi(\frac{\gamma_i}{\alpha_i}) + 1\right]}\right\} \frac{\delta}{N}. \tag{3.26}$$

We herein show that the above analytical lower bound can be derived directly based on the arguments in [19].

Recall [19, the last equation above (8)] that

$$V_i := \sum_{k=1}^{N} \frac{a_i(k)}{k} = \frac{2}{r}\alpha_i - \frac{1}{r(r-1)}\beta_i + \sum_{k=1}^{N} \frac{(r-k)(r-k-1)}{r(r-1)} \frac{a_i(k)}{k}, \tag{3.27}$$

where the last term

$$\sum_{k=1}^{N} \frac{(r-k)(r-k-1)}{r(r-1)} \frac{a_i(k)}{k} \geq 0. \tag{3.28}$$

Thus, the authors in [19] use

$$V_i \geq \frac{2}{r}\alpha_i - \frac{1}{r(r-1)}\beta_i \tag{3.29}$$

to determine the KAT bound as follows

$$P\left(\bigcup_{i} A_i\right) = \sum_i V_i \geq \max_{r_i \in \mathbb{N}} \sum_i \left[\frac{2}{r_i}\alpha_i - \frac{1}{r_i(r_i-1)}\beta_i\right] = \ell_{KAT}, \tag{3.30}$$

where the maximization is over the integer r_i's and the optimum is achieved at $r_i =$

$1 + \chi(\frac{\gamma_i}{\alpha_i})$. *Note that we can rewrite (3.27) as*

$$
\begin{aligned}
V_i = &\left[\frac{2}{r}\alpha_i - \frac{1}{r(r-1)}\beta_i + \frac{(r-N)(r-N-1)}{r(r-1)}\frac{a_i(N)}{N}\right] \\
&+ \sum_{k=1}^{N-1} \frac{(r-k)(r-k-1)}{r(r-1)}\frac{a_i(k)}{k},
\end{aligned}
\tag{3.31}
$$

where the last term is non-negative. Note that from (3.18), one can see that δ is the smallest possible value of $x = a_i(N)$ that guarantees the existence of the solution of (3.9), i.e. $\frac{\delta}{N} \leq \frac{a_i(N)}{N}$. Therefore, the lower bound of (3.26) can be obtained as follows:

$$
\begin{aligned}
P\left(\bigcup_i A_i\right) &= \sum_i V_i \\
&\geq \max_{r_i \in \mathbb{N}} \sum_i \left[\frac{2}{r_i}\alpha_i - \frac{1}{r_i(r_i-1)}\beta_i + \frac{(r_i-N)(r_i-N-1)}{r_i(r_i-1)}\frac{a_i(N)}{N}\right] \\
&\geq \sum_i \left\{\frac{2\alpha_i}{1+\chi(\frac{\gamma_i}{\alpha_i})} - \frac{\beta_i}{[1+\chi(\frac{\gamma_i}{\alpha_i})]\chi(\frac{\gamma_i}{\alpha_i})} + \frac{[1+\chi(\frac{\gamma_i}{\alpha_i})-N](\chi(\frac{\gamma_i}{\alpha_i})-N)}{[1+\chi(\frac{\gamma_i}{\alpha_i})]\chi(\frac{\gamma_i}{\alpha_i})}\frac{\delta}{N}\right\} \\
&= \ell_{KAT} + \left\{\sum_{i=1}^{N} \frac{\left[N-\chi(\frac{\gamma_i}{\alpha_i})\right]\left[N-\chi(\frac{\gamma_i}{\alpha_i})-1\right]}{\chi(\frac{\gamma_i}{\alpha_i})\left[\chi(\frac{\gamma_i}{\alpha_i})+1\right]}\right\}\frac{\delta}{N}.
\end{aligned}
\tag{3.32}
$$

3.3 Numerical Examples

In this section, we evaluate the new lower bounds using eight numerical examples. The first four examples are the same as in [19]. The last four examples, Systems V to VIII, are new and are shown in Table 3.1-3.4, respectively. As a reference, the existing DS bound [7], DC bound [8], the KAT bound [19] are included for comparison. Furthermore, the GK bound [13, 17], which exploits full information of all $P(A_i \cap A_j)$'s and $P(A_i)$'s, is also compared with the new bounds. The results are shown in Table 3.5. The gap of $\ell_{\text{NEW-2}} - \ell_{\text{KAT}}$ and the derived lower bound (3.21) are shown in Table 3.6.

One can see that the KAT bound is at least as good as the DS and DC bounds as already shown in [19]. The new bounds are at least as good as the KAT bound in all the examples, as expected. More specifically, the new numerical bound (3.1) is sharper than the KAT bound in all examples, and the new analytical bound (3.6) is sharper than the KAT bound for Systems V to VIII and identical to the KAT bound for Systems I to VI. Concerning the gap of new analytical bound and the KAT bound, the equality of (3.21) holds for Systems V, VII and VIII.

Moreover, from the numerical examples, we note that the GK bound [13, 17], which requires more information (all the information of individual $P(A_i \cap A_j)$ as well as $P(A_i)$'s), is not guaranteed to be sharper than the KAT bound[1] and the new bounds. For example, the GK bound is worse than the KAT bound as well as the new bounds in Systems V and VIII. It is better than the KAT bound but worse than the new bounds in System VI, better than the KAT bound and the new analytical bound but worse than the new numerical bound in System VII.

Finally, we note that all lower bounds considered in this work can be sharpered algorithmically by optimizing over subsets (e.g., see [14, 2, 15]).

[1]Another example in which the GK bound is looser than the KAT bound is given in [10].

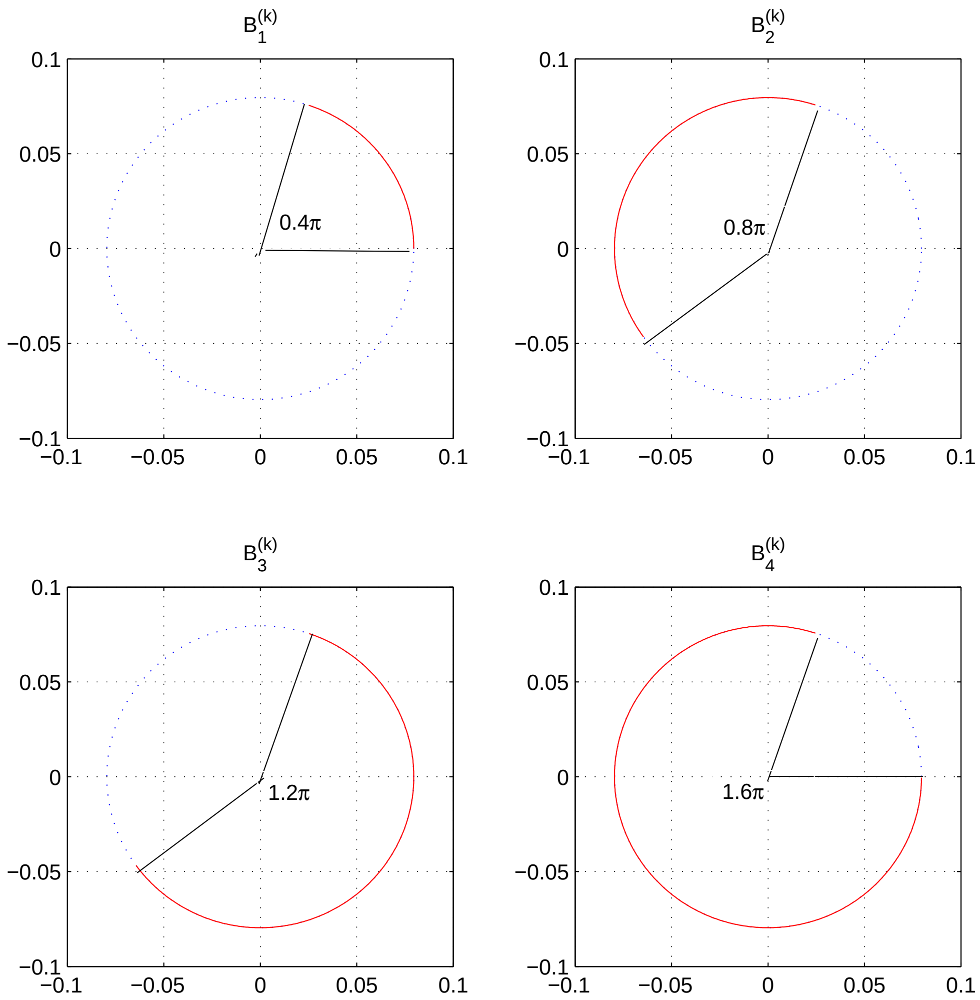

Figure 3.1: Example illustrating the construction of the proof of Theorem 1 for $N = 4$ and $k = 2$.

Table 3.1: System V.

Outcomes ω_i	$p(\omega_i)$	A_1	A_2	A_3
ω_0	0.145			$\times$
ω_1	0.045	$\times$		$\times$
ω_2	0.01	$\times$	$\times$	$\times$
ω_3	0.045	$\times$	$\times$	
ω_4	0.145		$\times$	

Table 3.2: System VI.

Outcomes ω_i	$p(\omega_i)$	A_1	A_2	A_3	A_4
ω_0	0.0962	$\times$			$\times$
ω_1	0.0446				$\times$
ω_2	0.0581		$\times$		$\times$
ω_3	0.0225	$\times$	$\times$	$\times$	$\times$
ω_4	0.0385	$\times$			
ω_5	0.0071	$\times$		$\times$	$\times$
ω_6	0.0582		$\times$		

Table 3.3: System VII.

Outcomes ω_i	$p(\omega_i)$	A_1	A_2	A_3	A_4
ω_0	0.1832	$\times$			
ω_1	0.1219			$\times$	
ω_2	0.0337	$\times$	$\times$	$\times$	$\times$
ω_3	0.0256		$\times$	$\times$	
ω_4	0.0682				$\times$
ω_5	0.0389		$\times$	$\times$	$\times$
ω_6	0.0631			$\times$	$\times$

Table 3.4: System VIII.

Outcomes ω_i	$p(\omega_i)$	A_1	A_2	A_3	A_4
ω_0	0.0330				$\times$
ω_1	0.0705	$\times$	$\times$	$\times$	
ω_2	0.0876	$\times$		$\times$	$\times$
ω_3	0.0608	$\times$	$\times$		$\times$
ω_4	0.0865	$\times$	$\times$	$\times$	$\times$
ω_5	0.0621		$\times$	$\times$	$\times$
ω_6	0.0181		$\times$		
ω_7	0.0898	$\times$		$\times$	
ω_8	0.0770		$\times$	$\times$	

Table 3.5: Comparison of lower bounds.

System	$P\left(\bigcup_{i=1}^{N} A_i\right)$	ℓ_{DS}	ℓ_{DC}	ℓ_{KAT}	ℓ_{GK}	$\ell_{\text{NEW-2}}$	$\ell_{\text{NEW-1}}$
I	0.7890	0.7007	0.7087	0.7247	0.7601	0.7247	0.7487
II	0.6740	0.6150	0.6154	0.6227	0.6510	0.6227	0.6398
III	0.7890	0.6933	0.7048	0.7222	0.7508	0.7222	0.7427
IV	0.9687	0.8879	0.8757	0.8909	0.9231	0.8909	0.9044
V	0.3900	0.3800	0.3495	0.3833	0.3813	0.3900	0.3900
VI	0.3252	0.2706	0.2720	0.2769	0.2972	0.3205	0.3252
VII	0.5346	0.3989	0.4186	0.4434	0.4750	0.4562	0.5090
VIII	0.5854	0.5395	0.5352	0.5412	0.5390	0.5464	0.5513

Table 3.6: Comparison of the new analytical lower bound (3.6) $\ell_{\text{NEW-2}}$ with the KAT bound ℓ_{KAT}.

System	ℓ_{KAT}	$\ell_{\text{NEW-2}}$	$\ell_{\text{NEW-2}} - \ell_{\text{KAT}}$	Lower bound on the gap (3.21)
V	0.3833	0.3900	0.0067	0.0067
VI	0.2769	0.3205	0.0436	0.0206
VII	0.4434	0.4562	0.0128	0.0128
VIII	0.5412	0.5464	0.0051	0.0051

Chapter 4

New Bounds using $\{P(A_i)\}$ and $\{\sum_j c_j P(A_i \cap A_j)\}$

In this chapter, we consider bounds that are established by $\{P(A_i)\}$ and $\{\sum_j c_j P(A_i \cap A_j)\}$. We first assume $\boldsymbol{c} = (c_1, \ldots, c_N)^T$ is a given weight or parameter vector and derive a new class of lower bounds which has at most a pseudo-polynomial computational complexity and can be sharper than the GK bound in some cases. Then, we discuss methods for choosing $\boldsymbol{c}$, which will lead to lower bounds that use $\{P(A_i)\}$ and $\{P(A_i \cap A_j)\}$. Finally, we show the following regarding the existing GK bound: i) the GK bound cannot be improved via optimization over subsets of events; ii) the GK bound can be implemented iteratively.

4.1 New Class of Lower Bounds

4.1.1 New Expressions for $P\left(\bigcup_{i=1}^N A_i\right)$

For simplicity, assume the events $\{A_1, \ldots, A_N\}$ are in a finite probability space $(\Omega, \mathscr{F}, P)$, where N is a fixed positive integer. Denote $\mathscr{B}$ as the collection of all non-empty subsets of $\{1, 2, \ldots, N\}$ and let $B \in \mathscr{B}$ be a non-empty subset of $\{1, 2, \ldots, N\}$, we use ω_B to denote the outcome such that $\omega_B \in A_i$ for all $i \in B$ and $\omega_B \notin A_i$ for all $i \notin B$, $i = 1, \ldots, N$. Using this notation, $\{\omega_B : i \in B\}$ is the collection of all the outcomes in A_i, and similarly $P(A_i) = \sum_{\omega \in A_i} p(\omega)$ can be written as $P(A_i) = \sum_{B \in \mathscr{B}: i \in B} p(\omega_B)$.

For simplicity, we use p_B to denote $p(\omega_B)$:

$$p_B := p(\omega_B). \tag{4.1}$$

Then we have

$$P\left(\bigcup_{i=1}^{N} A_i\right) = \sum_{B \in \mathscr{B}} p_B. \tag{4.2}$$

Suppose there are N functions $f_i(B), i = 1, \ldots, N$ that $\sum_{i=1}^{N} f_i(B) = 1$ for any $B \in \mathscr{B}$ (i.e., for any outcome ω_B). If we further assume that $f_i(B) = 0$ if $i \notin B$ (i.e., $\omega_B \notin A_i$), one can get

$$\begin{aligned} P\left(\bigcup_{i=1}^{N} A_i\right) &= \sum_{B \in \mathscr{B}} \left(\sum_{i=1}^{N} f_i(B)\right) p_B \\ &= \sum_{i=1}^{N} \sum_{B \in \mathscr{B}} f_i(B) p_B = \sum_{i=1}^{N} \sum_{B \in \mathscr{B}: i \in B} f_i(B) p_B. \end{aligned} \tag{4.3}$$

Note that if we define

$$f_i(B) = \begin{cases} \frac{1}{|B|} = \frac{1}{\deg(\omega_B)} & \text{if } i \in B \\ 0 & \text{if } i \notin B \end{cases} \tag{4.4}$$

then $\sum_{i=1}^{N} f_i(B) = 1$ is satisfied and equation (4.3) becomes

$$P\left(\bigcup_{i=1}^{N} A_i\right) = \sum_{i=1}^{N} \sum_{B\in\mathscr{B}:i\in B} f_i(B)p_B = \sum_{i=1}^{N} \sum_{B\in\mathscr{B}:i\in B} \frac{p_B}{|B|} = \sum_{i=1}^{N} \sum_{\omega\in A_i} \frac{p(\omega)}{\deg(\omega)}. \tag{4.5}$$

If we define

$$f_i(B) = \begin{cases} \frac{c_i}{\sum_{k\in B} c_k} & \text{if } i \in B \\ 0 & \text{if } i \notin B \end{cases} \tag{4.6}$$

where the parameter vector $\boldsymbol{c} = (c_1, \ldots, c_N)$ satisfies $\sum_{k\in B} c_k \neq 0$ for all $B \in \mathscr{B}$, (therefore $c_i \neq 0, i = 1, \ldots, N$) then again $\sum_i f_i(\omega) = 1$ is satisfied, and we can get from (4.3) that

$$P\left(\bigcup_{i=1}^{N} A_i\right) = \sum_{i=1}^{N} \sum_{B\in\mathscr{B}:i\in B} f_i(B)p_B = \sum_{i=1}^{N} \sum_{B\in\mathscr{B}:i\in B} \frac{c_i p_B}{\sum_{k\in B} c_k} = \sum_{i=1}^{N} \sum_{\omega\in A_i} \frac{c_i p(\omega)}{\sum_{\{k:\omega\in A_k\}} c_k}, \tag{4.7}$$

yielding the following lemma (to the best of our knowledge, this lemma is novel).

Lemma 7. *Suppose $\{\omega_B, B \in \mathscr{B}\}$ are all the $2^N - 1$ outcomes in $\bigcup_i A_i$. Let $\boldsymbol{c} = (c_1, \ldots, c_N)^T \in \mathbb{R}^N$ satisfies*

$$\sum_{k\in B} c_k \neq 0, \quad \textit{for all} \quad B \in \mathscr{B} \tag{4.8}$$

then we have

$$P\left(\bigcup_{i=1}^{N} A_i\right) = \sum_{i=1}^{N} \sum_{B\in\mathscr{B}:i\in B} \frac{c_i p_B}{\sum_{k\in B} c_k} = \sum_{i=1}^{N} \sum_{\omega\in A_i} \frac{c_i p(\omega)}{\sum_{\{k:\omega\in A_k\}} c_k}. \tag{4.9}$$

Note that (4.9) holds for any $\boldsymbol{c}$ that satisfies (4.8), which is clearly a generalized expression of (4.5).

4.1.2 Lower Bounds via the Cauchy-Schwarz Inequality

In this subsection, we use (4.3) to establish relations to the lower bounds of [6] and [11]. Note that in order for the following Cauchy-Schwarz inequalities to hold, we have to make a further assumption on $f_i(\cdot)$, that

$$f_i(B) > 0, \quad i = 1, \ldots, N, \quad B \in \mathscr{B}. \tag{4.10}$$

Note that when $f_i(B)$ is defined by $\boldsymbol{c}$, then condition (4.10) is stronger than the original condition (4.8). If $f_i(B)$ is defined by (4.6), condition (4.10) is then equivalent to requiring that $c_i > 0$ for all i.

Relation to the Cohen-Merhav bound [6]

Let $m_i(\omega_B)$ be non-negative real functions. Then by the Cauchy-Schwarz inequaility,

$$\left[\sum_{B:i\in B} f_i(B)p_B\right]\left[\sum_{B:i\in B} \frac{p_B}{f_i(B)} m_i^2(\omega_B)\right] \geq \left[\sum_{B:i\in B} p_B m_i(\omega_B)\right]^2. \tag{4.11}$$

Thus, using (4.3), we have

$$P\left(\bigcup_{i=1}^{N} A_i\right) = \sum_{i=1}^{N}\sum_{B:i\in B} f_i(B)p_B \geq \sum_{i=1}^{N} \frac{\left[\sum_{B:i\in B} p_B m_i(\omega_B)\right]^2}{\sum_{B:i\in B} \frac{p_B}{f_i(B)} m_i^2(\omega_B)}. \tag{4.12}$$

If we define $f_i(B)$ by (4.4), then the above inequality reduces to

$$P\left(\bigcup_{i=1}^{N} A_i\right) \geq \sum_{i=1}^{N} \frac{\left[\sum_{B:i\in B} p_B m_i(\omega_B)\right]^2}{\sum_{B:i\in B} p_B m_i^2(\omega_B)|B|} = \sum_{i} \frac{\left[\sum_{\omega\in A_i} p(\omega)m_i(\omega)\right]^2}{\sum_j \sum_{\omega\in A_i\cap A_j} p(\omega)m_i^2(\omega)}, \tag{4.13}$$

where the equality holds when $m_i(\omega) = \frac{1}{\deg(\omega)}$ (i.e., $m_i(\omega_B) = \frac{1}{|B|}$), which was first shown by Cohen and Merhav in [6, Theorem 2.1].

When $m_i(\omega) = c_i > 0$, (4.3) reduces to the DC bound [8]

$$P\left(\bigcup_{i=1}^{N} A_i\right) \geq \sum_i \frac{[c_i P(A_i)]^2}{\sum_j c_i^2 P(A_i \cap A_j)} = \sum_i \frac{P(A_i)^2}{\sum_j P(A_i \cap A_j)} = \ell_{\mathrm{DC}}. \tag{4.14}$$

Note that as remarked in [11], the DC bound can be seen as a special case of the lower bound

$$P\left(\bigcup_{i=1}^{N} A_i\right) \geq \frac{\left[\sum_i c_i P(A_i)\right]^2}{\sum_i \sum_j c_i^2 P(A_i \cap A_j)}, \tag{4.15}$$

when $c_i = \frac{P(A_i)}{\sum_j P(A_i \cap A_j)}$. This is because

$$\begin{aligned}\frac{\left[\sum_i \left(\frac{P(A_i)}{\sum_j P(A_i \cap A_j)}\right) P(A_i)\right]^2}{\sum_i \sum_j \left(\frac{P(A_i)}{\sum_j P(A_i \cap A_j)}\right)^2 P(A_i \cap A_j)} &= \frac{\left(\sum_i \frac{P(A_i)^2}{\sum_j P(A_i \cap A_j)}\right)^2}{\sum_i \left\{\left(\frac{P(A_i)}{\sum_j P(A_i \cap A_j)}\right)^2 \sum_j P(A_i \cap A_j)\right\}} \\ &= \frac{\ell_{\mathrm{DC}}^2}{\ell_{\mathrm{DC}}} = \ell_{\mathrm{DC}}.\end{aligned} \tag{4.16}$$

Note that although $c_i > 0$ is not assumed in (4.15), one can always replace c_i by $|c_i|$ in (4.15) if $c_i < 0$ to get a sharper bound.

However, the lower bound in (4.15) is looser than the following two (left-most) lower bounds (which we later derive in (4.23) and (4.25)):

$$\sum_{i=1}^{N} \frac{c_i^2 P(A_i)^2}{c_i \sum_k c_k P(A_i \cap A_k)} \geq \frac{\left[\sum_i c_i P(A_i)\right]^2}{\sum_i \sum_k c_i c_k P(A_i \cap A_k)} \geq \frac{\left[\sum_i c_i P(A_i)\right]^2}{\sum_i \sum_j c_i^2 P(A_i \cap A_j)}, \tag{4.17}$$

where $c_i > 0$ for all i and the last inequality can be proved using $2c_i c_j \leq c_i^2 + c_j^2$.

Relation to the Gallot-Kounias bound [11]

By the Cauchy-Schwarz inequality, which is equivalent to assuming $m_i(\omega) = 1$ in (4.11), we have

$$\left[\sum_{B:i\in B} f_i(B)p_B\right]\left[\sum_{B:i\in B} \frac{p_B}{f_i(B)}\right] \geq \left[\sum_{B:i\in B} p_B\right]^2 = P(A_i)^2. \tag{4.18}$$

Using $f_i(B)$ defined using $\boldsymbol{c}$ in (4.6) (note that the condition in (4.10) is equivalent to $c_i > 0$ for all i), we have

$$\left[\sum_{B:i\in B} \frac{c_i p_B}{\sum_{k\in B} c_k}\right]\left[\sum_{B:i\in B} \left(\frac{\sum_{k\in B} c_k}{c_i}\right) p_B\right] \geq P(A_i)^2. \tag{4.19}$$

Note that

$$\sum_{B:i\in B} \left(\frac{\sum_{k\in B} c_k}{c_i}\right) p_B = \frac{1}{c_i}\sum_{k=1}^{N} \sum_{B:i\in B, k\in B} c_k p_B = \frac{\sum_k c_k P(A_i\cap A_k)}{c_i}. \tag{4.20}$$

Therefore, we have

$$\left[\sum_{B:i\in B} \frac{c_i p_B}{\sum_{k\in B} c_k}\right]\left[\frac{\sum_k c_k P(A_i\cap A_k)}{c_i}\right] \geq P(A_i)^2. \tag{4.21}$$

Then for all i,

$$\sum_{B:i\in B} \frac{c_i p_B}{\sum_{k\in B} c_k} \geq \frac{c_i^2 P(A_i)^2}{c_i \sum_k c_k P(A_i\cap A_k)} \tag{4.22}$$

By summing (4.22) over i, we get another new lower bound:

$$P\left(\bigcup_i A_i\right) \geq \sum_{i=1}^{N} \frac{c_i^2 P(A_i)^2}{c_i \sum_k c_k P(A_i\cap A_k)}. \tag{4.23}$$

Note that we can use Cauchy-Schwarz Inequality again:

$$\left[\sum_{i=1}^{N} \frac{c_i^2 P(A_i)^2}{c_i \sum_k c_k P(A_i \cap A_k)}\right] \left[\sum_i c_i \sum_k c_k P(A_i \cap A_k)\right] \geq \left[\sum_i c_i P(A_i)\right]^2, \tag{4.24}$$

which yields

$$P\left(\bigcup_i A_i\right) \geq \sum_{i=1}^{N} \frac{c_i^2 P(A_i)^2}{c_i \sum_k c_k P(A_i \cap A_k)} \geq \frac{\left[\sum_i c_i P(A_i)\right]^2}{\sum_i \sum_k c_i c_k P(A_i \cap A_k)}. \tag{4.25}$$

Since the above inequality holds for any positive $\boldsymbol{c}$, we have

$$P\left(\bigcup_i A_i\right) \geq \max_{\boldsymbol{c} \in \mathbb{R}_+^N} \sum_{i=1}^{N} \frac{c_i^2 P(A_i)^2}{c_i \sum_k c_k P(A_i \cap A_k)} \geq \max_{\boldsymbol{c} \in \mathbb{R}_+^N} \frac{\left[\sum_i c_i P(A_i)\right]^2}{\sum_i \sum_k c_i c_k P(A_i \cap A_k)}. \tag{4.26}$$

One can show that by computing the partial derivative with respect to c_i and set it to zero that

$$\max_{\boldsymbol{c} \in \mathbb{R}^N} \sum_{i=1}^{N} \frac{c_i^2 P(A_i)^2}{c_i \sum_k c_k P(A_i \cap A_k)} = \max_{\boldsymbol{c} \in \mathbb{R}^N} \frac{\left[\sum_i c_i P(A_i)\right]^2}{\sum_i \sum_k c_i c_k P(A_i \cap A_k)} = \ell_{\mathrm{GK}}, \tag{4.27}$$

where ℓ_{GK} is the Gallot-Kounias bound [11], and the optimal $\tilde{\mathbf{c}}$ can be obtained from $\boldsymbol{\Sigma}\tilde{\boldsymbol{c}} = \boldsymbol{\alpha}$ (see Section 2.3.2). Thus, we conclude that the lower bounds in (4.26) are equal to the GK bound [11] if $\tilde{\boldsymbol{c}} \in \mathbb{R}_+^N$; otherwise, the lower bounds in (4.26) are weaker than the GK bound.

4.1.3 New Class of Lower Bounds $\boldsymbol{\ell}_{\textbf{NEW-3}}(\boldsymbol{c})$

We have the following theorem.

Theorem 3. *For any given* $\mathbf{c}$ *that satisfies (4.8), a new lower bound on the union* *probability is given by*

$$P\left(\bigcup_{i=1}^{N} A_i\right) \geq \sum_{i=1}^{N} \ell_i(\boldsymbol{c}) =: \ell_{NEW\text{-}3}(\boldsymbol{c}), \tag{4.28}$$

where

$$\ell_i(\boldsymbol{c}) = P(A_i)\left(\frac{c_i}{\sum_{k\in B_1^{(i)}} c_k} + \frac{c_i}{\sum_{k\in B_2^{(i)}} c_k} - \frac{c_i \sum_k c_k P(A_i\cap A_k)}{P(A_i)\left(\sum_{k\in B_1^{(i)}} c_k\right)\left(\sum_{k\in B_2^{(i)}} c_k\right)}\right), \tag{4.29}$$

where $B_1^{(i)}$ *and* $B_2^{(i)}$ *are subsets of* $\{1,\ldots,N\}$ *that satisfy the following conditions.*

1. *If* $\frac{\sum_k c_k P(A_i\cap A_k)}{c_i P(A_i)} \geq 0$ *and* $\min_{\{B:i\in B\}} \frac{\sum_{k\in B} c_k}{c_i} < 0$*, then*

$$\begin{aligned} B_1^{(i)} &= \arg\max_{\{B:i\in B\}} \frac{\sum_{k\in B} c_k}{c_i} \quad s.t. \quad \frac{\sum_{k\in B} c_k}{c_i} < 0, \\ B_2^{(i)} &= \arg\max_{\{B:i\in B\}} \frac{\sum_{k\in B} c_k}{c_i}. \end{aligned} \tag{4.30}$$

2. *If* $\frac{\sum_k c_k P(A_i\cap A_k)}{c_i P(A_i)} \geq 0$ *and* $\min_{\{B:i\in B\}} \frac{\sum_{k\in B} c_k}{c_i} \geq 0$*, then*

$$\begin{aligned} B_1^{(i)} &= \arg\max_{\{B:i\in B\}} \frac{\sum_{k\in B} c_k}{c_i} \quad s.t. \quad \frac{\sum_{k\in B} c_k}{c_i} \leq \frac{\sum_k c_k P(A_i\cap A_k)}{c_i P(A_i)}, \\ B_2^{(i)} &= \arg\min_{\{B:i\in B\}} \frac{\sum_{k\in B} c_k}{c_i} \quad s.t. \quad \frac{\sum_{k\in B} c_k}{c_i} \geq \frac{\sum_k c_k P(A_i\cap A_k)}{c_i P(A_i)}. \end{aligned} \tag{4.31}$$

3. *If* $\frac{\sum_k c_k P(A_i\cap A_k)}{c_i P(A_i)} < 0$ *and* $\frac{\sum_k c_k P(A_i\cap A_k)}{c_i P(A_i)} < \left\{\max_{\{B:i\in B\}} \frac{\sum_{k\in B} c_k}{c_i}, \quad s.t. \ \frac{\sum_{k\in B} c_k}{c_i} < 0\right\}$*, then*

$$\begin{aligned} B_1^{(i)} &= \arg\max_{\{B:i\in B\}} \frac{\sum_{k\in B} c_k}{c_i}, \quad s.t. \ \frac{\sum_{k\in B} c_k}{c_i} < 0, \\ B_2^{(i)} &= \arg\min_{\{B:i\in B\}} \frac{\sum_{k\in B} c_k}{c_i}. \end{aligned} \tag{4.32}$$

4. *If* $\frac{\sum_k c_k P(A_i \cap A_k)}{c_i P(A_i)} < 0$ *and* $\frac{\sum_k c_k P(A_i \cap A_k)}{c_i P(A_i)} \geq \left\{ \max_{\{B: i \in B\}} \frac{\sum_{k \in B} c_k}{c_i}, \quad s.t. \ \frac{\sum_{k \in B} c_k}{c_i} < 0 \right\}$, *then*

$$\begin{aligned} B_1^{(i)} &= \arg \max_{\{B: i \in B\}} \frac{\sum_{k \in B} c_k}{c_i}, \\ B_2^{(i)} &= \arg \max_{\{B: i \in B\}} \frac{\sum_{k \in B} c_k}{c_i} \quad s.t. \quad \frac{\sum_{k \in B} c_k}{c_i} \leq \frac{\sum_k c_k P(A_i \cap A_k)}{c_i P(A_i)}. \end{aligned} \tag{4.33}$$

Proof. We note that $\ell_i(\boldsymbol{c})$ is the solution of

$$\begin{aligned} \min_{\{p_B: i \in B\}} & \sum_{B: i \in B} \frac{c_i p_B}{\sum_{k \in B} c_k} \\ \text{s.t.} & \sum_{B: i \in B} p_B = P(A_i), \\ & \sum_{B: i \in B} \left(\frac{\sum_{k \in B} c_k}{c_i} \right) p_B = \frac{1}{c_i} \sum_k c_k P(A_i \cap A_k), \\ & p_B \geq 0, \quad \text{for all} \quad B \in \mathscr{B} \quad \text{such that} \quad i \in B. \end{aligned} \tag{4.34}$$

From (4.34) we have that

$$\sum_{B: i \in B} \frac{c_i p_B}{\sum_{k \in B} c_k} \geq \ell_i(\boldsymbol{c}). \tag{4.35}$$

Summing (4.35) over i and using (4.9) we directly yield

$$P\left(\bigcup_{i=1}^N A_i \right) \geq \sum_{i=1}^N \ell_i(\boldsymbol{c}). \tag{4.36}$$

The solution of (4.34) is given in Appendix B.1. □

Remark 11. *We can solve (4.34) by solving its dual problem*

$$\begin{aligned} \max_{q_1,q_2} \quad & q_1 P(A_i) + q_2 \sum_k w_k P(A_i \cap A_k) \\ s.t. \quad & q_1 + (\sum_{k\in B'} w_k) q_2 \le \frac{1}{\sum_{k\in B'} w_k}, \quad \forall B' \in \mathscr{B} : i \in B', \end{aligned} \tag{4.37}$$

where $w_k := \frac{c_k}{c_i}$. *We give an alternative proof of Theorem 3 by solving this dual problem for* $\boldsymbol{c} \in \mathbb{R}_+^N$, *i.e., the case (4.31), in Appendix B.2.*

Remark 12 (**The new bound $\boldsymbol{\ell}_{\textbf{NEW-3}}(\boldsymbol{c})$ v.s. the GK bound $\boldsymbol{\ell}_{\textbf{GK}}$**). *For any* $\boldsymbol{c} \in \mathbb{R}_+^N$, *we have these relations between different lower bounds:*

$$\ell_{NEW\text{-}3}(\boldsymbol{c}) \ge \sum_{i=1}^N \frac{c_i^2 P(A_i)^2}{c_i \sum_k c_k P(A_i \cap A_k)} \ge \frac{\left[\sum_i c_i P(A_i)\right]^2}{\sum_i \sum_k c_i c_k P(A_i \cap A_k)} \ge \frac{\left[\sum_i c_i P(A_i)\right]^2}{\sum_i \sum_j c_i^2 P(A_i \cap A_j)}. \tag{4.38}$$

Note that if $\tilde{\mathbf{c}}$ *obtained by the GK bound satisfies* $\tilde{\mathbf{c}} \in \mathbb{R}_+^N$, *then* $\ell_{NEW\text{-}3}(\tilde{\mathbf{c}}) \ge \ell_{GK}$. *This can be proven by first noting that the two constraints of (4.34) and the Cauchy-Schwarz inequality yield (4.22). Then by (4.26), we can get that* ℓ_{GK} *is a lower bound of* $\ell_{NEW\text{-}3}(\tilde{\mathbf{c}})$.

Remark 13 (**The new bound $\boldsymbol{\ell}_{\textbf{NEW-3}}(\boldsymbol{c})$ v.s. the KAT bound $\boldsymbol{\ell}_{\textbf{KAT}}$**). *One can easily verify that* $\ell_{NEW\text{-}3}(\kappa\mathbf{1}) = \ell_{KAT}$, *where* $\mathbf{1}$ *is the all-one vector of size* N *and* κ *is any non-zero constant.*

Lemma 8. *When* $\boldsymbol{c} \in \mathbb{R}_+^N$, *the lower bound* $\ell_{NEW\text{-}3}(\boldsymbol{c})$ *can be computed in pseudo-polynomial time, and can be arbitrarily closely approximated by an algorithm running in polynomial time.*

Proof. The problems in (4.30) to (4.33) are exactly the 0/1 knapsack problem with mass equals to value [24] (the corresponding decision problem is also called subset sum problem). Unfortunately, the 0/1 knapsack problem is NP-hard in general.

However, if $\boldsymbol{c} \in \mathbb{R}_+^N$, i.e, the case (4.31), there exists a dynamic programming solution which runs in pseudo-polynomial time [24], i.e., polynomial in N, but exponential in the number of bits required to represent $\frac{\sum_k c_k P(A_i \cap A_k)}{c_i P(A_i)}$. Furthermore, there is a fully polynomial-time approximation scheme (FPTAS), which finds a solution that is correct within a factor of $(1-\epsilon)$ of the optimal solution [24]. The running time is bounded by a polynomial and $1/\epsilon$ where ϵ is a bound on the correctness of the solution.

Therefore, if $\boldsymbol{c} \in \mathbb{R}_+^N$, one can get a lower bound for $\ell_i(\boldsymbol{c})$ in polynomial time which can be arbitrarily close to $\ell_i(\boldsymbol{c})$ by setting ϵ small enough, i.e.,

$$\ell_i(\boldsymbol{c}) \geq \ell_i^L(\boldsymbol{c}, \epsilon), \quad \lim_{\epsilon \to 0^+} \ell_i^L(\boldsymbol{c}, \epsilon) = \ell_i(\boldsymbol{c}). \tag{4.39}$$

The details are as follows. First, assume $\hat{B}_1$ and $\hat{B}_2$ are obtained by the FPTAS which satisfy

$$(1-\epsilon) \sum_{k \in B_1^{(i)}} c_k \leq \sum_{k \in \hat{B}_1^{(i)}} c_k \leq \sum_{k \in B_1^{(i)}} c_k, \quad \sum_{k \in B_2^{(i)}} c_k \leq \sum_{k \in \hat{B}_2^{(i)}} c_k \leq (1+\epsilon) \sum_{k \in B_2^{(i)}} c_k. \tag{4.40}$$

Then we have

$$\begin{aligned} \sum_{k \in B_1^{(i)}} c_k &\leq \min \left\{ \frac{\sum_{k \in \hat{B}_1^{(i)}} c_k}{1-\epsilon}, \frac{\sum_k c_k P(A_i \cap A_k)}{P(A_i)} \right\} =: b_1^{(i)}, \\ \sum_{k \in B_2^{(i)}} c_k &\geq \max \left\{ \frac{\sum_{k \in B_2^{(i)}} c_k}{1+\epsilon}, \frac{\sum_k c_k P(A_i \cap A_k)}{P(A_i)} \right\} =: b_2^{(i)}. \end{aligned} \tag{4.41}$$

Then one can get the arbitrarily close lower bound for $\ell_i(\boldsymbol{c})$ as

$$\ell_i(\boldsymbol{c}) \geq \ell_i^L(\boldsymbol{c}, \epsilon) := P(A_i) \left(\frac{c_i}{b_1^{(i)}} + \frac{c_i}{b_2^{(i)}} - \frac{c_i \sum_k c_k P(A_i \cap A_k)}{P(A_i) b_1^{(i)} b_2^{(i)}} \right). \tag{4.42}$$

Therefore, we can get a lower bound for $P\left(\bigcup_{i=1}^N A_i\right)$ that is arbitrarily close to $\ell_{\text{NEW-3}}(\boldsymbol{c})$ in polynomial time:

$$P\left(\bigcup_{i=1}^{N} A_i\right) \geq \sum_i \ell_i(\boldsymbol{c}) \geq \sum_i \ell_i^L(\boldsymbol{c}, \epsilon). \tag{4.43}$$

□

Remark 14 (**New class of upper bounds $\hbar_{\text{NEW-4}}(\boldsymbol{c})$**)**.** *We can also derive an upper bound by maximizing, instead of minimizing, the objective function of (4.34).*

For any given $\boldsymbol{c} \in \mathbb{R}^+$, a upper bound can be obtained by

$$\hbar(\boldsymbol{c}) = \sum_{i=1}^{N} \hbar_i(\boldsymbol{c}), \tag{4.44}$$

where $\hbar_i(\boldsymbol{c})$ is defined by

$$\begin{aligned} \hbar_i(\boldsymbol{c}) := \max_{\{p_B : i \in B\}} & \sum_{B: i \in B} \frac{c_i p_B}{\sum_{k \in B} c_k} \\ \textit{s.t.} & \sum_{B: i \in B} p_B = P(A_i), \\ & \sum_{B: i \in B} \left(\frac{\sum_{k \in B} c_k}{c_i} \right) p_B = \frac{1}{c_i} \sum_k c_k P(A_i \cap A_k), \\ & p_B \geq 0, \quad \textit{for all} \quad B \in \mathscr{B} \quad \textit{such that} \quad i \in B. \end{aligned} \tag{4.45}$$

The resulting upper bound is given by

$$\begin{aligned} P\left(\bigcup_i A_i\right) &\leq \sum_i \left\{ P(A_i) \left[\frac{c_i}{\min_k c_k} + \frac{c_i}{\sum_k c_k} - \frac{c_i^2}{(\min_k c_k) \sum_k c_k} \frac{\sum_k c_k P(A_i \cap A_k)}{c_i P(A_i)} \right] \right\} \\ &= \left(\frac{1}{\min_k c_k} + \frac{1}{\sum_k c_k} \right) \sum_i c_i P(A_i) - \frac{1}{(\min_k c_k) \sum_k c_k} \sum_i \sum_k c_i c_k P(A_i \cap A_k), \\ &=: \hbar_{NEW\text{-}4}(\boldsymbol{c}). \end{aligned} \tag{4.46}$$

The partial derivative of $\hbar(\boldsymbol{c})$ w.r.t. c_j such that $c_j \neq \min_k c_k$ is given by

$$\begin{aligned} \frac{\partial \hbar(\boldsymbol{c})}{c_j} = \frac{P(A_j)}{\min_k c_k} &+ \frac{P(A_j) \sum_k c_k - \sum_i c_i P(A_i)}{(\sum_k c_k)^2} \\ &- \frac{1}{\min_k c_k} \frac{2 \left[\sum_k c_k P(A_j \cap A_k)\right] (\sum_k c_k) - \sum_i \sum_k c_i c_k P(A_i \cap A_k)}{(\sum_k c_k)^2}. \end{aligned} \tag{4.47}$$

Thus,

$$\begin{aligned} (\min_k c_k)(\sum_k c_k)^2 \frac{\partial \hbar(\boldsymbol{c})}{c_j} &= P(A_j)(\sum_k c_k)^2 + P(A_j)(\sum_k c_k)(\min_k c_k) - (\min_k c_k) \sum_i c_i P(A_i) \\ &\quad - 2(\sum_k c_k) \left[\sum_k c_k P(A_j \cap A_k) \right] + \sum_i \sum_k c_i c_k P(A_i \cap A_k). \end{aligned} \tag{4.48}$$

It is conjectured that the above partial derivatives w.r.t any $c_j \neq \min_k c_k$ are always positive, and hence $\hbar(\boldsymbol{c})$ is no less than (2.29), i.e. $\hbar_{NEW\text{-}4} \geq \hbar_{NEW\text{-}1} \geq \hbar_{NEW\text{-}3}$.

4.1.4 Heuristic and optimal choices for $\boldsymbol{c}$

First, note that if the $\tilde{\boldsymbol{c}}$ obtained by the GK bound satisfies $\tilde{\boldsymbol{c}} \in \mathbb{R}_+^N$, then one good choice for $\boldsymbol{c}$ is $\boldsymbol{c} = \tilde{\boldsymbol{c}}$ since in this case we have already proved in Remark 12 that

$\ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}}) \geq \ell_{\text{GK}}$. Otherwise, $\ell_{\text{NEW-3}}(\boldsymbol{c})$ has to be computed in exponential time. Furthermore, $\ell_{\text{NEW-3}}(\boldsymbol{c})$ might be very poor especially for the cases in (B.5) and (B.7) if $b_1 \to 0^-$, the objective function of (B.2) goes to $-\infty$. Then a heuristic choice for $\boldsymbol{c}$ is to have its components given by $\tilde{c}_i^+ = \max(\tilde{c}_i, \epsilon)$, where $\epsilon > 0$ is close to zero; we will denote it by $\tilde{\boldsymbol{c}}^+$. Then $\tilde{\boldsymbol{c}}^+ \in \mathbb{R}_+^N$ and hence the solution of (B.2) always falls into the case of (B.6) and therefore $\ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}}^+)$ can be computed in pseudo-polynomial time and approximated in polynomial time.

We will also consider in the numerical examples another heuristic method for choosing $\boldsymbol{c}$. Specifically, we choose $\boldsymbol{c}$ as $\boldsymbol{c} = \tilde{\boldsymbol{c}} + \kappa\mathbf{1}$, where κ is chosen via a line search. Since $\tilde{\boldsymbol{c}}$ is obtained by the GK bound and $\boldsymbol{c} = \kappa\mathbf{1}$ yields the KAT bound, $\boldsymbol{c} = \tilde{\boldsymbol{c}} + \kappa\mathbf{1}$ is a line passing through those two possible $\boldsymbol{c}$'s. Since the computational load for a line search can be however high, we only use it to demonstrate that the lower bounds can be further improved by optimizing $\boldsymbol{c}$.

Finally, we define the best bound in the class of $\ell_{\text{NEW-3}}(\boldsymbol{c})$ which is achieved by using $\boldsymbol{c} = \boldsymbol{c}_{\text{opt}}$, although how to find $\boldsymbol{c}_{\text{opt}}$ is still open.

Theorem 4 (**The best bound in the class of $\boldsymbol{\ell_{\text{NEW-3}}(c)}$**).

$$P\left(\bigcup_{i=1}^{N} A_i\right) \geq \max_{\boldsymbol{c}} \ell_{\textit{NEW-3}}(\boldsymbol{c}) = \ell_{\textit{NEW-3}}(\boldsymbol{c}_{opt}), \tag{4.49}$$

the maximum of which is range over all $\boldsymbol{c}$*'s that satisfy (4.8). The optimal* $\boldsymbol{c}_{opt}$ *can* *be obtained by the following non-convex optimization problem:*

$$\boldsymbol{c}_{opt} = \arg \max_{\boldsymbol{c}, \{p_i, q_i\}} \quad \sum_i p_i c_i P(A_i) + \sum_i q_i \sum_k c_k P(A_i \cap A_k)$$
$$s.t. \quad p_i + (\sum_{k \in B'} c_k) q_i \leq \frac{1}{\sum_{k \in B'} c_k}, \quad \forall B' \in \mathscr{B} : i \in B', \quad i = 1, \ldots, N. \tag{4.50}$$

Proof. Similar to (4.37), for a given $\boldsymbol{c}$, the $\ell_{\text{NEW-3}}(\boldsymbol{c})$ is the solution of the following problem

$$\max_{\{p_i, q_i\}} \quad \sum_i \left\{ p_i c_i P(A_i) + q_i \sum_k c_k P(A_i \cap A_k) \right\}$$
$$\text{s.t.} \quad p_i + (\sum_{k \in B'} c_k) q_i \leq \frac{1}{\sum_{k \in B'} c_k}, \quad \forall B' \in \mathscr{B} : i \in B', \quad i = 1, \ldots, N. \tag{4.51}$$

Therefore, by maximizing (4.51) over $\boldsymbol{c}$, we directly get $\boldsymbol{c}_{\text{opt}}$ as in (4.50). □

Note that it is very difficult to get the solution $\boldsymbol{c}_{\text{opt}}$ since (4.50) is non-convex. However, we note that any feasible point of (4.50) leads to a (sub-optimal) lower bound. Also, by further constraining c_i to be nonnegative for all i, any feasible point corresponds to a lower bound that can be computed by a polynomial-time approximation algorithm. In the numerical examples, we randomly generate $\boldsymbol{c} \in \mathbb{R}_+^N$ for a large number samples and choose the best one to illustrate the bounds' performance.

4.1.5 Another Class of Lower Bounds, $\ell_{\text{NEW-4}}(\boldsymbol{c})$

We only consider $\boldsymbol{c} \in \mathbb{R}_+^N$ in this subsection. Then one can further improve the lower bound $\ell_{\text{NEW-3}}(\boldsymbol{c})$ to get the following new class of lower bounds.

Theorem 5. *Defining* $\mathscr{B}^- = \mathscr{B} \setminus \{1, \dots, N\}$, $\tilde{\gamma}_i := \sum_k c_k P(A_i \cap A_k)$, $\tilde{\alpha}_i := P(A_i)$ *and*

$$\tilde{\delta} := \left[\frac{\tilde{\gamma}_i - \left(\sum_k c_k - \min_k c_k\right) \tilde{\alpha}_i}{\min_k c_k} \right]^+, \tag{4.52}$$

where $\boldsymbol{c} \in \mathbb{R}_+^N$, *another class of lower bounds is given by*

$$\ell_{\text{NEW-4}}(\boldsymbol{c}) := \tilde{\delta} + \sum_{i=1}^N \ell_i'(\boldsymbol{c}, \tilde{\delta}), \tag{4.53}$$

where

$$\ell_i'(\boldsymbol{c}, x) = [P(A_i) - x] \left(\frac{c_i}{\sum_{k \in B_1^{(i)}} c_k} + \frac{c_i}{\sum_{k \in B_2^{(i)}} c_k} - \frac{c_i \sum_k c_k \left[P(A_i \cap A_k) - x\right]}{[P(A_i) - x] \left(\sum_{k \in B_1^{(i)}} c_k\right) \left(\sum_{k \in B_2^{(i)}} c_k\right)} \right), \tag{4.54}$$

and

$$\begin{aligned} B_1^{(i)} &= \arg \max_{\{B \in \mathscr{B}^- : i \in B\}} \frac{\sum_{k \in B} c_k}{c_i} \quad s.t. \quad \frac{\sum_{k \in B} c_k}{c_i} \le \frac{\sum_k c_k \left[P(A_i \cap A_k) - x\right]}{c_i \left[P(A_i) - x\right]}, \\ B_2^{(i)} &= \arg \min_{\{B \in \mathscr{B}^- : i \in B\}} \frac{\sum_{k \in B} c_k}{c_i} \quad s.t. \quad \frac{\sum_{k \in B} c_k}{c_i} \ge \frac{\sum_k c_k \left[P(A_i \cap A_k) - x\right]}{c_i \left[P(A_i) - x\right]}. \end{aligned} \tag{4.55}$$

Proof. Let $x = p_{\{1,\dots,N\}}$ and define $\mathscr{B}^- = \mathscr{B} \setminus \{1, \dots, N\}$, then consider $\sum_i \ell_i'(\boldsymbol{c}, x) + x$

as a new lower bound where where $\ell'_i(\boldsymbol{c}, x)$ is defined by

$$\begin{aligned}\ell'_i(\boldsymbol{c}, x) := \min_{\{p_B : i \in B, B \in \mathscr{B}^-\}} & \sum_{B: i \in B, B \in \mathscr{B}^-} \frac{c_i p_B}{\sum_{k \in B} c_k} \\ \text{s.t.} \quad & \sum_{B: i \in B, B \in \mathscr{B}^-} p_B = P(A_i) - x, \\ & \sum_{B: i \in B, B \in \mathscr{B}^-} \left(\frac{\sum_{k \in B} c_k}{c_i} \right) p_B = \frac{1}{c_i} \sum_k c_k \left[P(A_i \cap A_k) - x \right], \\ & p_B \geq 0, \quad \text{for all} \quad B \in \mathscr{B}^- \quad \text{such that} \quad i \in B.\end{aligned} \tag{4.56}$$

The solution of (4.56) exists if and only if

$$\min_k c_k \leq \frac{\tilde{\gamma}_i - (\sum_k c_k) x}{\tilde{\alpha}_i - x} \leq \sum_k c_k - \min_k c_k, \tag{4.57}$$

which gives

$$\left[\frac{\tilde{\gamma}_i - \left(\sum_k c_k - \min_k c_k \right) \tilde{\alpha}_i}{\min_k c_k} \right]^+ \leq x \leq \frac{\tilde{\gamma}_i - (\min_k c_k) \tilde{\alpha}_i}{\sum_k c_k - \min_k c_k}. \tag{4.58}$$

Therefore, the new lower bound can be written as

$$\min_x \left[x + \sum_{i=1}^N \ell'_i(\boldsymbol{c}, x) \right], \quad \text{s.t.} \quad \left[\frac{\tilde{\gamma}_i - \left(\sum_k c_k - \min_k c_k \right) \tilde{\alpha}_i}{\min_k c_k} \right]^+ \leq x \leq \frac{\tilde{\gamma}_i - (\min_k c_k) \tilde{\alpha}_i}{\sum_k c_k - \min_k c_k}. \tag{4.59}$$

Similar to solving (4.34) in the proof of $\ell_{\text{NEW-2}}$, we can prove that the objective function of (4.59) is non-decreasing with x; this proof is given in Appendix B.3.

Therefore, defining $\tilde{\delta}$ as in (4.52), the new lower bound can be written as

$$\ell_{\text{NEW-4}}(\boldsymbol{c}) = \tilde{\delta} + \sum_{i=1}^{N} \ell_i'(\boldsymbol{c}, \tilde{\delta}), \tag{4.60}$$

where $\ell_i'(\boldsymbol{c}, \tilde{\delta})$ can be obtained using the solution for $\ell_i(\boldsymbol{c})$ in (4.34) with $b = \frac{\sum_k c_k P(A_i \cap A_k)}{c_i P(A_i)}$ replaced by $\tilde{b} = \frac{\sum_k c_k \left[P(A_i \cap A_k) - \tilde{\delta}\right]}{c_i \left[P(A_i) - \tilde{\delta}\right]}$. □

Remark 15 (**$\boldsymbol{\ell}_{\textbf{NEW-4}}(\boldsymbol{c})$ v.s. $\boldsymbol{\ell}_{\textbf{NEW-3}}(\boldsymbol{c})$**). *Note that $\ell_{NEW\text{-}3}(\boldsymbol{c}) = \sum_{i=1}^{N} \ell_i(\boldsymbol{c})$ where $\ell_i(\boldsymbol{c})$ is the solution of (4.34). The optimal variable $p_{\{1,\ldots,N\}}$ in (4.34) is not required to be the same for each $\ell_i(\boldsymbol{c}), i = 1, \ldots, N$. The lower bound $\ell_{NEW\text{-}4}(\boldsymbol{c})$, however, is the solution of the same problem as for $\ell_{NEW\text{-}3}(\boldsymbol{c})$ with the additional constraint that the optimal variable $p_{\{1,\ldots,N\}}$ in (4.34) has the same value for each $\ell_i(\boldsymbol{c}), i = 1, \ldots, N$. Therefore, if $\mathbf{c} \in \mathbb{R}_+^N$, $\ell_{NEW\text{-}3}(\boldsymbol{c})$ is the solution of a relaxed problem to the problem for obtaining $\ell_{NEW\text{-}4}(\boldsymbol{c})$; thus $\ell_{NEW\text{-}4}(\boldsymbol{c}) \geq \ell_{NEW\text{-}3}(\boldsymbol{c})$. Also, since $\mathbf{c} \in \mathbb{R}_+^N$, the solution of (4.55) can be computed in pseudo-polynomial time and has a polynomial-time approximation algorithm.*

Remark 16 (**Improved class of upper bounds $\hbar_{\textbf{NEW-5}}(\boldsymbol{c})$**). *We can improve the upper bound $\hbar_{NEW\text{-}4}$ in (4.46) by letting $x = p_{\{1,\ldots,N\}}$. Defining $\mathscr{B}^- = \mathscr{B} \setminus \{1, \ldots, N\}$, then*

$$\hbar'(\boldsymbol{c}) = \max_x \left[x + \sum_{i=1}^{N} \hbar_i'(\boldsymbol{c}, x) \right], \tag{4.61}$$

where $\hbar_i'(\boldsymbol{c}, x)$ *is defined by*

$$
\begin{aligned}
\hbar_i'(\boldsymbol{c}, x) := \max_{\{p_B : i \in B, B \in \mathscr{B}^-} & \sum_{B : i \in B, B \in \mathscr{B}^-} \frac{c_i p_B}{\sum_{k \in B} c_k} \\
s.t. \quad & \sum_{B : i \in B, B \in \mathscr{B}^-} p_B = P(A_i) - x, \\
& \sum_{B : i \in B, B \in \mathscr{B}^-} \left(\frac{\sum_{k \in B} c_k}{c_i} \right) p_B = \frac{1}{c_i} \sum_k c_k \left[P(A_i \cap A_k) - x \right], \\
& p_B \geq 0, \quad \textit{for all} \quad B \in \mathscr{B}^- \quad \textit{such that} \quad i \in B.
\end{aligned}
\tag{4.62}
$$

The solution of $\hbar_i'(\boldsymbol{c}, x)$ *is independent with* x*:*

$$
\begin{aligned}
\hbar_i'(\boldsymbol{c}, x) &= (P(A_i) - x) \left(\frac{c_i}{\min_k c_k} + \frac{c_i}{\sum_k c_k - \min_k c_k} \right) \\
&\quad - \frac{c_i}{(\min_k c_k)(\sum_k c_k - \min_k c_k)} \sum_k c_k \left(P(A_i \cap A_k) - x \right), \\
&= P(A_i) \left(\frac{c_i}{\min_k c_k} + \frac{c_i}{\sum_k c_k - \min_k c_k} \right) \\
&\quad - \frac{c_i}{(\min_k c_k)(\sum_k c_k - \min_k c_k)} \sum_k c_k P(A_i \cap A_k),
\end{aligned}
\tag{4.63}
$$

and the solution exists if and only if for all i

$$
\min_k c_k \leq \frac{\sum_k c_k P(A_i \cap A_k) - (\sum_k c_k) x}{P(A_i) - x} \leq \sum_k c_k - \min_k c_k. \tag{4.64}
$$

Thus, we get

$$\begin{aligned}&\left\{\max_i \frac{\sum_k c_k P(A_i \cap A_k) - \left(\sum_k c_k - \min_k c_k\right) P(A_i)}{\min_k c_k}\right\}^+ \\ &\le x \le \min_i \frac{\sum_k c_k P(A_i \cap A_k) - (\min_k c_k) P(A_i)}{\sum_k c_k - \min_k c_k}\end{aligned} \tag{4.65}$$

Therefore, we get the upper bound

$$\begin{aligned}P\left(\bigcup_i A_i\right) &\le \min_i \left\{\frac{\sum_k c_k P(A_i \cap A_k) - (\min_k c_k) P(A_i)}{\sum_k c_k - \min_k c_k}\right\} \\ &+ \left(\frac{1}{\min_k c_k} + \frac{1}{\sum_k c_k - \min_k c_k}\right) \sum_i c_i P(A_i) \\ &- \frac{1}{(\min_k c_k)(\sum_k c_k - \min_k c_k)} \sum_i \sum_k c_i c_k P(A_i \cap A_k), \\ &=: \hbar_{NEW\text{-}5}(\boldsymbol{c}).\end{aligned} \tag{4.66}$$

Clearly, the upper bound $\hbar_{NEW\text{-}5}(\boldsymbol{c})$ in (4.66) is always sharper than $\hbar_{NEW\text{-}4}$ in (4.46), however, it is conjectured to be always looser than $\hbar_{NEW\text{-}3}$ in (3.20).

4.2 Numerical Examples

In the numerical examples, $\tilde{\boldsymbol{c}}$ is obtained by the GK bound; the elements of $\tilde{\boldsymbol{c}}^+$ are given by $\{\tilde{c}_i^+ = \max(\tilde{c}_i, \epsilon), i = 1, \ldots, N\}$ where $\epsilon > 0$ is small enough so that if $\tilde{\boldsymbol{c}} \in \mathbb{R}_+^N$ then $\tilde{\boldsymbol{c}}^+ = \tilde{\boldsymbol{c}}$.

We present $\ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}})$, $\ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}}^+)$, $\ell_{\text{NEW-4}}(\tilde{\boldsymbol{c}}^+)$ and $\max_\kappa \ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}}+\kappa\mathbf{1})$ in Table 4.1. In three examples (Systems II, III and VIII), $\tilde{\boldsymbol{c}} \in \mathbb{R}_+^N$; therefore $\ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}}) = \ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}}^+)$. In two examples (Systems VI and VII), $\ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}})$ gives a negative value so we ignore it and replace it by 0. The lower bound $\max_\kappa \ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}} + \kappa\mathbf{1})$ is done by searching κ

from -1 to 1 with a fixed step length 0.005 (so that 401 points are used in total). We also randomly generated 100,000 samples of $\boldsymbol{c} \in \mathbb{R}_+^N$ to compute $\ell_{\text{NEW-3}}(\boldsymbol{c})$ and $\ell_{\text{NEW-4}}(\boldsymbol{c})$ and the largest bounds were selected and denoted as $\ell_{\text{NEW-3}}(\boldsymbol{c}_{\text{Rand}}^+)$ and $\ell_{\text{NEW-4}}(\boldsymbol{c}_{\text{Rand}}^+)$.

From the results, one can see $\ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}}^+)$ is always sharper than $\ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}})$ and is sharper than ℓ_{GK} in most of the examples except for System VI. The line search $\max_\kappa \ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}} + \kappa\mathbf{1})$ is shaper than $\ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}}^+)$ in most of the examples except for System V. Since $\tilde{\boldsymbol{c}}^+ \in \mathbb{R}_+^N$, the class of lower bounds $\ell_{\text{NEW-4}}(\tilde{\boldsymbol{c}}^+)$ is always sharper than $\ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}}^+)$, as expected.

In Table 4.2, we compared $\ell_{\text{NEW-3}}(\boldsymbol{c})$ and $\ell_{\text{NEW-4}}(\boldsymbol{c})$ with randomly generated $\boldsymbol{c} \in \mathbb{R}_+^N$. One can see that in System VI, the maximum $\ell_{\text{NEW-4}}(\boldsymbol{c})$ is 0.3203 which is sharper than the maximum $\ell_{\text{NEW-3}}(\boldsymbol{c})$ which is 0.3022. Also, the percentage for $\ell_{\text{NEW-4}}(\boldsymbol{c})$ is strictly larger than $\ell_{\text{NEW-3}}(\boldsymbol{c})$ and the average of $\frac{\ell_{\text{NEW-4}}(\boldsymbol{c})}{\ell_{\text{NEW-3}}(\boldsymbol{c})}$ are shown in Table 4.2.

4.3 Comments on the GK Bound

Finally, we conclude this chapter with two comments on the GK bound.

4.3.1 Applying the GK bound to subsets of events

We note that many existing lower bounds, which do not fully explore available information, can be further improved algorithmically via optimization over subsets, as in [2, 14]. However, in this section, we prove that the GK bound cannot be improved by applying it to subsets of $\{A_1, \dots, A_N\}$.

Table 4.1: Comparison of lower bounds (* indicates $\tilde{\boldsymbol{c}} \in \mathbb{R}_+^N$ and a bold number indicates exact agreement with the optimal lower bound (5.1) of exponential complexity in N.)

System	I	II*	III*	IV	V	VI	VII	VIII*
N	6	6	6	7	3	4	4	4
$P\left(\bigcup_{i=1}^N A_i\right)$	0.7890	0.6740	0.7890	0.9687	0.3900	0.3252	0.5346	0.5854
ℓ_{KAT}	0.7247	0.6227	0.7222	0.8909	0.3833	0.2769	0.4434	0.5412
ℓ_{GK}	0.7601	0.6510	0.7508	0.9231	0.3813	0.2972	0.4750	0.5390
$\ell_{\text{NEW-2}}$	0.7247	0.6227	0.7222	0.8909	**0.3900**	0.3205	0.4562	0.5464
$\ell_{\text{NEW-1}}$	0.7487	0.6398	0.7427	0.9044	**0.3900**	**0.3252**	**0.5090**	0.5531
$\ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}})$	0.6359	0.6517*	0.7512*	0.7908	0.3865	0	0	0.5412*
$\ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}}^+)$	0.7638	0.6517*	0.7512*	0.9231	**0.3900**	0.2951	0.4905	0.5412*
$\ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}} + \kappa\mathbf{1})$	0.7577	0.6539	0.7557	0.9235	0.3899	0.2993	0.4949	0.5412
$\ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}}^+_{\text{Rand}})$	0.7783	0.6633	0.7810	0.9501	**0.3900**	0.3022	0.4992	0.5666
$\ell_{\text{NEW-4}}(\tilde{\boldsymbol{c}}^+)$	0.7638	0.6517	0.7512	0.9231	**0.3900**	0.2951	0.4905	0.5412
$\ell_{\text{NEW-4}}(\tilde{\boldsymbol{c}}^+_{\text{Rand}})$	0.7783	0.6633	0.7810	0.9501	**0.3900**	0.3203	0.4992	0.5666

Table 4.2: Comparison of $\ell_{\text{NEW-3}}(\boldsymbol{c})$ and $\ell_{\text{NEW-4}}(\boldsymbol{c})$ with randomly generated $\boldsymbol{c} \in \mathbb{R}_+^N$ (a bold number indicates coincidence with optimal lower bound (5.1) of exponential complexity in N).

System	V	VI	VII	VIII*
N	3	4	4	4
$P\left(\bigcup_{i=1}^N A_i\right)$	0.3900	0.3252	0.5346	0.5854
$\max \ell_{\text{NEW-3}}(\boldsymbol{c})$	**0.3900**	0.3022	0.4992	0.5666
$\max \ell_{\text{NEW-4}}(\boldsymbol{c})$	**0.3900**	0.3203	0.4992	0.5666
Average $\frac{\ell_{\text{NEW-4}}(\boldsymbol{c})}{\ell_{\text{NEW-3}}(\boldsymbol{c})}$	1.0011	1.065	1.0006	1.0000
Percentage $\ell_{\text{NEW-4}}(\boldsymbol{c}) > \ell_{\text{NEW-3}}(\boldsymbol{c})$	7.82 %	69.6%	3.87%	0.54 %

Lemma 9. *For any given $M \geq N$, the GK bound is the solution of the following problem:*

$$\begin{aligned} &\min_{\{\boldsymbol{x} \in \mathbb{R}^{M\times 1}, \boldsymbol{A} \in \mathbb{R}^{N\times M}\}} \|\boldsymbol{x}\|^2 \\ &s.t. \quad \boldsymbol{A}\boldsymbol{x} = \boldsymbol{\alpha}, \quad \boldsymbol{A}\boldsymbol{A}^T = \boldsymbol{\Sigma} \in \mathbb{R}^{N\times N}. \end{aligned} \tag{4.67}$$

Proof. We can always write $\boldsymbol{x}$ as

$$\boldsymbol{x} = \boldsymbol{A}^T\boldsymbol{k}_1 + \boldsymbol{A}_\perp^T\boldsymbol{k}_2, \tag{4.68}$$

where $\boldsymbol{k}_1 \in \mathbb{R}^{N\times 1}$, $\boldsymbol{k}_2 \in \mathbb{R}^{(M-N)\times 1}$, and $\boldsymbol{A}_\perp \in \mathbb{R}^{(M-N)\times M}$ satisfies $\boldsymbol{A}\boldsymbol{A}_\perp^T = \boldsymbol{0}_{N\times(M-N)}$. Particularly, let $\boldsymbol{L}\boldsymbol{L}^T$ be the Cholesky decomposition of $\boldsymbol{\Sigma}$, then $\boldsymbol{A} = \left(\boldsymbol{L}, \boldsymbol{0}_{N\times(M-N)}\right)\boldsymbol{Q}$ where $\boldsymbol{Q}$ is any orthogonal matrix is the solution of (4.67).

Then

$$\|\boldsymbol{x}\|^2 = \boldsymbol{k}_1^T\boldsymbol{A}\boldsymbol{A}^T\boldsymbol{k}_1 + \boldsymbol{k}_2^T\boldsymbol{A}_\perp\boldsymbol{A}_\perp^T\boldsymbol{k}_2 = \boldsymbol{k}_1^T\boldsymbol{\Sigma}\boldsymbol{k}_1 + \boldsymbol{k}_2^T\boldsymbol{A}_\perp\boldsymbol{A}_\perp^T\boldsymbol{k}_2. \tag{4.69}$$

The first constraint $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{\alpha}$ implies $\boldsymbol{A}\boldsymbol{A}^T\boldsymbol{k}_1 = \boldsymbol{\alpha}$, i.e., $\boldsymbol{k}_1 = \boldsymbol{\Sigma}^{-1}\boldsymbol{\alpha}$. Therefore, the minimum of $\|\boldsymbol{x}\|^2$ is achieved at $\boldsymbol{k}_2 = \boldsymbol{0}$, so that

$$\min_{\boldsymbol{k}_1,\boldsymbol{k}_2} \|\boldsymbol{x}\|^2 = \boldsymbol{k}_1^T\boldsymbol{\Sigma}\boldsymbol{k}_1 = \boldsymbol{\alpha}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\alpha}. \tag{4.70}$$

□

Theorem 6. *The GK bound cannot be improved via optimization over subsets of* $\{A_1, A_2, \ldots, A_N\}$.

Proof. Denoting $\boldsymbol{A} = \begin{pmatrix} \boldsymbol{a}_1^T \\ \boldsymbol{a}_2^T \\ \vdots \\ \boldsymbol{a}_N^T \end{pmatrix}$, the first constraint of (4.67) is equivalent to N constraints $\boldsymbol{a}_i^T\boldsymbol{x} = \alpha_i, i = 1, \ldots, N$, and the second constraint of (4.67) is equivalent to N^2 constraints $\boldsymbol{a}_i^T\boldsymbol{a}_j = \boldsymbol{\Sigma}_{ij}, i = 1, \ldots, N, j = 1, \ldots, N$.

By selecting a subset of $\{1, 2, \ldots, N\}$, the resulting GK bound is the solution of a relaxed problem of (4.67) with a subset of constraints on $\boldsymbol{x}$ and $\boldsymbol{a}_i, i = 1, \ldots, N$. Since the objective value of the relaxed problem must be no more than the original problem (4.67), the GK bound using a subset cannot be higher than the GK bound using full information. $\square$

4.3.2 Iterative implementation of the GK bound

Theorem 7. *The GK bound can be computed iteratively. More specifically, for* $n = 1, \ldots, N$, *denote* $\ell_{GK}(n)$ *as the GK bound using the information of* $A_1, \ldots, A_n : \boldsymbol{\alpha}_n = (P(A_1), \ldots, P(A_n))^T$, $\boldsymbol{\beta}_n = (P(A_1 \cap A_n), \ldots, P(A_{n-1} \cap A_n))^T$ *and* $\boldsymbol{\Sigma}_n$, *the* $n \times n$ *upper left sub-matrix of* $\boldsymbol{\Sigma}$, *then if* $\alpha_n - \boldsymbol{\beta}_n^H \boldsymbol{\Sigma}_{n-1}^{-1} \boldsymbol{\beta}_n > 0$, *we have*

$$\ell_{GK}(n) = \ell_{GK}(n-1) + \frac{1}{\alpha_n - \boldsymbol{\beta}_n^H \boldsymbol{\Sigma}_{n-1}^{-1} \boldsymbol{\beta}_n} \boldsymbol{\alpha}_n^T \begin{pmatrix} \boldsymbol{b}_n \boldsymbol{b}_n^T & \boldsymbol{b}_n \\ \boldsymbol{b}_n^T & 1 \end{pmatrix} \boldsymbol{\alpha}_n, \tag{4.71}$$

where $\boldsymbol{b}_n = -\boldsymbol{\Sigma}_{n-1}^{-1} \boldsymbol{\beta}_n$.

The matrix $\boldsymbol{\Sigma}_n$ *is not invertible if and only if* $\alpha_n - \boldsymbol{\beta}_n^H \boldsymbol{\Sigma}_{n-1}^{-1} \boldsymbol{\beta}_n = 0$. *The last case* $\alpha_n - \boldsymbol{\beta}_n^H \boldsymbol{\Sigma}_{n-1}^{-1} \boldsymbol{\beta}_n < 0$ *never happens, i.e., the following inequality holds*

$$\begin{aligned} P(A_n) \geq\, & (P(A_1 \cap A_n), \ldots, P(A_{n-1} \cap A_n)) \cdot \\ & \begin{pmatrix} P(A_1 \cap A_1) & \ldots & P(A_1 \cap A_{n-1}) \\ P(A_2 \cap A_1) & \ldots & P(A_2 \cap A_{n-1}) \\ \vdots & \ldots & \vdots \\ P(A_{n-1} \cap A_1) & \ldots & P(A_N \cap A_{n-1}) \end{pmatrix}^{-1} \begin{pmatrix} P(A_1 \cap A_n) \\ P(A_2 \cap A_n) \\ \vdots \\ P(A_{n-1} \cap A_n) \end{pmatrix}, \end{aligned} \tag{4.72}$$

for $n = 1, \ldots, N$.

Proof. Note that

$$\mathbf{\Sigma}_n = \begin{pmatrix} \mathbf{\Sigma}_{n-1} & \boldsymbol{\beta}_n \\ \boldsymbol{\beta}_n^T & \alpha_n \end{pmatrix}. \tag{4.73}$$

and by the matrix inverse lemma for a Hermitian matrix [16], we have

$$\mathbf{\Sigma}_n^{-1} = \begin{pmatrix} \mathbf{\Sigma}_{n-1}^{-1} & \mathbf{0}_n \\ \mathbf{0}_n^T & 0 \end{pmatrix} + \frac{1}{\alpha_n - \boldsymbol{\beta}_n^H \mathbf{\Sigma}_{n-1}^{-1} \boldsymbol{\beta}_n} \begin{pmatrix} \boldsymbol{b}_n \boldsymbol{b}_n^T & \boldsymbol{b}_n \\ \boldsymbol{b}_n^T & 1 \end{pmatrix} \tag{4.74}$$

Substituting to $\ell_{\mathrm{GK}}(n) = \boldsymbol{\alpha}_n \mathbf{\Sigma}_n^{-1} \boldsymbol{\alpha}_n$, $\ell_{\mathrm{GK}}(n)$ can be computed using $\ell_{\mathrm{GK}}(n-1)$.

Since we have proved $\ell_{\mathrm{GK}}(n) \geq \ell_{\mathrm{GK}}(n-1)$ in Theorem 6, the inequality is directly from $\alpha_n - \boldsymbol{\beta}_n^H \mathbf{\Sigma}_{n-1}^{-1} \boldsymbol{\beta}_n \geq 0$ in (4.71) of Theorem 7. $\square$

Chapter 5

New Bounds using $\{P(A_i)\}$ and $\{P(A_i \cap A_j)\}$

We derive new numerical lower/upper bounds of $P\left(\bigcup_{i=1}^{N} A_i\right)$ using $\{P(A_i)\}$ and $\{P(A_i \cap A_j)\}$ by solving a linear programming problem with $\frac{(N-1)^3+N+3}{2}$ variables, which coincide with the optimal lower/upper bounds when $N \leq 7$. The new numerical lower/upper bounds are guaranteed to be sharper than $\ell_{\text{NEW-1}}$, which is the optimal lower bound using $\{P(A_i)\}$ and $\{\sum_j P(A_i \cap A_j)\}$.

We also derive the generalized version of the KAT bound [19] when $\{P(A_i)\}$ and $\{\sum_j c_{ij} P(A_i \cap A_j)\}$ are used for any given parameter set $\{c_{ij}\}$. Then we show that the generalized KAT bound is upper bounded by the KAT bound. Similarly, the generalized version of $\ell_{\text{NEW-2}}$ using $\{P(A_i)\}$ and $\{\sum_j c_{ij} P(A_i \cap A_j)\}$ can also be derived, which is also upper bounded by $\ell_{\text{NEW-2}}$.

5.1 New Numerical Lower/Upper Bounds

5.1.1 A Relaxed Problem of the optimal LP

As in Chapter 4, we consider a finite probability space for simplicity, and denote by $\mathscr{B}$ as the collection of all non-empty subsets of $\{1, 2, \ldots, N\}$, and ω_B as the outcome that belongs to $\{A_i, i \in B\}$ and not to $\{A_i, i \notin B\}$. Let p_B stand for $p(\omega_B)$, for $B \in \mathscr{B}$. Consider p_B as variables; then the following (exhaustive) LP problem with 2^N number of variables gives the optimal lower/upper bound established using $\{P(A_i)\}$ and $\{P(A_i \cap A_j)\}$:

$$\begin{aligned} \min_{\{p_B, B\in\mathscr{B}\}} / \max_{\{p_B, B\in\mathscr{B}\}} & \sum_{B\in\mathscr{B}} p_B, \\ \text{s.t.} \quad & \sum_{i,j\in B, B\in\mathscr{B}} p_B = P(A_i \cap A_j), \quad i,j \in \{1,\ldots,N\}, \\ & p_B \geq 0, B \in \mathscr{B}. \end{aligned} \tag{5.1}$$

The optimality of (5.1) can be easily proved by showing its achievability: for each p_B, construct an outcome ω_B such that $p(\omega_B) = p_B$ and let $\omega_B \in A_i, \forall i \in B$. However, the computational complexity of the optimal lower bound (5.1) is exponential.

Now we consider relaxed versions of (5.1). Assume integer $M < N$ and define 2^M functions $f_1(i_1, \ldots, i_M, k)$ to $f_{2^M}(i_1, \ldots, i_M, k)$ for $i_1, i_2, \ldots, i_M, k \in \{1, 2, \ldots, N\}$ as follows

$$\begin{aligned} f_1(i_1,\ldots,i_M,k) &= \sum_{B: i_1,\ldots,i_M \in B, |B|=k} p_B, \\ f_2(i_1,\ldots,i_M,k) &= \sum_{B: i_1,\ldots,i_{M-1} \in B, i_M \notin B, |B|=k} p_B, \\ &\vdots \\ f_{2^M}(i_1,\ldots,i_M,k) &= \sum_{B: i_1,\ldots,i_M \notin B, |B|=k} p_B. \end{aligned} \tag{5.2}$$

That is, for all outcomes that have degree k (i.e., for all $B \in \mathscr{B}$ that $|B| = k$), the functions $f_1(i_1, \ldots, i_M, k)$ to $f_{2^M}(i_1, \ldots, i_M, k)$ divide $\sum_{B\in\mathscr{B}:|B|=k} p_B$ into 2^M groups, each corresponding to a subset of $\{i_1, \ldots, i_M\}$ that B contains (i.e., the outcomes are in a subset of $\{A_{i_1}, A_{i_2}, \ldots, A_{i_M}\}$).

Now we replace the constraints $p_B \geq 0, \forall B \in \mathscr{B}$ in (5.1) by $f_m(i_1, \ldots, i_M, k) \geq 0, m = 1, \ldots, 2^M$ to formulate the following relaxed LP problem.

$$\begin{aligned} \min_{\{p_B, B\in\mathscr{B}\}} / \max_{\{p_B, B\in\mathscr{B}\}} & \sum_{B\in\mathscr{B}} p_B, \\ \text{s.t.} \quad & \sum_{i,j\in B, B\in\mathscr{B}} p_B = P(A_i \cap A_j), \quad i,j \in \{1,\ldots,N\}, \\ & f_m(i_1,\ldots,i_M,k) \geq 0, \quad \forall m \in \{1,\ldots,2^M\}, \\ & \forall i_1,\ldots,i_M,k \in \{1,\ldots,N\}. \end{aligned} \tag{5.3}$$

Clearly, (5.3) is a relaxed problem of (5.1) since all the constraints of (5.3) must be satisfied if $p_B \geq 0, \forall B \in \mathscr{B}$. Thus, the optimal value of (5.3) is a lower/upper bound of $P\left(\bigcup_{i=1}^N A_i\right)$.

Lemma 10. *The solution of problem (5.3) coincides with the optimal lower/upper bound by (5.1) when $N \leq 2M+1$.*

Proof. Since (5.3) is a relaxed problem of (5.1), we just need to show that the constraints of (5.3) reduce to $p_B \geq 0, \forall B \in \mathscr{B}$ when $N \leq 2M+1$.

Note that when $1 \leq k \leq M$, there exists one function $f_m(i_1, \ldots, i_M, k)$ that is defined as $\sum_{B\in\mathscr{B}, i_1,\ldots,i_k\in B, i_{k+1},\ldots,i_M\notin B, |B|=k} p_B$. For simplicity, let $f_{m'}$ be such function, i.e.,

$$f_{m'}(i_1,\ldots,i_M,k) = \sum_{B\in\mathscr{B}, i_1,\ldots,i_k\in B, i_{k+1},\ldots,i_M\notin B, |B|=k} p_B. \tag{5.4}$$

Then the constraint

$$f_{m'}(i_1,\ldots,i_M,k) \geq 0 \tag{5.5}$$

reduces to

$$p_{\{i_1,\ldots,i_k\}} \geq 0, \tag{5.6}$$

which is equivalent to $p_B \geq 0, \forall |B| = k$ since $i_1, \ldots, i_k \in \{1, \ldots, N\}$.

Similarly, when $N-M \leq k \leq N$, there exists one function $f_{m''}(i_1, \ldots, i_M, k)$ given by

$$f_{m''}(i_1, \ldots, i_M, k) = \sum_{B \in \mathscr{B}, i_1, \cdots, i_{N-k} \notin B, i_{N-k+1}, \ldots, i_M \in B, |B|=k} p_B. \tag{5.7}$$

Then the constraint

$$f_{m''}(i_1, \ldots, i_M, k) \geq 0 \tag{5.8}$$

reduces to

$$p_{B''} \geq 0, \tag{5.9}$$

where $B'' = \{1, \ldots, N\} \backslash \{i_1, \ldots, i_{N-k}\}$. Note that this is equivalent to $p_B \geq 0, \forall |B| = k$ since $i_1, \ldots, i_{N-k} \in \{1, \ldots, N\}$.

Finally, if $M \geq (N-M) - 1$, the union of $\{1, \ldots, M\}$ and $\{N-M, \ldots, N\}$ is $\{1, \ldots, N\}$ and so all possible values of k are included. Therefore, all the constraints in $p_B \geq 0, B \in \mathscr{B}$ can be obtained by requiring $f_m(i_1, \ldots, i_M, k) \geq 0, m = 1, \ldots, 2^M$. Thus, the problem (5.1) is equivalent to (5.3). □

5.1.2 A Case Study for $M = 3$

In the rest of this chapter, we focus on a particular case with $M = 3$. We show that when $M = 3$, problem (5.3) can be solved by an LP problem with $\frac{(N-1)^3+N+3}{2}$ variables. Note that problem (5.3) has an exponential number of variables $\{p_B, B \in \mathscr{B}\}$. In this subsection, we show that problem (5.3) shares the same solution as a relaxed problem which still has exponential number of variables when $M = 3$. In the next subsection, we show that the later relaxed problem can be solved by an LP problem with $\frac{(N-1)^3+N+3}{2}$ variables.

Defining $2^M = 8$ functions, $f_1, \ldots, f_8$, by the following:

$$
\begin{aligned}
f_1(i,j,l,k) &= \sum_{B: i,j,l \in B, |B|=k} p_B, \\
f_2(i,j,l,k) &= \sum_{B: i,j \in B, l \notin B, |B|=k} p_B, \\
f_3(i,j,l,k) &= \sum_{B: i,l \in B, j \notin B, |B|=k} p_B, \\
f_4(i,j,l,k) &= \sum_{B: j,l \in B, i \notin B, |B|=k} p_B, \\
f_5(i,j,l,k) &= \sum_{B: i \in B, j,l \notin B, |B|=k} p_B, \\
f_6(i,j,l,k) &= \sum_{B: j \in B, i,l \notin B, |B|=k} p_B, \\
f_7(i,j,l,k) &= \sum_{B: l \in B, i,j \notin B, |B|=k} p_B, \\
f_8(i,j,l,k) &= \sum_{B: i,j,l \notin B, |B|=k} p_B,
\end{aligned}
\tag{5.10}
$$

the problem (5.3) becomes

$$
\begin{aligned}
&\min_{\{p_B, B \in \mathscr{B}\}} \Big/ \max_{\{p_B, B \in \mathscr{B}\}} \sum_{B \in \mathscr{B}} p_B, \\
&\qquad \text{s.t.} \quad \sum_{i,j \in B, B \in \mathscr{B}} p_B = P(A_i \cap A_j), \quad i,j \in \{1,\ldots,N\}, \\
&\qquad\qquad f_m(i,j,l,k) \geq 0, \quad m \in \{1,\ldots,8\}, \quad i,j,l,k \in \{1,\ldots,N\}.
\end{aligned}
\tag{5.11}
$$

Now, we consider a relaxed version of (5.11) as follows:

$$
\begin{aligned}
&\min_{\{p_B, B\in\mathscr{B}\}} / \max_{\{p_B, B\in\mathscr{B}\}} \sum_{B\in\mathscr{B}} p_B, \\
&\qquad \text{s.t.} \qquad \sum_{i,j\in B, B\in\mathscr{B}} p_B = P(A_i\cap A_j), \quad i,j\in\{1,\dots,N\}, \\
&\qquad\qquad\qquad \begin{pmatrix}
1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 1 & 0
\end{pmatrix}
\begin{pmatrix}
f_1(i,j,l,k) \\ f_2(i,j,l,k) \\ f_3(i,j,l,k) \\ f_4(i,j,l,k) \\ f_5(i,j,l,k) \\ f_6(i,j,l,k) \\ f_7(i,j,l,k) \\ f_8(i,j,l,k)
\end{pmatrix} \geq \mathbf{0}, \\
&\qquad\qquad\qquad \forall i,j,l,k\in\{1,\dots,N\}.
\end{aligned}
\tag{5.12}
$$

Clearly, (5.12) is a relaxed version of (5.11) and therefore a relaxed version of (5.1). In the following lemma, we prove that (5.12) and (5.11) give the same solution, i.e., the lower/upper bounds obtained by solving the two problems are identical.

Lemma 11. *The optimal feasible point of (5.11) is also optimal in (5.12).*

Proof. In order to show the optimal feasible point of (5.11) is also optimal in (5.12), it suffices to show for any feasible point of (5.12), we are able to find a feasible point of (5.11) that gives the same value of the objective function. That is, for any $\{p_B, B \in \mathscr{B}\}$ that satisfies the constraint of (5.12), there exists a feasible point of (5.11), $\{p'_B, B \in \mathscr{B}\}$, that satisfies $f_m(i,j,l,k) \geq 0, i,j,l,k \in \{1,\ldots,M\}, m \in \{1,\ldots,8\}$ as well as $\sum_{B\in\mathscr{B}} p'_B = \sum_{B\in\mathscr{B}} p_B$.

We consider different values of k. According to the proof of Lemma 10, it is direct to verify for $k \in \{1,2,3,N-3,N-2,N-1,N\}$ the constraints of (5.12) are equivalent to $p_B \geq 0, |B| = k$. Therefore, if $\{p_B, |B| \in \{1,2,3,N-3,N-2,N-1,N\}\}$ come from a feasible point of (5.12), they also satisfy the constraints in (5.11).

Next, we only consider the case $4 \leq k \leq N-4$. Suppose $k = \tilde{k}$ is given such that $4 \leq \tilde{k} \leq N-4$, and there are variables $\{p_B, |B| = \tilde{k}\}$ which are from a feasible point of (5.12). If $\{p_B, |B| = \tilde{k}\}$ also satisfy the constraints on $f_1,\ldots,f_8$ for $k = \tilde{k}$ in (5.11), we simply let $p'_B = p_B, |B| = \tilde{k}$. On the other hand, if $\{p_B, |B| = \tilde{k}\}$ do not satisfy the constraints on $f_1,\ldots,f_8$ in (5.11) for $k = \tilde{k}$ then there are integers $\tilde{i},\tilde{j},\tilde{l}$ that $f_m(\tilde{i},\tilde{j},\tilde{l},\tilde{k}) < 0$ hold for at least one $m \in \{1,\ldots,8\}$.

Note that the matrix in the last constraint of (5.12) does not have full rank, for any value τ: vector $(\tau,-\tau,-\tau,-\tau,\tau,\tau,\tau,-\tau)^T$ lies in the null space of the matrix in the constraint. Therefore, it is possible to introduce a particular transformation on the values of $\{p_B\}$ such that after the transformation, the value of the objective function of (5.12) is not changed and the equality constraints in (5.12) are still satisfied. The only terms that have changed are the values of $f_m(\tilde{i},\tilde{j},\tilde{l},\tilde{k})$ for a particular $(\tilde{i},\tilde{j},\tilde{l},\tilde{k})$.

We define the transformation in the following.

For given $\tilde{i}, \tilde{j}, \tilde{l}$, we first pick one B_1 such that $|B_1| = \tilde{k}$ and $\tilde{i}, \tilde{j}, \tilde{l} \in B_1$. Since $\tilde{k} \leq N-4$, there exists $\hat{i}, \hat{j}, \hat{l} \notin B_1$. We replace some of $\tilde{i}, \tilde{j}, \tilde{l}$ by some of $\hat{i}, \hat{j}, \hat{l}$, respectively, to get $B_2, \ldots, B_8$ as follows (the notation $\ldots$ denotes other integers in the subset that are remain the same):

$$\begin{aligned}
B_1 &= \{\tilde{i}, \tilde{j}, \tilde{l}, \ldots\} \\
B_2 &= \{\tilde{i}, \tilde{j}, \hat{l}, \ldots\} \\
B_3 &= \{\tilde{i}, \hat{j}, \tilde{l}, \ldots\} \\
B_4 &= \{\hat{i}, \tilde{j}, \tilde{l}, \ldots\} \\
B_5 &= \{\tilde{i}, \hat{j}, \hat{l}, \ldots\} \\
B_6 &= \{\hat{i}, \tilde{j}, \hat{l}, \ldots\} \\
B_7 &= \{\hat{i}, \hat{j}, \tilde{l}, \ldots\} \\
B_8 &= \{\hat{i}, \hat{j}, \hat{l}, \ldots\}
\end{aligned} \tag{5.13}$$

Let $\{p_B^{(0)}\}$ be the values of variables $\{p_B\}$ before transformation, and $\{p_B^{(1)}\}$ be the values of variables $\{p_B\}$ after the first transformation, we assign values to $p_{B_m}^{(1)}, m =$

$1, \ldots, 8$ as follows:

$$\begin{pmatrix} p_{B_1}^{(1)} \\ p_{B_2}^{(1)} \\ p_{B_3}^{(1)} \\ p_{B_4}^{(1)} \\ p_{B_5}^{(1)} \\ p_{B_6}^{(1)} \\ p_{B_7}^{(1)} \\ p_{B_8}^{(1)} \end{pmatrix} \Leftarrow \begin{pmatrix} p_{B_1}^{(0)} \\ p_{B_2}^{(0)} \\ p_{B_3}^{(0)} \\ p_{B_4}^{(0)} \\ p_{B_5}^{(0)} \\ p_{B_6}^{(0)} \\ p_{B_7}^{(0)} \\ p_{B_8}^{(0)} \end{pmatrix} + \begin{pmatrix} \tau \\ -\tau \\ -\tau \\ -\tau \\ \tau \\ \tau \\ \tau \\ -\tau \end{pmatrix}, \tag{5.14}$$

for any τ. For other $B \notin \{B_1, \ldots, B_8\}$, we simply set $p_B^{(1)} = p_B^{(0)}$.

Now it can be verified that if $\{p_B^{(0)}\}$ is a feasible point of (5.12), after the transformation the value of the objective function is not changed, i.e., $\sum_B p_B^{(0)} = \sum_B p_B^{(1)}$ and all the equality constraints in (5.12) are still satisfied. Also, the values of functions $f_m(i,j,l,k)$ are not changed if one of the elements of (i,j,l,k) is not equal to the corresponding elements of $(\tilde{i},\tilde{j},\tilde{l},\tilde{k})$. The only terms that were changed are

$$\begin{pmatrix} f_1^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}) \\ f_2^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}) \\ f_3^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}) \\ f_4^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}) \\ f_5^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}) \\ f_6^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}) \\ f_7^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}) \\ f_8^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}) \end{pmatrix} \Leftarrow \begin{pmatrix} f_1^{(0)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}) + \tau \\ f_2^{(0)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}) - \tau \\ f_3^{(0)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}) - \tau \\ f_4^{(0)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}) - \tau \\ f_5^{(0)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}) + \tau \\ f_6^{(0)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}) + \tau \\ f_7^{(0)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}) + \tau \\ f_8^{(0)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}) - \tau \end{pmatrix}, \tag{5.15}$$

where $f_m^{(0)}, m = 1, \ldots, 8$ denotes the value of function f_m before the transformation and $f_m^{(1)}, m = 1, \ldots, 8$ denotes the value of function f_m after the first transformation.

Note that $f_m^{(1)}$ still satisfies the last constraint in (5.12) for any value of τ. Therefore, $\{p_B^{(1)}\}$ is still a feasible point of (5.12) that shares the same value of the objective function with $\{p_B^{(0)}\}$.

Starting from a feasible point of (5.12), the transformation defined in (5.14) can be used to get another feasible point of (5.12) without changing the value of the objective function. Therefore, it suffices to show that for any optimal feasible point of (5.12), if there are integers $(\tilde{i}, \tilde{j}, \tilde{l}, \tilde{k})$ and the inequality $f_m^{(0)}(\tilde{i}, \tilde{j}, \tilde{l}, \tilde{k}) < 0$ holds for at least one $m \in \{1, \ldots, 8\}$, we are able to find another feasible point after t transformations such that

$$f_m^{(t)}(\tilde{i}, \tilde{j}, \tilde{l}, \tilde{k}) \geq 0, \quad m = 1, \ldots, 8. \tag{5.16}$$

We show that $t \leq 2$, i.e., at most two transformations are needed. The details are as follows.

1. Suppose $f_m^{(0)}(\tilde{i}, \tilde{j}, \tilde{l}, \tilde{k}) < 0$ holds for at least one $m \in \{1, \ldots, 8\}$. Defining

$$\tau_1 = \min\left\{ f_2^{(0)}(\tilde{i}, \tilde{j}, \tilde{l}, \tilde{k}), f_3^{(0)}(\tilde{i}, \tilde{j}, \tilde{l}, \tilde{k}), f_4^{(0)}(\tilde{i}, \tilde{j}, \tilde{l}, \tilde{k}) \right\}, \tag{5.17}$$

after the first transformation, according to (5.15), we have

$$\min\left\{ f_2^{(1)}(\tilde{i}, \tilde{j}, \tilde{l}, \tilde{k}), f_3^{(1)}(\tilde{i}, \tilde{j}, \tilde{l}, \tilde{k}), f_4^{(1)}(\tilde{i}, \tilde{j}, \tilde{l}, \tilde{k}) \right\} = 0. \tag{5.18}$$

Furthermore, by the first four rows of the matrix constraint in (5.12), one can get

$$f_1^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}) + \min\left\{f_2^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}), f_3^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}), f_4^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k})\right\} \geq 0, \qquad (5.19)$$

which is equivalent to $f_1^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}) \geq 0$.

Finally, by the last nine rows of the matrix constraint in (5.12), one can get

$$\begin{aligned} &\min\left\{f_5^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}), f_6^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}), f_7^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k})\right\} \\ &\quad + \min\left\{f_2^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}), f_3^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}), f_4^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k})\right\} \geq 0, \end{aligned} \qquad (5.20)$$

which means

$$\min\left\{f_5^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}), f_6^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}), f_7^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k})\right\} \geq 0. \qquad (5.21)$$

The only function left is $f_8^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k})$ since we only have

$$f_8^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}) + \min\left\{f_5^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}), f_6^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}), f_7^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k})\right\} \geq 0 \qquad (5.22)$$

after the first transformation. In case $f_8^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}) \geq 0$ after the first transformation, then we have already obtained a new feasible point of (5.12) that satisfies $f_m^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}) \geq 0$ for all m.

2. On the other hand, if $f_8^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}) < 0$ after the first transformation, let $\tau_2 = f_8^{(1)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k})$, then after the second transformation, according to (5.15), one can verify that $f_8^{(2)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}) = 0$ and all

$$f_m^{(2)}(\tilde{i},\tilde{j},\tilde{l},\tilde{k}) \geq 0, \quad m = 1, \ldots, 8, \qquad (5.23)$$

are satisfied.

□

Note that even though it results in the same solution as (5.11), the problem (5.12) still has an exponential number of variables. Next, we show that we can solve (5.12) by solving an LP problem with only $\frac{(N-1)^3+N+3}{2}$ variables.

5.1.3 New Numerical Bounds

In this subsection, we show that (5.12) can be solved by an LP problem with only $\frac{(N-1)^3+N+3}{2}$ variables. Define

$$a_{ij}(k) := P\left(\{x \in A_i \cap A_j, \deg(x) = k\}\right), \quad i, j, k \in \{1, \cdots, N\}. \tag{5.24}$$

Then the following properties directly hold for $a_{ij}(k)$:

$$a_{ij}(1) = P\left(\{x \in A_i \cap A_j, \deg(x) = 1\}\right) = 0, \quad \text{for all} \quad i \neq j, \tag{5.25}$$

$$a_{ij}(k) = a_{ji}(k) \tag{5.26}$$

and

$$a_{ii}(k) = P\left(\{x \in A_i \cap A_i, \deg(x) = k\}\right) = a_i(k). \tag{5.27}$$

Also, we have

$$\sum_{k=1}^{N} a_{ij}(k) = P(A_i \cap A_j). \tag{5.28}$$

Furthermore, we can write

$$\sum_{j=1}^{N} \frac{a_{ij}(k)}{k} = P\left(\{x \in A_i, \deg(x) = k\}\right) = a_i(k). \tag{5.29}$$

Substituting (5.29) into the expression of $P\left(\bigcup_{i=1}^{N} A_i\right)$ using $a_i(k)$, we directly obtain the following equalities

$$P(A_i) = \sum_{k=1}^{N} a_i(k) = \sum_{k=1}^{N}\left(\sum_{j=1}^{N} \frac{a_{ij}(k)}{k}\right), \tag{5.30}$$

and

$$P\left(\bigcup_i A_i\right) = \sum_{k=1}^{N}\sum_{i=1}^{N} \frac{a_i(k)}{k} = \sum_{k=1}^{N}\sum_{i=1}^{N} \frac{1}{k}\left(\sum_{j=1}^{N} \frac{a_{ij}(k)}{k}\right) = \sum_{k=1}^{N}\sum_{i=1}^{N}\sum_{j=1}^{N} \frac{a_{ij}(k)}{k^2}. \tag{5.31}$$

In the following, we show that one can formulate an LP problem with $\{a_{ij}(k)\}$ as variables that is equivalent to problem (5.12)

Theorem 8. *The solution (denoted by $\ell_{NEW\text{-}5}/\hbar_{NEW\text{-}6}$) of the following LP problem with N^3 variables is the same as the solution of (5.12), which gives a lower/upper* *bound for* $P\left(\bigcup_i A_i\right)$.

$$
\begin{aligned}
\ell_{NEW\text{-}5}/\hbar_{NEW\text{-}6} := \min_{\{a_{ij}(k)\}} / \max_{\{a_{ij}(k)\}} \quad & \sum_k \sum_i \sum_j \frac{a_{ij}(k)}{k^2} \\
s.t. \quad & \sum_k \sum_j \frac{a_{ij}(k)}{k} = P(A_i), \quad i = 1, \cdots, N, \\
& \sum_k a_{ij}(k) = P(A_i \cap A_j), \quad i = 1, \cdots, N, \quad j = 1, \cdots, N, \\
& a_{ij}(k) = a_{ji}(k), \quad i = 1, \cdots, N, \quad j = 1, \cdots, N, \quad k = 1, \cdots, N, \\
& \sum_{m=1}^{N} \frac{a_{im}(k)}{k} \geq a_{ij}(k), \quad i = 1, \cdots, N, \quad j = 1, \cdots, N, \quad k = 1, \cdots, N, \\
& \sum_m \sum_n \frac{a_{nm}(k)}{k^2} - \sum_m \frac{a_{im}(k)}{k} \geq \sum_n \frac{a_{nj}(k)}{k} - a_{ij}(k), \quad i, j, k = 1, \cdots, N, \\
& \sum_n \frac{a_{nl}(k)}{k} \geq a_{il}(k) + a_{jl}(k) - a_{ij}(k), \quad i, j, l, k = 1, \cdots, N, \\
& \sum_m \sum_n \frac{a_{nm}(k)}{k^2} + a_{ij}(k) + a_{il}(k) + a_{jl}(k) \geq \sum_m \frac{a_{im}(k) + a_{jm}(k) + a_{lm}(k)}{k}, \\
& \qquad i, j, l, k = 1, \cdots, N, \\
& a_{ij}(k) \geq 0, \quad i = 1, \cdots, N, \quad j = 1, \cdots, N, \quad k = 1, \cdots, N.
\end{aligned}
\tag{5.32}
$$

Furthermore, the number of variables of (5.32) can be reduced to $\frac{(N-1)^3+N+3}{2}$.

Proof. First, we show that problem (5.32) is equivalent to (5.12).

Noting that $a(k)$ and $a_i(k)$ can be written as linear functions of $a_{ij}(k)$. Also, from their definitions, $a(k)$, $a_i(k)$ and $a_{ij}(k)$ can be written as linear functions of

$\{p_B, B \in \mathscr{B}\}$:

$$
\begin{aligned}
a(k) &= \sum_{|B|=k} p_B, \\
a_i(k) &= \sum_{i\in B, |B|=k} p_B, \\
a_{ij}(k) &= \sum_{i,j\in B, |B|=k} p_B.
\end{aligned}
\tag{5.33}
$$

Since the objective function and the equality constraints in (5.12) can be easily written in terms of $a_{ij}(k)$, it suffices to show that the matrix constraint in (5.12) can also be written as constraints on $a_{ij}(k)$.

By symmetry, we only need to show that $f_1(i,j,l,k) + f_2(i,j,l,k)$, $f_3(i,j,l,k) + f_5(i,j,l,k)$, $f_7(i,j,l,k)+f_8(i,j,l,k)$, $f_2(i,j,l,k)+f_7(i,j,l,k)$ and $f_1(i,j,l,k)+f_8(i,j,l,k)$ can be expressed using $a_{ij}(k)$. Other rows of the matrix constraint in (5.12) can be directly obtained by changing the order of the indices (i,j,l). The details are in the following:

$$
\begin{aligned}
a_{ij}(k) &= \sum_{i,j\in B, |B|=k} p_B = f_1(i,j,l,k) + f_2(i,j,l,k), \\
a_i(k) - a_{ij}(k) &= \sum_{i\in B, j\notin B, |B|=k} p_B = f_3(i,j,l,k) + f_5(i,j,l,k),
\end{aligned}
\tag{5.34}
$$

$$
\begin{aligned}
&a(k) - a_i(k) - a_j(k) + a_{ij}(k) \\
&\quad = \sum_{i\notin B, |B|=k} p_B - \sum_{j\in B, i\notin B, |B|=k} p_B \\
&\quad = \sum_{i,j\notin B, |B|=k} p_B \\
&\quad = f_7(i,j,l,k) + f_8(i,j,l,k),
\end{aligned}
\tag{5.35}
$$

$$
\begin{aligned}
&a_l(k) + a_{ij}(k) - a_{il}(k) - a_{jl}(k) \\
&= \sum_{l \in B, |B|=k} p_B + \sum_{i,j \in B, |B|=k} p_B - \sum_{i,l \in B, |B|=k} p_B - \sum_{\{j,l\} \in B, |B|=k} p_B \\
&= \left(\sum_{\{l,i,j\} \in B, |B|=k} p_B + \sum_{i,j \in B, l \notin B, |B|=k} p_B + \sum_{\{l,j\} \in B, i \notin B, |B|=k} p_B + \sum_{i,j \notin B, l \in B, |B|=k} p_B \right) \\
&\quad + \left(\sum_{l,i,j \in B, |B|=k} p_B + \sum_{i,j \in B, l \notin B, |B|=k} p_B \right) \\
&\quad - \left(\sum_{l,i,j \in B, |B|=k} p_B + \sum_{l,i \in B, j \notin B, |B|=k} p_B \right) \\
&\quad - \left(\sum_{l,i,j \in B, |B|=k} p_B + \sum_{l,j \in B, i \notin B, |B|=k} p_B \right) \\
&\quad = \sum_{i,j \in B, l \notin B, |B|=k} p_B + \sum_{i,j \notin B, l \in B, |B|=k} p_B = f_2(i,j,l,k) + f_7(i,j,l,k),
\end{aligned}
\tag{5.36}
$$

$$
\begin{aligned}
&a(k) - a_l(k) - a_i(k) - a_j(k) + a_{ij}(k) + a_{il}(k) + a_{jl}(k) \\
&= [a_{ij}(k)] + [a(k) - a_i(k) - a_j(k) + a_{ij}(k)] - [a_l(k) + a_{ij}(k) - a_{il}(k) - a_{jl}(k)] \\
&= f_1(i,j,l,k) + f_2(i,j,l,k) + f_7(i,j,l,k) + f_8(i,j,l,k) - f_2(i,j,l,k) + f_7(i,j,l,k) \\
&= f_1(i,j,l,k) + f_8(i,j,l,k).
\end{aligned}
\tag{5.37}
$$

Therefore, the problem (5.32) with N^3 variables is equivalent to (5.12).

Next, we show the number of variables of (5.32) can be reduced to $\frac{(N-1)^3+N+3}{2}$. First, for $k = 1$, we can obtain $a_{ij}(1) = 0$ for $i \neq j$, which is previously given by (5.25), from the LP problem (5.32). This is because from the constraint $\sum_k a_{ij}(k) =$

$P(A_i \cap A_j)$ of (5.32), we have

$$\sum_k a_{ii}(k) = P(A_i), i = 1, \cdots, N, \tag{5.38}$$

by setting $j = i$. However, by another constraint, $\sum_{m=1}^{N} \frac{a_{im}(k)}{k} \geq a_{ij}(k)$ in (5.32), we have

$$P(A_i) = \sum_k a_{ii}(k) \leq \sum_k \sum_j \frac{a_{ij}(k)}{k} = P(A_i), \tag{5.39}$$

thus, we have

$$a_{ii}(k) = \sum_j \frac{a_{ij}(k)}{k}, \quad k = 1, \cdots, N. \tag{5.40}$$

Letting $k = 1$, we have

$$a_{ii}(1) = \sum_j a_{ij}(1) = a_{ii}(1) + \sum_{j \neq i} a_{ij}(1). \tag{5.41}$$

Since $a_{ij}(k) \geq 0$, the constraints (5.25) directly holds. Furthermore, we note that for $k = N$, the variables $a_{ij}(N)$ are equal and so they can be reduced to 1 variable. Finally, using the constraint $a_{ij}(k) = a_{ji}(k)$ in (5.32), we can further reduce the number of variables. In conclusion, the number of variables for different values of k are

$$\begin{cases} N & \text{if } k = 1 \\ \frac{N(N-1)}{2} & \text{if } k = 2, \ldots, N-1 \\ 1 & \text{if } k = N \end{cases} \tag{5.42}$$

Thus, the total number of variables is $N + \frac{N(N-1)(N-2)}{2} + 1$. $\square$

It can be readily shown that the new lower bound by (5.32) is sharper than the lower bounds $\ell_{\text{NEW-1}}$ and $\ell_{\text{NEW-2}}$ in Chapter 3 (see also [26, 27]).

Denoting the lower bound obtained by (5.32) as $\ell_{\text{NEW-5}}$, then we have the following lemma.

Lemma 12. *The lower bound $\ell_{\text{NEW-5}}$ obtained by (5.32) is no less than the lower bound $\ell_{\text{NEW-1}}$, which is optimal lower bound using $\{P(A_i)\}$ and $\{\sum_j P(A_i \cap A_j)\}$.*

Proof. For any feasible point of (5.32), defining variable $a_i(k)$ using (5.29), it can be readily verified that all the constraints in the LP problem formulated in (3.1) are satisfied. Therefore, the LP problem (3.1) can be seen as a relaxed version of (5.32). □

Lemma 13 (**Optimality of $\boldsymbol{\ell_{\text{NEW-5}}}$ for $\boldsymbol{N \leq 7}$**)**.** *The lower bound obtained by (5.32) is an optimal lower bound when $N \leq 7$.*

Proof. Since (5.32) shares the same solution with (5.11) which is (5.3) with $M = 3$. According to Lemma 10, the lower bound obtained by (5.32) is optimal when $N \leq 2M + 1 = 7$. □

5.2 Generalized KAT-type Lower Bounds

Note that both the existing KAT bound and the analytical bound $\ell_{\text{NEW-2}}$ (of Chapter 3) are established using $\{P(A_i)\}$ and $\{\sum_j P(A_i \cap A_j)\}$. Consider the general case that $\{P(A_i)\}$ and $\{\sum_j c_{ij} P(A_i \cap A_j)\}$ are available, for some given $\{c_{ij}\}$. In this case, neither the KAT bound nor $\ell_{\text{NEW-2}}$ can be computed. However, we could formulate a similar problem using the definition of $\{a_{ij}(k)\}$ which could lead to a KAT-type lower bound.

For example, we can solve the following relaxed problem of (5.32)

$$
\begin{aligned}
\min_{\{a_{ij}(k)\}} \quad & \sum_k \sum_i \sum_j \frac{a_{ij}(k)}{k^2} \\
\text{s.t.} \quad & \sum_k \sum_j \frac{a_{ij}(k)}{k} = P(A_i), \quad i = 1, \cdots, N, \\
& \sum_j c_{ij} \sum_k a_{ij}(k) = \sum_j c_{ij} P(A_i \cap A_j), \quad i = 1, \cdots, N, \\
& a_{ii}(k) = \sum_j \frac{a_{ij}(k)}{k}, \quad k = 1, \cdots, N, \\
& a_{ij}(k) \geq 0, \quad i = 1, \cdots, N, \quad j = 1, \cdots, N, \quad k = 1, \cdots, N,
\end{aligned}
\tag{5.43}
$$

the solution of which, $\ell_{\text{NEW-6}}$, satisfies

$$
P\left(\bigcup_i A_i\right) \geq \ell_{\text{NEW-6}} := \sum_i \ell_i, \tag{5.44}
$$

where ℓ_i is obtained by fixing i and solving the following subproblem for each $i = 1, \ldots, N$:

$$
\begin{aligned}
\ell_i := \min_{\{a_{ij}(k)\}} \quad & \sum_k \sum_j \frac{a_{ij}(k)}{k^2} \\
\text{s.t.} \quad & \sum_k \sum_j \frac{a_{ij}(k)}{k} = P(A_i), \\
& \sum_j \sum_k c_{ij} a_{ij}(k) = \sum_j c_{ij} P(A_i \cap A_j), \\
& a_{ii}(k) = \sum_j \frac{a_{ij}(k)}{k}, \quad k = 1, \cdots, N, \\
& a_{ij}(k) \geq 0, \quad j = 1, \cdots, N, \quad k = 1, \cdots, N.
\end{aligned}
\tag{5.45}
$$

The solution of ℓ_i in (5.45) is given by the minimum of two values. The first is

$$\min_{k\in\{2,\dots,N\}} \quad \alpha_i - \frac{1}{k}\frac{\beta_i}{c_{i\tilde{j}}} = \alpha_i \left\{ 1 - \frac{1}{k}\frac{1}{c_{i\tilde{j}}}\frac{\beta_i}{\alpha_i} \right\}, \tag{5.46}$$

where $\tilde{j}$ is a function of k:

$$\tilde{j} := \arg\min_j \left\{ c_{ij} \geq \frac{1}{k-1}\frac{\beta_i}{\alpha_i} \right\}, \tag{5.47}$$

and the second is

$$\min_{k_1,k_2\in\{2,\dots,N\}} \quad \alpha_i \left\{ \frac{k_2\left[\tilde{c}_{ij_2}(k_2-1) - \frac{\beta_i}{\alpha_i}\right] + k_1\left[\frac{\beta_i}{\alpha_i} - \tilde{c}_{ij_1}(k_1-1)\right]}{k_1k_2\left[\tilde{c}_{ij_2}(k_2-1) - \tilde{c}_{ij_2}(k_1-1)\right]} \right\}, \tag{5.48}$$

where

$$\tilde{c}_{ij_1} = \begin{cases} \arg\min_{c_{ij}} c_{ij} & \text{if } k_2 > k_1 \\ \arg\min_{c_{ij}} \left\{ \frac{\beta_i}{\alpha_i} - (k_1-1)c_{ij} \geq 0 \right\} & \text{if } k_2 < k_1 \end{cases} \tag{5.49}$$

and

$$\tilde{c}_{ij_2} = \begin{cases} \arg\min_{c_{ij}} \left\{ (k_2-1)c_{ij} - \frac{\beta_i}{\alpha_i} \geq 0 \right\} & \text{if } k_2 > k_1 \\ \arg\max_{c_{ij}} c_{ij} & \text{if } k_2 < k_1. \end{cases} \tag{5.50}$$

Therefore,

$$\ell_i = \min\{(5.46), (5.48)\}, \tag{5.51}$$

The details of solving (5.45) are given in Appendix C.1.

Remark 17. *When $c_{i1} = c_{i2} = \cdots = c_{iN}$ hold for all i, the generalized KAT lower bound $\ell_{NEW\text{-}6}$ reduces to the KAT bound.*

Unfortunately, we can show that $\ell_{\text{NEW-6}}$ is upper bounded by the KAT bound.

Lemma 14. *$\ell_{NEW\text{-}6} \le \ell_{KAT}$, where the equality holds if for any given i, the values of c_{ij} for all j are equal.*

Proof. The dual problem of (5.45) can be written as

$$\begin{aligned} \ell_i = \max_{q_1,q_2} \quad & q_1 P(A_i) + q_2 \sum_{j:j\neq i} c_{ij} P(A_i \cap A_j) \\ \text{s.t.} \quad & q_1 \le 1, \\ & \frac{1}{k} q_1 + c_{ij} q_2 \le \frac{1}{k(k-1)}, \quad k = 2, \ldots, N-1, \quad \forall j \neq i. \end{aligned} \tag{5.52}$$

An upper bound of ℓ_i is given by maximizing ℓ_i over all possible $\{c_{ij}\}$, i.e.

$$\begin{aligned} \ell_i \le \ell_i^U := \max_{q_1,q_2,\{c_{ij}\}} \quad & q_1 P(A_i) + q_2 \sum_{j:j\neq i} c_{ij} P(A_i \cap A_j) \\ \text{s.t.} \quad & q_1 \le 1, \\ & \frac{1}{k} q_1 + c_{ij} q_2 \le \frac{1}{k(k-1)}, \quad k = 2, \ldots, N-1, \quad \forall j \neq i. \end{aligned} \tag{5.53}$$

Denoting $\tilde{q}_{ij} := c_{ij} q_2$, the above problem becomes

$$\begin{aligned} \ell_i \le \ell_i^U = \max_{q_1,\{\tilde{q}_{ij}\}} \quad & q_1 P(A_i) + \sum_{j:j\neq i} \tilde{q}_{ij} P(A_i \cap A_j) \\ \text{s.t.} \quad & q_1 \le 1, \\ & \frac{1}{k} q_1 + \tilde{q}_{ij} \le \frac{1}{k(k-1)}, \quad k = 2, \ldots, N-1, \quad \forall j \neq i. \end{aligned} \tag{5.54}$$

Note that for any given q_1, the constraints for $\tilde{q}_{ij}$ are the same for any j, which are

$$\tilde{q}_{ij} \le \frac{1}{k(k-1)} - \frac{1}{k} q_1, \quad k = 2, \ldots, N-1, \quad \forall j \neq i, \tag{5.55}$$

and the objective function is monotone increasing function of $\tilde{q}_{ij}$ for any j. Therefore, the problem can be reduced to

$$\begin{aligned} \ell_i \le \ell_i^U = \max_{q_1} \quad & q_1 P(A_i) + \sum_{j:j\neq i} \left[\max_k \left(\frac{1}{k(k-1)} - \frac{1}{k} q_1 \right) \right] P(A_i \cap A_j) \\ \text{s.t.} \quad & q_1 \le 1, \end{aligned} \tag{5.56}$$

which is equivalent to $\tilde{q}_{ij}$ are equal for all j, i.e. using $P(A_i)$ and $\sum_{j\neq i} P(A_i \cap A_j)$. Therefore

$$\ell_{\text{NEW-6}} = \sum_i \ell_i \le \sum_i \ell_i^U = \ell_{\text{KAT}}. \tag{5.57}$$

□

Similarly, we can also consider generalization of the analytical bound $\ell_{\text{NEW-2}}$ to solve the following problem

$$\begin{aligned} \min_{\{a_{ij}(k)\}} \quad & \sum_k \sum_i \sum_j \frac{a_{ij}(k)}{k^2} \\ \text{s.t.} \quad & \sum_k \sum_j \frac{a_{ij}(k)}{k} = P(A_i), \quad i = 1, \cdots, N, \\ & \sum_j c_{ij} \sum_k a_{ij}(k) = \sum_j c_{ij} P(A_i \cap A_j), \quad i = 1, \cdots, N, \\ & \sum_{m=1}^N \frac{a_{im}(N)}{N} \ge a_{ij}(N), \quad i = 1, \cdots, N, \quad j = 1, \cdots, N, \\ & a_{ii}(k) = \sum_j \frac{a_{ij}(k)}{k}, \quad k = 1, \cdots, N, \\ & a_{ij}(k) \ge 0, \quad i = 1, \cdots, N, \quad j = 1, \cdots, N, \quad k = 1, \cdots, N, \end{aligned} \tag{5.58}$$

which can be rewritten as

$$\begin{aligned}
\min_{\{a_{ij}(k)\}} \quad & \sum_k \sum_i \sum_j \frac{a_{ij}(k)}{k^2} \\
\text{s.t.} \quad & \sum_k \sum_j \frac{a_{ij}(k)}{k} = P(A_i), \quad i = 1, \cdots, N, \\
& \sum_j \sum_k c_{ij} a_{ij}(k) = \sum_j c_{ij} P(A_i \cap A_j), \quad i = 1, \cdots, N, \\
& a_{11}(N) = a_{12}(N) = \cdots = a_{N1}(N) = \cdots = a_{NN}(N), \\
& a_{ii}(k) = \sum_j \frac{a_{ij}(k)}{k}, \quad k = 1, \cdots, N, \\
& a_{ij}(k) \geq 0, \quad i = 1, \cdots, N, \quad j = 1, \cdots, N, \quad k = 1, \cdots, N.
\end{aligned} \tag{5.59}$$

Fixing i, $\{a_{ij}(k)\}$ is $N \times N$ variables with indices j and k. Then, by solving the following LP as a function of x

$$\begin{aligned}
\ell_i(x) := \min_{\{a_{ij}(k)\}} \quad & \sum_k \sum_j \frac{a_{ij}(k)}{k^2} \\
\text{s.t.} \quad & \sum_k \sum_j \frac{a_{ij}(k)}{k} = P(A_i), \\
& \sum_j \sum_k c_{ij} a_{ij}(k) = \sum_j c_{ij} P(A_i \cap A_j), \\
& x = a_{i1}(N) = a_{i2}(N) = \cdots = a_{iN}(N) \geq 0, \\
& a_{ii}(k) = \sum_j \frac{a_{ij}(k)}{k}, \quad k = 1, \cdots, N, \\
& a_{ij}(k) \geq 0, \quad j = 1, \cdots, N, \quad k = 1, \cdots, N.
\end{aligned} \tag{5.60}$$

We can therefore solve (5.59) and get another lower bound as

$$P\left(\bigcup_i A_i\right) \geq \min_x \sum_i \ell_i(x) =: \ell_{\text{NEW-7}}, \tag{5.61}$$

where the minimum ranges over $x \geq 0$ when the solutions of the LP problems (5.45) all exist. Since the solution of (5.59) can be obtained based on the solution of (5.58), we herein ignore the derivations.

Remark 18. *If $c_{i1} = c_{i2} = \cdots = c_{iN}$ for all i, the lower bound $\ell_{NEW\text{-}7}$ reduces to the analytical lower bound $\ell_{NEW\text{-}2}$.*

Remark 19. *Similar to the proof of Lemma 14, one can show that the lower bound obtained by (5.58) is upper bounded $\ell_{NEW\text{-}2}$, i.e., $\ell_{NEW\text{-}7} \leq \ell_{NEW\text{-}2}$. We herein ignore the derivations.*

5.3 Numerical Examples

Lower bounds are compared in Table 5.1, including existing bounds (the KAT bound ℓ_{KAT}, the GK bound ℓ_{GK} and the stepwise lower bound ℓ_{Stepwise} described in Chapter 2), the new lower bounds $\ell_{\text{NEW-1}}$ and $\ell_{\text{NEW-2}}$ of Chapter 3, the new lower bounds $\ell_{\text{NEW-3}}$ and $\ell_{\text{NEW-4}}$ of Chapter 4, and the new lower bound $\ell_{\text{NEW-5}}$ in this chapter.

We use the same notation as in Chapter 4: $\tilde{\boldsymbol{c}}$ is obtained by the GK bound and the elements of $\tilde{\boldsymbol{c}}^+$ are given by $\{\tilde{c}_i^+ = \max(\tilde{c}_i, \epsilon), i = 1, \ldots, N\}$ where $\epsilon > 0$ is small enough so that if $\tilde{\boldsymbol{c}} \in \mathbb{R}_+^N$ then $\tilde{\boldsymbol{c}}^+ = \tilde{\boldsymbol{c}}$. In three examples (Systems II, III and VIII), $\tilde{\boldsymbol{c}} \in \mathbb{R}_+^N$, therefore $\ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}}) = \ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}}^+)$. In two examples (Systems VI and VII), $\ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}})$ gives a negative value so we ignore it and replace it by 0. The lower bound $\max_\kappa \ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}}+\kappa\mathbf{1})$ is computed by searching κ from -1 to 1 with a fixed step length

0.005 (with 401 points used in total). We also randomly generated $100,000$ samples of $\boldsymbol{c} \in \mathbb{R}_+^N$ to compute $\ell_{\text{NEW-3}}(\boldsymbol{c})$ and $\ell_{\text{NEW-4}}(\boldsymbol{c})$ and the largest bounds were selected and denoted as $\ell_{\text{NEW-3}}(\boldsymbol{c}^+_{\text{Rand}})$ and $\ell_{\text{NEW-4}}(\boldsymbol{c}^+_{\text{Rand}})$. The class of new lower bounds $\ell_{\text{NEW-6}}$ and $\ell_{\text{NEW-7}}$ are not included in these numerical examples since we have shown that $\ell_{\text{NEW-6}}$ is not sharper than ℓ_{KAT} and $\ell_{\text{NEW-7}}$ is not sharper than $\ell_{\text{NEW-2}}$. A bold number in the table indicates coincidence with the optimal lower bound using $\{P(A_i)\}$ and $\{P(A_i \cap A_j)\}$, which is the solution of (5.1).

According to the numerical examples, since $N \leq 7$, the new lower bound $\ell_{\text{NEW-5}}$ coincides with the optimal lower bound in all eight systems, as expected by Lemma 13.

The upper bounds are compared in Table 5.2, including the existing bounds (the union upper bound $\hbar_{\text{Union}}$ and the Greedy upper bound $\hbar_{\text{Greedy}}$ described in Chapter 2), the new upper bounds $\hbar_{\text{NEW-1}}$ (of Chapter 2), $\hbar_{\text{NEW-2}}$ and $\hbar_{\text{NEW-3}}$ (of Chapter 3) and the new upper bound $\hbar_{\text{NEW-6}}$ of this chapter. The class of $\hbar_{\text{NEW-6}}$ and $\hbar_{\text{NEW-5}}$ are not included in Table 5.2 since they are conjectured to be always looser than $\hbar_{\text{NEW-1}}$ and $\hbar_{\text{NEW-3}}$, respectively. All the upper bounds shown in Table 5.2 are not truncated by 1, and a bold number indicates coincidence with the optimal upper bound (5.1).

Again, we can see that the new upper bound coincides with the optimal upper bound in all eight systems, as expected by Lemma 13 since $N \leq 7$.

Finally, we provide additional examples for $N > 7$ to illustrate cases where the new lower and upper bounds, $\ell_{\text{NEW-5}}$ and $\hbar_{\text{NEW-6}}$, do not always coincide with the optimal upper/lower bounds of (5.1). The two additional systems (System IX with $N = 8$ and System X with $N = 10$) are given in Appendix C.2, and the lower and upper bounds for these two systems are given in Table 5.3. The optimal lower and upper bounds of (5.1) are denoted as ℓ_{OPT} and $\hbar_{\text{OPT}}$, respectively.

Table 5.1: Comparison of lower bounds (* indicates $\tilde{\boldsymbol{c}} \in \mathbb{R}_+^N$ and a bold number indicates coincidence with the optimal bound (5.1) of exponential complexity in N).

System	I	II*	III*	IV	V	VI	VII	VIII*
N	6	6	6	7	3	4	4	4
$P\left(\bigcup_{i=1}^N A_i\right)$	0.7890	0.6740	0.7890	0.9687	0.3900	0.3252	0.5346	0.5854
ℓ_{KAT}	0.7247	0.6227	0.7222	0.8909	0.3833	0.2769	0.4434	0.5412
ℓ_{GK}	0.7601	0.6510	0.7508	0.9231	0.3813	0.2972	0.4750	0.5390
$\ell_{\text{NEW-2}}$	0.7247	0.6227	0.7222	0.8909	**0.3900**	0.3205	0.4562	0.5464
$\ell_{\text{NEW-1}}$	0.7487	0.6398	0.7427	0.9044	**0.3900**	**0.3252**	**0.5090**	0.5531
$\ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}})$	0.6359	0.6517*	0.7512*	0.7908	0.3865	0	0	0.5412*
$\ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}}^+)$	0.7638	0.6517*	0.7512*	0.9231	**0.3900**	0.2951	0.4905	0.5412*
$\ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}} + \kappa\mathbf{1})$	0.7577	0.6539	0.7557	0.9235	0.3899	0.2993	0.4949	0.5412
$\ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}}^+_{\text{Rand}})$	0.7783	0.6633	0.7810	0.9501	**0.3900**	0.3022	0.4992	0.5666
$\ell_{\text{NEW-4}}(\tilde{\boldsymbol{c}}^+)$	0.7638	0.6517	0.7512	0.9231	**0.3900**	0.2951	0.4905	0.5412
$\ell_{\text{NEW-4}}(\tilde{\boldsymbol{c}}^+_{\text{Rand}})$	0.7783	0.6633	0.7810	0.9501	**0.3900**	0.3203	0.4992	0.5666
ℓ_{Stepwise}	**0.7890**	**0.6740**	**0.7890**	**0.9687**	**0.3900**	0.3027	0.5009	**0.5673**
$\ell_{\text{NEW-5}}$	**0.7890**	**0.6740**	**0.7890**	**0.9687**	**0.3900**	**0.3252**	**0.5090**	**0.5673**

Table 5.2: Comparison of upper bounds (* indicates $\tilde{\boldsymbol{c}} \in \mathbb{R}_+^N$ and a bold number indicates coincidence with the optimal bound of (5.1) of exponential complexity in N. All upper bounds are not truncated by 1.)

System	I	II*	III*	IV	V	VI	VII	VIII*
N	6	6	6	7	3	4	4	4
$P\left(\bigcup_{i=1}^N A_i\right)$	0.7890	0.6740	0.7890	0.9687	0.3900	0.3252	0.5346	0.5854
$\hbar_{\text{Union}}$	2.07	1.716	1.916	2.4181	0.5	0.5612	0.8022	1.5737
$\hbar_{\text{NEW-1}}$	1.3907	1.1870	1.3320	1.7974	0.4200	0.4059	0.5984	0.8093
$\hbar_{\text{NEW-3}}$	1.3744	1.1356	1.2820	1.7763	0.4125	0.3814	0.5642	0.7813
$\hbar_{\text{NEW-2}}$	1.28	0.9310	1.1330	1.5047	**0.3900**	**0.3252**	**0.5346**	**0.7070**
$\hbar_{\text{Greedy}}$	1.144	0.8910	1.0780	1.4568	0.4450	**0.3252**	**0.5346**	**0.7070**
$\hbar_{\text{NEW-6}}$	**0.8550**	**0.8130**	**0.9550**	**1.0703**	**0.3900**	**0.3252**	**0.5346**	**0.7070**

From Table 5.3, one can see that the new lower and upper bounds, $\ell_{\text{NEW-5}}$ and $\hbar_{\text{NEW-6}}$ do not coincide with ℓ_{OPT} and $\hbar_{\text{OPT}}$ in these two systems. However, they are still sharper than all other tested lower/upper bounds that can be computed in polynomial time.

Table 5.3: Additional Systems (Examples for $N > 7$).

System	IX	X
N	8	10
$P\left(\bigcup_{i=1}^{N} A_i\right)$	0.5051	0.5261
ℓ_{KAT}	0.4391	0.4847
ℓ_{GK}	0.4381	0.4852
$\ell_{\text{NEW-2}}$	0.4391	0.4847
$\ell_{\text{NEW-1}}$	0.4393	0.4847
$\ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}})$	0.4381	0.4852
$\ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}}^{+})$	0.4381	0.4852
$\ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}} + \kappa\mathbf{1})$	0.4381	0.4852
$\ell_{\text{NEW-3}}(\tilde{\boldsymbol{c}}^{+}_{\text{Rand}})$	0.4381	0.4852
$\ell_{\text{NEW-4}}(\tilde{\boldsymbol{c}}^{+})$	0.4381	0.4852
$\ell_{\text{NEW-4}}(\tilde{\boldsymbol{c}}^{+}_{\text{Rand}})$	0.4381	0.4852
ℓ_{Stepwise}	0.4349	0.4758
$\ell_{\text{NEW-5}}$	0.4400	0.4874
ℓ_{OPT} (5.1)	**0.4421**	**0.4878**
$\hbar_{\text{Union}}$	2.1101	2.7491
$\hbar_{\text{NEW-1}}$	1.0975	1.4542
$\hbar_{\text{NEW-3}}$	1.0705	14180
$\hbar_{\text{NEW-2}}$	0.9566	1.2652
$\hbar_{\text{Greedy}}$	0.8735	1.1581
$\hbar_{\text{NEW-6}}$	0.7362	0.9887
$\hbar_{\text{OPT}}$ (5.1)	**0.7359**	**0.9831**

Appendices

Appendix A

New Bounds using $\{P(A_i)\}$ and $\{\sum_j P(A_i \cap A_j)\}$

A.1 Uniqueness of the optimal feasible point of the KAT LP problem (2.22)

Since we can solve the KAT LP problem (2.22) by separating $i = 1, \ldots, N$, we only need to consider if the following LP has a unique optimal feasible point:

$$\min_{\boldsymbol{x}} \boldsymbol{p}^T \boldsymbol{x}, \quad \text{s.t.} \quad \boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}, \quad \boldsymbol{I}\boldsymbol{x} \geq \boldsymbol{0}, \tag{A.1}$$

where $\boldsymbol{p} = (1, \frac{1}{2}, \ldots, \frac{1}{N})^T$, $\boldsymbol{x} = (x_1, \ldots, x_N)^T$, $\boldsymbol{b} = (\alpha, \gamma)^T$, $\boldsymbol{I}$ is the $N \times N$ identity matrix, and

$$\boldsymbol{A} = \begin{pmatrix} 1 & 1 & \ldots & 1 \\ 1 & 2 & \ldots & N \end{pmatrix}. \tag{A.2}$$

First, the optimum of LP is achieved at one vertex, which is denoted by $\{x_k = 0, k \neq k_1, k \neq k_2\}$ and $x_{k_1} \geq 0, x_{k_2} \geq 0, k_2 > k_1$ such that

$$x_{k_1} + x_{k_2} = \alpha, \quad k_1 x_{k_1} + k_2 x_{k_2} = \gamma, \tag{A.3}$$

or $x_{k_1} = \frac{k_2\alpha-\gamma}{k_2-k_1}$ and $x_{k_2} = \frac{\gamma-k_1\alpha}{k_2-k_1}$. The optimal k_1^* and k_2^* are chosen to minimize the objective function

$$\{k_1^*, k_2^*\} = \arg\min_{k_1,k_2} \quad \boldsymbol{p}^T\boldsymbol{x} = \frac{x_{k_1}}{k_1} + \frac{x_{k_2}}{k_2} \tag{A.4}$$

Denote $\mathscr{K}$ as the set of all integer tuples (k_1, k_2) such that $1 \leq k_1 < k_2 \leq N$, and $\mathscr{K}_*$ be the set of optimum (k_1^*, k_2^*). Then using a similar approach to the proof of Theorem 2, we can show that if $\frac{\gamma}{\alpha}$ is not an integer, $\mathscr{K}_* = \{(\lfloor\frac{\gamma}{\alpha}\rfloor, \lfloor\frac{\gamma}{\alpha}\rfloor + 1)\}$ has only one optimal solution of (k_1^*, k_2^*). If $\frac{\gamma}{\alpha}$ is an integer, $\mathscr{K}_* = \{(\frac{\gamma}{\alpha}, \frac{\gamma}{\alpha} + 1), (\frac{\gamma}{\alpha} - 1, \frac{\gamma}{\alpha})\}$, both lead to the same solution of $\boldsymbol{x}$. Note that using a similar approach as the one adopted in A.2, by computing the derivative with respect to k_1 and k_2, we have that

$$\frac{x_{k_1^*}}{k_1^*} + \frac{x_{k_2^*}}{k_2^*} = \min_{(k_1,k_2)\in\mathscr{K}} \frac{x_{k_1}}{k_1} + \frac{x_{k_2}}{k_2} < \min_{(k_1,k_2)\in\mathscr{K}\setminus\mathscr{K}_*} \frac{x_{k_1}}{k_1} + \frac{x_{k_2}}{k_2} \tag{A.5}$$

for any $(k_1^*, k_2^*) \in \mathscr{K}_*$. Note that the strict inequality implies there exists $\epsilon^* > 0$ such that

$$\frac{x_{k_1^*}}{k_1^*} + \frac{x_{k_2^*}}{k_2^*} + \epsilon^* \leq \min_{(k_1,k_2)\in\mathscr{K}\setminus\mathscr{K}_*} \frac{x_{k_1}}{k_1} + \frac{x_{k_2}}{k_2}. \tag{A.6}$$

Now we prove the uniqueness of the LP problem by [21, Theorem 1], which is to show that for any given non-zero vector $\boldsymbol{q}$, the optimal feasible point of (A.1) is also optimal for the following perturbed LP problem by properly choosing $\epsilon > 0$:

$$\min_{\boldsymbol{x}} (\boldsymbol{p} + \epsilon\boldsymbol{q})^T\boldsymbol{x}, \quad \text{s.t.} \quad \boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}, \quad \boldsymbol{I}\boldsymbol{x} \geq \boldsymbol{0}. \tag{A.7}$$

Since the constraints remain the same, it suffices to show the optimal (k_1^*, k_2^*) are also optimal for the perturbed problem, i.e.,

$$(\frac{1}{k_1^*} + \epsilon q_{k_1^*})x_{k_1^*} + (\frac{1}{k_2^*} + \epsilon q_{k_2^*})x_{k_2^*} = \min_{(k_1,k_2)\in\mathscr{K}} \left[(\frac{1}{k_1} + \epsilon q_{k_1})x_{k_1} + (\frac{1}{k_2} + \epsilon q_{k_2})x_{k_2}\right] \quad \text{(A.8)}$$

which is enough to show

$$(\frac{1}{k_1^*} + \epsilon q_{k_1^*})x_{k_1^*} + (\frac{1}{k_2^*} + \epsilon q_{k_2^*})x_{k_2^*} \leq \min_{(k_1,k_2)\in\mathscr{K}\setminus\mathscr{K}_*} \left[(\frac{1}{k_1} + \epsilon q_{k_1})x_{k_1} + (\frac{1}{k_2} + \epsilon q_{k_2})x_{k_2}\right] \quad \text{(A.9)}$$

Note that

$$(\frac{1}{k_1^*} + \epsilon q_{k_1^*})x_{k_1^*} + (\frac{1}{k_2^*} + \epsilon q_{k_2^*})x_{k_2^*} \leq \left(\frac{x_{k_1^*}}{k_1^*} + \frac{x_{k_2^*}}{k_2^*}\right) + \epsilon \left[\max_{(k_1,k_2)\in\mathscr{K}} (q_{k_1}x_{k_1} + q_{k_2}x_{k_2})\right] \quad \text{(A.10)}$$

and

$$\begin{aligned} &\min_{(k_1,k_2)\in\mathscr{K}\setminus\mathscr{K}_*} \left[(\frac{1}{k_1} + \epsilon q_{k_1})x_{k_1} + (\frac{1}{k_2} + \epsilon q_{k_2})x_{k_2}\right] \\ &\geq \min_{(k_1,k_2)\in\mathscr{K}\setminus\mathscr{K}_*} \left(\frac{x_{k_1}}{k_1} + \frac{x_{k_2}}{k_2}\right) + \epsilon \left[\min_{(k_1,k_2)\in\mathscr{K}} (q_{k_1}x_{k_1} + q_{k_2}x_{k_2})\right] \end{aligned} \quad \text{(A.11)}$$

Therefore, by choosing

$$\epsilon = \frac{\epsilon^*}{\max_{(k_1,k_2)\in\mathscr{K}} (q_{k_1}x_{k_1} + q_{k_2}x_{k_2}) - \min_{(k_1,k_2)\in\mathscr{K}} (q_{k_1}x_{k_1} + q_{k_2}x_{k_2})}, \quad \text{(A.12)}$$

equation (A.9) can be obtained by (A.10), (A.11) and (A.6).

A.2 Proof that $\frac{a_i(k_1)}{k_1} + \frac{a_i(k_2)}{k_2}$ is non-decreasing with k_2 and non-increasing with k_1 (between (3.13) and (3.14))

Let $k := \frac{\gamma_i - Nx}{\alpha_i - x}$, then

$$a_i(k_1) = \frac{k_2(\alpha_i - x) - (\gamma_i - Nx)}{k_2 - k_1} = (\alpha_i - x)\frac{k_2 - \frac{\gamma_i - Nx}{\alpha_i - x}}{k_2 - k_1} = (\alpha_i - x)\frac{k_2 - k}{k_2 - k_1}. \quad \text{(A.13)}$$

Similarly, we have

$$a_i(k_2) = \frac{(\gamma_i - Nx) - k_1(\alpha_i - x)}{k_2 - k_1} = (\alpha_i - x)\frac{k - k_1}{k_2 - k_1}. \quad \text{(A.14)}$$

Since $\alpha_i - x$ is a constant here and $k_1 \leq k \leq k_2$, we only need to consider

$$\begin{aligned}
\frac{1}{\alpha_i - x}\left[\frac{a_i(k_1)}{k_1} + \frac{a_i(k_2)}{k_2}\right] &= \frac{1}{k_1}\frac{k_2 - k}{k_2 - k_1} + \frac{1}{k_2}\frac{k - k_1}{k_2 - k_1} \\
&= \frac{1}{k_2 - k_1}\left[\left(\frac{k_2}{k_1} - \frac{k}{k_1}\right) + \left(\frac{k}{k_2} - \frac{k_1}{k_2}\right)\right] \\
&= \frac{1}{k_2 - k_1}\left(\frac{k_2^2 - k_1^2}{k_1 k_2} + \frac{k_1 - k_2}{k_1 k_2}k\right) \\
&= \frac{1}{k_1} + \frac{1}{k_2} - \frac{k}{k_1 k_2}
\end{aligned} \quad \text{(A.15)}$$

The derivatives w.r.t. k_1 and k_2 can be obtained as follows:

$$\frac{1}{k_1^2}\left(\frac{k}{k_2} - 1\right) \leq 0, \quad \frac{1}{k_2^2}\left(\frac{k}{k_1} - 1\right) \geq 0. \quad \text{(A.16)}$$

Therefore, the function is non-increasing with k_1 and non-decreasing with k_2.

A.3 Proof that $\frac{\gamma_i - Nx}{\alpha_i - x}$ is a non-increasing function of x

Note that by definition of γ_i and α_i, we know $\gamma_i \leq N\alpha_i$.

$$\begin{aligned}\left(\frac{\gamma_i - Nx}{\alpha_i - x}\right)' &= \frac{(-N)(\alpha_i - x) - (\gamma_i - Nx)(-1)}{(\alpha_i - x)^2} \\ &= \frac{(\gamma_i - Nx) - N(\alpha_i - x)}{(\alpha_i - x)^2} \\ &\leq \frac{(N\alpha_i - Nx) - N(\alpha_i - x)}{(\alpha_i - x)^2} = 0.\end{aligned} \tag{A.17}$$

Clearly, if $\gamma_i < N\alpha_i$, the function $\frac{\gamma_i - Nx}{\alpha_i - x}$ is a strictly decreasing function of x.

A.4 Proof that $f_i(x+h) - f_i(x)$ and $f_i(x) - f_i(x-h)$ are positive

By (3.16), we can write

$$\begin{aligned} f_i(x) &= \frac{2(n-1)+1}{(n-1)n}(\alpha_i - x) - \frac{1}{(n-1)n}(\gamma_i - Nx) + \frac{x}{N} \\ f_i(x+h) &= \frac{2(n-1)+1}{(n-1)n}(\alpha_i - x - h) - \frac{1}{(n-1)n}(\gamma_i - Nx - Nh) + \frac{x+h}{N} \\ f_i(x-h) &= \frac{2n+1}{n(n+1)}(\alpha_i - x + h) - \frac{1}{n(n+1)}(\gamma_i - Nx + Nh) + \frac{x-h}{N} \end{aligned} \tag{A.18}$$

Substituting $\gamma_i - Nx = n(\alpha_i - x)$, we get

$$\begin{aligned}
f_i(x) &= \left[\frac{2n-1}{(n-1)n} - \frac{n}{(n-1)n}\right](\alpha_i - x) + \frac{x}{N} = \frac{1}{n}(\alpha_i - x) + \frac{x}{N} \\
f_i(x+h) &= f_i(x) - \frac{2(n-1)+1}{(n-1)n}h + \frac{N}{(n-1)n}h + \frac{1}{N}h \\
f_i(x-h) &= \left[\frac{2n+1}{n(n+1)} - \frac{n}{n(n+1)}\right](\alpha_i - x) + \left[\frac{2n+1}{n(n+1)} - \frac{N}{n(n+1)}\right]h + \frac{x-h}{N} \\
&= f_i(x) + \left[\frac{2n+1}{n(n+1)} - \frac{N}{n(n+1)} - \frac{1}{N}\right]h
\end{aligned} \tag{A.19}$$

Therefore, we have

$$\begin{aligned}
f_i(x+h) - f_i(x) &= h\left(\frac{N-2n+1}{(n-1)n} + \frac{1}{N}\right) \\
&= h\left[\frac{N-n}{(n-1)n} - \frac{1}{n} + \frac{1}{N}\right] \\
&= h\frac{N-n}{n}\left(\frac{1}{n-1} - \frac{1}{N}\right) > 0,
\end{aligned} \tag{A.20}$$

and

$$\begin{aligned}
f_i(x) - f_i(x-h) &= \left[\frac{N}{n(n+1)} + \frac{1}{N} - \frac{1}{n+1} - \frac{1}{n}\right]h \\
&= \left[\frac{N-n}{n(n+1)} - \frac{N-n}{Nn}\right]h \\
&= \frac{N-n}{n}\left(\frac{1}{n+1} - \frac{1}{N}\right)h > 0.
\end{aligned} \tag{A.21}$$

Appendix B

New Bounds using $\{P(A_i)\}$ and $\{\sum_j c_j P(A_i \cap A_j)\}$

B.1 The solution of (4.34)

Note that we can solve (4.34) using the same technique used in Chapter 3 (see also [26]). Assume two subsets B_1 and B_2 such that $p_{B_1} \geq 0$ and $p_{B_2} \geq 0$, then denoting

$$b := \frac{\sum_k c_k P(A_i \cap A_k)}{c_i P(A_i)}, \quad b_1 := \frac{\sum_{k \in B_1} c_k}{c_i}, \quad b_2 := \frac{\sum_{k \in B_2} c_k}{c_i}, \tag{B.1}$$

then problem (4.34) reduces to

$$\begin{aligned} \ell_i(\boldsymbol{c}) = \min_{\{p_{B_1}, p_{B_2}\}} \quad & \frac{p_{B_1}}{b_1} + \frac{p_{B_2}}{b_2} \\ \text{s.t.} \quad & p_{B_1} + p_{B_2} = P(A_i), \\ & b_1 p_{B_1} + b_2 p_{B_2} = bP(A_i), \\ & p_{B_1} \geq 0, \quad p_{B_2} \geq 0. \end{aligned} \tag{B.2}$$

According to Appendix A.2 (see also [26, Appendix B]) that one can get

$$\ell_i(\boldsymbol{c}) = \min_{\{b_1,b_2:b_1\le b\le b_2\}} \quad P(A_i)\left(\frac{1}{b_1}+\frac{1}{b_2}-\frac{b}{b_1b_2}\right), \tag{B.3}$$

and the partial derivative of $P(A_i)\left(\frac{1}{b_1}+\frac{1}{b_2}-\frac{b}{b_1b_2}\right)$ with respect to b_1 and b_2 are (see Appendix A.2 or [26, Appendix B, Eq. (B.3)]):

$$\begin{aligned}
\frac{\partial\left[P(A_i)\left(\frac{1}{b_1}+\frac{1}{b_2}-\frac{b}{b_1b_2}\right)\right]}{\partial b_1} &= \frac{P(A_i)}{b_1^2}\left(\frac{b-b_2}{b_2}\right),\\
\frac{\partial\left[P(A_i)\left(\frac{1}{b_1}+\frac{1}{b_2}-\frac{b}{b_1b_2}\right)\right]}{\partial b_2} &= \frac{P(A_i)}{b_2^2}\left(\frac{b-b_1}{b_1}\right).
\end{aligned} \tag{B.4}$$

Note that the partial derivatives are not continuous at $b_1 = 0$ and $b_2 = 0$. Therefore, the solution depends on the following different scenarios.

1. If $b \ge 0$ and $\min_{\{B:i\in B\}} \frac{\sum_{k\in B} c_k}{c_i} < 0$, the solutions of (B.3) are given by

$$\begin{aligned}
b_1 &= \max_{\{B:i\in B\}} \frac{\sum_{k\in B} c_k}{c_i} \quad \text{s.t.} \quad \frac{\sum_{k\in B} c_k}{c_i} < 0,\\
b_2 &= \max_{\{B:i\in B\}} \frac{\sum_{k\in B} c_k}{c_i}.
\end{aligned} \tag{B.5}$$

2. If $b \ge 0$ and $\min_{\{B:i\in B\}} \frac{\sum_{k\in B} c_k}{c_i} \ge 0$, the solutions of (B.3) are given by

$$\begin{aligned}
b_1 &= \max_{\{B:i\in B\}} \frac{\sum_{k\in B} c_k}{c_i} \quad \text{s.t.} \quad \frac{\sum_{k\in B} c_k}{c_i} \le b,\\
b_2 &= \min_{\{B:i\in B\}} \frac{\sum_{k\in B} c_k}{c_i} \quad \text{s.t.} \quad \frac{\sum_{k\in B} c_k}{c_i} \ge b.
\end{aligned} \tag{B.6}$$

3. If $b < 0$ and $b < \left\{\max_{\{B:i\in B\}} \frac{\sum_{k\in B} c_k}{c_i}, \quad \text{s.t.}\ \frac{\sum_{k\in B} c_k}{c_i} < 0\right\}$, the solutions of (B.3)

are given by

$$\begin{aligned} b_1 &= \max_{\{B:i\in B\}} \frac{\sum_{k\in B} c_k}{c_i}, \quad \text{s.t.} \quad \frac{\sum_{k\in B} c_k}{c_i} < 0, \\ b_2 &= \min_{\{B:i\in B\}} \frac{\sum_{k\in B} c_k}{c_i}. \end{aligned} \tag{B.7}$$

4. If $b < 0$ and $b \geq \left\{\max_{\{B:i\in B\}} \frac{\sum_{k\in B} c_k}{c_i}, \quad \text{s.t.} \quad \frac{\sum_{k\in B} c_k}{c_i} < 0\right\}$, the solutions of (B.3) are given by

$$\begin{aligned} b_1 &= \max_{\{B:i\in B\}} \frac{\sum_{k\in B} c_k}{c_i}, \\ b_2 &= \max_{\{B:i\in B\}} \frac{\sum_{k\in B} c_k}{c_i} \quad \text{s.t.} \quad \frac{\sum_{k\in B} c_k}{c_i} \leq b. \end{aligned} \tag{B.8}$$

B.2 Solving the dual problem of (4.34)

We can alternatively solve (4.34) by solving the dual problem. Here we give the proof for $\boldsymbol{c} \in \mathbb{R}^+$. The interesting property of the dual problem is that any feasible point of the dual problem is a lower bound, although it is still not clear how to use such property to get a lower bound with lower complexity.

Note that for the prime problem of the form

$$\min_{\boldsymbol{p}} \boldsymbol{c}^T \boldsymbol{p}, \quad \text{s.t.} \quad \boldsymbol{A}\boldsymbol{p} = \boldsymbol{b}, \quad \boldsymbol{p} \geq \boldsymbol{0}, \tag{B.9}$$

the dual problem is

$$\max_{\boldsymbol{q}} \boldsymbol{b}^T \boldsymbol{q}, \quad \text{s.t.} \quad \boldsymbol{A}^T \boldsymbol{q} \leq \boldsymbol{c}. \tag{B.10}$$

Therefore, we can write the dual problem of (4.34) as

$$
\begin{aligned}
\max_{q_1,q_2} \quad & q_1 P(A_i) + q_2 \sum_k w_k P(A_i \cap A_k) \\
\text{s.t.} \quad & q_1 + (\sum_{k \in B'} w_k) q_2 \le \frac{1}{\sum_{k \in B'} w_k}, \quad \forall B' \in \mathscr{B} : i \in B',
\end{aligned}
\tag{B.11}
$$

where

$$
w_k := \frac{c_k}{c_i}. \tag{B.12}
$$

The necessary condition for a vertex is that there exists $B_1, B_2 \in \mathscr{B} : B_1 \neq B_2, i \in B_1, i \in B_2$ so that equality holds for the constraints in (B.11); then we can get

$$
q_1 = \frac{1}{\sum_{k \in B_1} w_k} + \frac{1}{\sum_{k \in B_2} w_k}, \quad q_2 = -\frac{1}{(\sum_{k \in B_1} w_k)(\sum_{k \in B_2} w_k)}. \tag{B.13}
$$

Hence, (B.11) is equivalent to

$$
\begin{aligned}
\max_{B_1,B_2} \quad & \frac{(\sum_{k \in B_1} w_k + \sum_{k \in B_2} w_k) P(A_i) - \sum_k w_k P(A_i \cap A_k)}{(\sum_{k \in B_1} w_k)(\sum_{k \in B_2} w_k)} \\
\text{s.t.} \quad & \frac{1}{\sum_{k \in B_1} w_k} + \frac{1}{\sum_{k \in B_2} w_k} - \frac{\sum_{k \in B'} w_k}{(\sum_{k \in B_1} w_k)(\sum_{k \in B_2} w_k)} \le \frac{1}{\sum_{k \in B'} w_k}, \\
& \forall B' \in \mathscr{B} : i \in B'.
\end{aligned}
\tag{B.14}
$$

Using the definition of b, b_1 and b_2 in (B.1) and defining $b' = \sum_{k \in B'} w_k$, we have

$$
\begin{aligned}
\max_{b_1,b_2} \quad & P(A_i) \left(\frac{1}{b_1} + \frac{1}{b_2} - \frac{b}{b_1 b_2} \right) \\
\text{s.t.} \quad & \frac{1}{b_1} + \frac{1}{b_2} \le \frac{b'}{b_1 b_2} + \frac{1}{b'}, \quad \forall b'.
\end{aligned}
\tag{B.15}
$$

Since we assumed $\boldsymbol{c} \in \mathbb{R}^+$ so b, b_1, b_2 and b' are all positive, the constraints imply

$$\min\{\frac{b'}{b_1 b_2}, \frac{1}{b'}\} \le \frac{1}{b_1} \le \frac{1}{b_2} \le \max\{\frac{b'}{b_1 b_2}, \frac{1}{b'}\}, \quad \forall b', \tag{B.16}$$

and from (B.4) we know that

$$b_1 \le b \le b_2. \tag{B.17}$$

Therefore, the solution of (B.11) is (B.6).

B.3 Proof that the objective function of (4.59) is non-decreasing with $\boldsymbol{x}$

The proof is similar to the proof of Theorem 2. First, we prove

$$\ell_i'(\boldsymbol{c}, x) = [P(A_i) - x] \left(\frac{c_i}{\sum_{k \in B_1^{(i)}} c_k} + \frac{c_i}{\sum_{k \in B_2^{(i)}} c_k} - \frac{c_i \sum_k c_k \left[P(A_i \cap A_k) - x\right]}{[P(A_i) - x] \left(\sum_{k \in B_1^{(i)}} c_k\right) \left(\sum_{k \in B_2^{(i)}} c_k\right)} \right), \tag{B.18}$$

is continuous when $\exists B' \in \mathscr{B}^-$ such that

$$\frac{\sum_k c_k \left[P(A_i \cap A_k) - x\right]}{c_i \left[P(A_i) - x\right]} = \frac{\sum_{k \in B'} c_k}{c_i}. \tag{B.19}$$

This can be proved similarly to (A.4) that

$$\lim_{h \to 0^+} \ell_i'(\boldsymbol{c}, x + h) = \lim_{h \to 0^+} \ell_i'(\boldsymbol{c}, x - h) = \frac{c_i}{\sum_{k \in B'} c_k}. \tag{B.20}$$

Then one can prove that when

$$\frac{\sum_{k \in B_2^{(i)}} c_k}{c_i} < \frac{\sum_k c_k \left[P(A_i \cap A_k) - x\right]}{c_i \left[P(A_i) - x\right]} < \frac{\sum_{k \in B_1^{(i)}} c_k}{c_i}, \tag{B.21}$$

the partial derivative of $\ell_i'(\boldsymbol{c}, x) + \frac{c_i}{\sum_k c_k} x$ w.r.t. x is non-negative:

$$\begin{aligned}
\frac{\partial\left(\ell_i'(\boldsymbol{c}, x) + \frac{c_i}{\sum_k c_k} x\right)}{\partial x} &= \frac{c_i}{\sum_k c_k} - \frac{c_i}{\sum_{k \in B_1^{(i)}} c_k} - \frac{c_i}{\sum_{k \in B_2^{(i)}} c_k} + \frac{c_i \sum_k c_k}{\left(\sum_{k \in B_1^{(i)}} c_k\right)\left(\sum_{k \in B_2^{(i)}} c_k\right)} \\
&= \frac{c_i \left(\sum_k c_k - \sum_{k \in B_1^{(i)}} c_k\right)\left(\sum_k c_k - \sum_{k \in B_2^{(i)}} c_k\right)}{\left(\sum_k c_k\right)\left(\sum_{k \in B_1^{(i)}} c_k\right)\left(\sum_{k \in B_2^{(i)}} c_k\right)} \\
&= \frac{c_i \left(\sum_{k \notin B_1^{(i)}} c_k\right)\left(\sum_{k \notin B_2^{(i)}} c_k\right)}{\left(\sum_k c_k\right)\left(\sum_{k \in B_1^{(i)}} c_k\right)\left(\sum_{k \in B_2^{(i)}} c_k\right)} \geq 0.
\end{aligned} \tag{B.22}$$

Therefore, the objective function of (4.59),

$$\sum_i \ell_i'(\boldsymbol{c}, x) + x = \sum_i \left(\ell_i'(\boldsymbol{c}, x) + \frac{c_i}{\sum_k c_k} x\right), \tag{B.23}$$

is non-decreasing with x.

Appendix C

New Bounds using $\{P(A_i)\}$ and $\{P(A_i \cap A_j)\}$

C.1 The solution of (5.43)

We can remove $a_{ii}(k), k > 1$ using $a_{ii}(k) = \sum_j \frac{a_{ij}(k)}{k}$ and then only consider $a_{ij}(k), i \neq j$:

$$\begin{aligned}
\ell_i = \min_{\{a_{ij}(k), i\neq j\}, a_i(1)} \quad & \sum_{k=2}^{N} \sum_{j, j\neq i} \frac{a_{ij}(k)}{(k-1)k} + a_i(1) \\
\text{s.t.} \quad & a_i(1) + \sum_{k=2}^{N} \sum_{j, i\neq j} \frac{a_{ij}(k)}{k-1} = P(A_i), \\
& \sum_{k=2}^{N} \sum_{j, j\neq i} c_{ij} a_{ij}(k) = \sum_{j, j\neq i} c_{ij} P(A_i \cap A_j), \\
& a_i(1) \geq 0, \\
& a_{ij}(k) \geq 0, j \neq i.
\end{aligned} \tag{C.1}$$

Considering the vertices of the above problem, for all the vertices that $a_i(1) > 0$, we obtain that the vertex yielding the minimal objective function is given by

$$\min_{j\neq i, k\in\{2,\dots,N\}} \alpha_i - \frac{\beta_i}{k c_{ij}}, \quad \text{s.t.} \quad c_{ij}(k-1) \geq \frac{\beta_i}{\alpha_i}, \tag{C.2}$$

where

$$\alpha_i := P(A_i), \quad \beta_i := \sum_{j, j \neq i} c_{ij} P(A_i \cap A_j). \tag{C.3}$$

Note that (C.2) can be easily solved by sorting $N-1$ values:

$$\min_{k \in \{2,\ldots,N\}} \quad \alpha_i - \frac{1}{k}\frac{\beta_i}{c_{i\tilde{j}}} = \alpha_i \left\{ 1 - \frac{1}{k}\frac{1}{c_{i\tilde{j}}}\frac{\beta_i}{\alpha_i} \right\}, \tag{C.4}$$

where $\tilde{j}$ is a function of k:

$$\tilde{j} := \arg\min_j \left\{ c_{ij} \geq \frac{1}{k-1}\frac{\beta_i}{\alpha_i} \right\}, \tag{C.5}$$

In the vertices that $a_i(1) = 0$, we get the optimal vertex as

$$\begin{aligned} \min_{k_1, k_2 \in \{2,\ldots,N\}, j_1 \neq i, j_2 \neq i,} \quad & \frac{\alpha_i}{k_1} - \frac{k_2 - k_1}{(k_2 - 1)k_1 k_2} \frac{\beta_i(k_2 - 1) - c_{ij_1}\alpha_i(k_1 - 1)(k_2 - 1)}{c_{ij_2}(k_2 = 1) - c_{ij_1}(k_1 - 1)} \\ \text{s.t.} \quad & (k_2 - 1)\alpha_i \geq \frac{\beta_i(k_2 - 1) - c_{ij_1}\alpha_i(k_1 - 1)(k_2 - 1)}{c_{ij_2}(k_2 - 1) - c_{ij_1}(k_1 - 1)} \geq 0, \end{aligned} \tag{C.6}$$

which can be rewritten as

$$\begin{aligned} \min_{k_1, k_2, j_1, j_2} \quad & \frac{k_2 c_{ij_2}(k_2 - 1) - k_1 c_{ij_1}(k_1 - 1)}{k_1 k_2 [c_{ij_2}(k_2 - 1) - c_{ij_2}(k_1 - 1)]}\alpha_i - \frac{k_2 - k_1}{k_1 k_2 [c_{ij_2}(k_2 - 1) - c_{ij_2}(k_1 - 1)]}\beta_i, \\ \text{s.t.} \quad & (k_2 - 1)c_{ij_2}\alpha_i \geq \beta_i \geq (k_1 - 1)c_{ij_1}\alpha_i, \end{aligned} \tag{C.7}$$

or more compactly,

$$\begin{aligned}
\min_{k_1,k_2,j_1,j_2} \quad & \alpha_i \left\{ \frac{k_2\left[c_{ij_2}(k_2-1)-\frac{\beta_i}{\alpha_i}\right]+k_1\left[\frac{\beta_i}{\alpha_i}-c_{ij_1}(k_1-1)\right]}{k_1k_2\left[c_{ij_2}(k_2-1)-c_{ij_2}(k_1-1)\right]} \right\} \\
\text{s.t.} \quad & (k_2-1)c_{ij_2} \geq \frac{\beta_i}{\alpha_i} \geq (k_1-1)c_{ij_1}.
\end{aligned} \tag{C.8}$$

Note that the objective function has the form

$$\alpha_i f := \alpha_i \frac{k_2 a + k_1 b}{k_1 k_2 (a+b)}, \quad a \geq 0, b \geq 0, \tag{C.9}$$

and it is easy to note that

$$\frac{\partial f}{\partial c_{ij_2}} \propto \frac{\partial f}{\partial a} = \frac{(k_2-k_1)b}{k_1k_2(a+b)^2}, \quad \frac{\partial f}{\partial c_{ij_1}} \propto -\frac{\partial f}{\partial b} = \frac{(k_2-k_1)a}{k_1k_2(a+b)^2} \tag{C.10}$$

Therefore, the optimal c_{ij_1} and c_{ij_1} can be written as functions of k_1 and k_2.

$$\tilde{c}_{ij_1} = \begin{cases} \arg\min_{c_{ij}} c_{ij} & \text{if } k_2 > k_1, \\ \arg\min_{c_{ij}} \left\{ \frac{\beta_i}{\alpha_i} - (k_1-1)c_{ij} \geq 0 \right\} & \text{if } k_2 < k_1, \end{cases} \tag{C.11}$$

and

$$\tilde{c}_{ij_2} = \begin{cases} \arg\min_{c_{ij}} \left\{ (k_2-1)c_{ij} - \frac{\beta_i}{\alpha_i} \geq 0 \right\} & \text{if } k_2 > k_1, \\ \arg\max_{c_{ij}} c_{ij} & \text{if } k_2 < k_1. \end{cases} \tag{C.12}$$

Then (C.8) can be solved by sorting the $(N-1)^2$ values:

$$\min_{k_1,k_2\in\{2,\ldots,N\}} \quad \alpha_i \left\{ \frac{k_2\left[\tilde{c}_{ij_2}(k_2-1)-\frac{\beta_i}{\alpha_i}\right]+k_1\left[\frac{\beta_i}{\alpha_i}-\tilde{c}_{ij_1}(k_1-1)\right]}{k_1k_2\left[\tilde{c}_{ij_2}(k_2-1)-\tilde{c}_{ij_2}(k_1-1)\right]} \right\}. \tag{C.13}$$

Therefore, the new lower bound $\ell_{\text{NEW-6}}$ is

$$P\left(\bigcup_i A_i\right) \geq \sum_i \ell_i = \sum_i \min\{(\text{C.4}), (\text{C.13})\} =: \ell_{\text{NEW-6}}. \tag{C.14}$$

C.2 Additional Examples: System IX to System X

Table C.1: System IX.

Outcomes ω_i	$p(\omega_i)$	A_1	A_2	A_3	A_4	A_5	A_6	A_7	A_8
ω_0	0.0100		×			×			
ω_1	0.0019	×	×			×			×
ω_2	0.0066		×		×			×	
ω_3	0.0069					×	×		
ω_4	0.0054	×	×	×		×			×
ω_5	0.0137		×		×		×	×	×
ω_6	0.0136				×	×		×	
ω_7	0.0120		×	×	×	×	×	×	
ω_8	0.0129	×	×	×	×	×		×	×
ω_9	0.0021		×		×				
ω_{10}	0.0106	×				×	×		×
ω_{11}	0.0036	×	×		×	×	×		×
ω_{12}	0.0062				×	×		×	
ω_{13}	0.0010				×	×		×	
ω_{14}	0.0043	×		×	×	×	×	×	×
ω_{15}	0.0081		×		×	×	×	×	

ω_{16}	0.0120	$\times$			$\times$				
ω_{17}	0.0102	$\times$	$\times$	$\times$					$\times$
ω_{18}	0.0008		$\times$		$\times$	$\times$	$\times$	$\times$	$\times$
ω_{19}	0.0075							$\times$	$\times$
ω_{20}	0.0026	$\times$		$\times$		$\times$			$\times$
ω_{21}	0.0087		$\times$				$\times$	$\times$	
ω_{22}	0.0129	$\times$	$\times$	$\times$					$\times$
ω_{23}	0.0074	$\times$	$\times$		$\times$	$\times$	$\times$	$\times$	$\times$
ω_{24}	0.0012	$\times$		$\times$	$\times$		$\times$		$\times$
ω_{25}	0.0070	$\times$	$\times$	$\times$	$\times$	$\times$			$\times$
ω_{26}	0.0063	$\times$			$\times$	$\times$	$\times$	$\times$	
ω_{27}	0.0091		$\times$		$\times$	$\times$	$\times$	$\times$	$\times$
ω_{28}	0.0058		$\times$		$\times$				
ω_{29}	0.0073		$\times$		$\times$	$\times$		$\times$	$\times$
ω_{30}	0.0080				$\times$	$\times$			
ω_{31}	0.0034	$\times$		$\times$	$\times$	$\times$	$\times$	$\times$	$\times$
ω_{32}	0.0030	$\times$	$\times$		$\times$		$\times$		
ω_{33}	0.0017	$\times$		$\times$					
ω_{34}	0.0011		$\times$	$\times$				$\times$	
ω_{35}	0.0128	$\times$	$\times$	$\times$	$\times$	$\times$		$\times$	$\times$
ω_{36}	0.0141	$\times$		$\times$	$\times$				
ω_{37}	0.0119		$\times$	$\times$		$\times$	$\times$		
ω_{38}	0.0087		$\times$	$\times$					$\times$

ω_{39}	0.0108	$\times$	$\times$	$\times$	$\times$	$\times$	$\times$		$\times$
ω_{40}	0.0070		$\times$				$\times$		$\times$
ω_{41}	0.0015			$\times$	$\times$	$\times$		$\times$	
ω_{42}	0.0127	$\times$	$\times$	$\times$		$\times$	$\times$		$\times$
ω_{43}	0.0084	$\times$		$\times$		$\times$	$\times$		
ω_{44}	0.0038	$\times$							$\times$
ω_{45}	0.0004	$\times$	$\times$	$\times$		$\times$	$\times$		$\times$
ω_{46}	0.0060	$\times$			$\times$	$\times$		$\times$	
ω_{47}	0.0089		$\times$				$\times$	$\times$	$\times$
ω_{48}	0.0032				$\times$				
ω_{49}	0.0030		$\times$	$\times$	$\times$	$\times$	$\times$		$\times$
ω_{50}	0.0026			$\times$	$\times$	$\times$		$\times$	$\times$
ω_{51}	0.0083	$\times$		$\times$	$\times$				
ω_{52}	0.0136			$\times$				$\times$	$\times$
ω_{53}	0.0135						$\times$		$\times$
ω_{54}	0.0101	$\times$	$\times$	$\times$	$\times$	$\times$		$\times$	$\times$
ω_{55}	0.0034			$\times$			$\times$	$\times$	$\times$
ω_{56}	0.0091		$\times$	$\times$	$\times$	$\times$	$\times$	$\times$	
ω_{57}	0.0062	$\times$	$\times$	$\times$	$\times$	$\times$		$\times$	$\times$
ω_{58}	0.0055	$\times$		$\times$		$\times$	$\times$		
ω_{59}	0.0117		$\times$			$\times$	$\times$		
ω_{60}	0.0023	$\times$			$\times$		$\times$		$\times$
ω_{61}	0.0014	$\times$	$\times$		$\times$	$\times$			$\times$

ω_{62}	0.0054	$\times$	$\times$	$\times$	$\times$		$\times$	$\times$	$\times$
ω_{63}	0.0143			$\times$	$\times$	$\times$			
ω_{64}	0.0036		$\times$						
ω_{65}	0.0137					$\times$	$\times$	$\times$	
ω_{66}	0.0070	$\times$			$\times$			$\times$	$\times$
ω_{67}	0.0112		$\times$			$\times$		$\times$	$\times$
ω_{68}	0.0141		$\times$	$\times$	$\times$				$\times$

Table C.2: System X.

Outcomes ω_i	$p(\omega_i)$	A_1	A_2	A_3	A_4	A_5	A_6	A_7	A_8	A_9	A_{10}
ω_0	0.0045	$\times$			$\times$	$\times$			$\times$		$\times$
ω_1	0.0048				$\times$				$\times$		
ω_2	0.0014				$\times$	$\times$	$\times$	$\times$		$\times$	
ω_3	0.0057	$\times$		$\times$	$\times$			$\times$		$\times$	
ω_4	0.0099								$\times$	$\times$	$\times$
ω_5	0.0006	$\times$		$\times$	$\times$			$\times$	$\times$		
ω_6	0.0033	$\times$		$\times$	$\times$			$\times$	$\times$	$\times$	
ω_7	0.0003	$\times$	$\times$			$\times$	$\times$	$\times$		$\times$	
ω_8	0.0072			$\times$	$\times$	$\times$		$\times$	$\times$		
ω_9	0.0064		$\times$			$\times$				$\times$	
ω_{10}	0.0103		$\times$			$\times$	$\times$	$\times$		$\times$	
ω_{11}	0.0074	$\times$	$\times$	$\times$	$\times$			$\times$	$\times$	$\times$	$\times$
ω_{12}	0.0091			$\times$	$\times$	$\times$	$\times$	$\times$	$\times$	$\times$	

ω_{13}	0.0057	$\times$		$\times$	$\times$	$\times$		$\times$	$\times$	$\times$	$\times$
ω_{14}	0.0111				$\times$	$\times$	$\times$	$\times$	$\times$		
ω_{15}	0.0071					$\times$	$\times$			$\times$	
ω_{16}	0.0117	$\times$			$\times$			$\times$	$\times$		$\times$
ω_{17}	0.0105				$\times$			$\times$			
ω_{18}	0.0099			$\times$		$\times$	$\times$			$\times$	$\times$
ω_{19}	0.0033	$\times$		$\times$	$\times$	$\times$	$\times$	$\times$	$\times$	$\times$	
ω_{20}	0.0058		$\times$	$\times$		$\times$		$\times$	$\times$	$\times$	
ω_{21}	0.0072	$\times$	$\times$		$\times$	$\times$	$\times$	$\times$			$\times$
ω_{22}	0.0110	$\times$		$\times$	$\times$		$\times$		$\times$		$\times$
ω_{23}	0.0041	$\times$		$\times$	$\times$					$\times$	$\times$
ω_{24}	0.0057	$\times$	$\times$					$\times$			
ω_{25}	0.0061			$\times$	$\times$		$\times$	$\times$	$\times$	$\times$	$\times$
ω_{26}	0.0089	$\times$			$\times$	$\times$	$\times$	$\times$		$\times$	$\times$
ω_{27}	0.0055									$\times$	
ω_{28}	0.0025						$\times$		$\times$		
ω_{29}	0.0058		$\times$	$\times$			$\times$	$\times$			$\times$
ω_{30}	0.0026	$\times$		$\times$	$\times$			$\times$		$\times$	$\times$
ω_{31}	0.0050	$\times$		$\times$	$\times$	$\times$	$\times$	$\times$		$\times$	
ω_{32}	0.0028		$\times$				$\times$		$\times$	$\times$	$\times$
ω_{33}	0.0085			$\times$	$\times$		$\times$	$\times$	$\times$	$\times$	$\times$
ω_{34}	0.0080	$\times$	$\times$	$\times$		$\times$	$\times$	$\times$		$\times$	
ω_{35}	0.0101	$\times$	$\times$			$\times$		$\times$	$\times$	$\times$	$\times$

ω_{36}	0.0075	$\times$		$\times$	$\times$	$\times$		$\times$	$\times$		
ω_{37}	0.0066		$\times$	$\times$	$\times$	$\times$			$\times$		
ω_{38}	0.0019	$\times$	$\times$	$\times$			$\times$			$\times$	$\times$
ω_{39}	0.0109		$\times$				$\times$	$\times$	$\times$		
ω_{40}	0.0067					$\times$			$\times$	$\times$	$\times$
ω_{41}	0.0058					$\times$		$\times$	$\times$	$\times$	
ω_{42}	0.0051	$\times$				$\times$		$\times$		$\times$	$\times$
ω_{43}	0.0111		$\times$	$\times$	$\times$	$\times$			$\times$	$\times$	$\times$
ω_{44}	0.0097			$\times$	$\times$	$\times$			$\times$		$\times$
ω_{45}	0.0115		$\times$			$\times$				$\times$	$\times$
ω_{46}	0.0080			$\times$	$\times$		$\times$	$\times$	$\times$		
ω_{47}	0.0042	$\times$	$\times$	$\times$	$\times$		$\times$	$\times$		$\times$	$\times$
ω_{48}	0.0065	$\times$	$\times$		$\times$	$\times$		$\times$	$\times$	$\times$	$\times$
ω_{49}	0.0010			$\times$	$\times$		$\times$		$\times$	$\times$	$\times$
ω_{50}	0.0063						$\times$	$\times$		$\times$	
ω_{51}	0.0041	$\times$		$\times$	$\times$	$\times$	$\times$	$\times$	$\times$	$\times$	
ω_{52}	0.0018		$\times$		$\times$		$\times$	$\times$		$\times$	
ω_{53}	0.0065	$\times$	$\times$		$\times$		$\times$		$\times$		$\times$
ω_{54}	0.0101	$\times$	$\times$		$\times$	$\times$	$\times$		$\times$		$\times$
ω_{55}	0.0109	$\times$			$\times$	$\times$		$\times$			
ω_{56}	0.0028	$\times$	$\times$	$\times$				$\times$			
ω_{57}	0.0082	$\times$	$\times$	$\times$		$\times$	$\times$	$\times$	$\times$		$\times$
ω_{58}	0.0014		$\times$	$\times$	$\times$			$\times$			

ω_{59}	0.0026		$\times$	$\times$	$\times$	$\times$	$\times$				$\times$
ω_{60}	0.0039	$\times$			$\times$		$\times$	$\times$			$\times$
ω_{61}	0.0056			$\times$	$\times$	$\times$	$\times$			$\times$	$\times$
ω_{62}	0.0106										
ω_{63}	0.0073	$\times$		$\times$	$\times$	$\times$	$\times$	$\times$		$\times$	
ω_{64}	0.0024	$\times$	$\times$				$\times$				$\times$
ω_{65}	0.0049	$\times$			$\times$	$\times$			$\times$	$\times$	
ω_{66}	0.0015	$\times$	$\times$		$\times$	$\times$	$\times$		$\times$		$\times$
ω_{67}	0.0112	$\times$	$\times$	$\times$					$\times$		$\times$
ω_{68}	0.0073	$\times$	$\times$	$\times$	$\times$	$\times$			$\times$		
ω_{69}	0.0032	$\times$	$\times$	$\times$					$\times$		$\times$
ω_{70}	0.0035	$\times$			$\times$				$\times$		
ω_{71}	0.0091	$\times$				$\times$		$\times$		$\times$	$\times$
ω_{72}	0.0049	$\times$					$\times$	$\times$	$\times$		
ω_{73}	0.0063		$\times$	$\times$	$\times$		$\times$				$\times$
ω_{74}	0.0062		$\times$	$\times$			$\times$				$\times$
ω_{75}	0.0096					$\times$		$\times$	$\times$	$\times$	$\times$
ω_{76}	0.0012	$\times$	$\times$		$\times$	$\times$	$\times$				$\times$
ω_{77}	0.0111			$\times$				$\times$			$\times$
ω_{78}	0.0062		$\times$		$\times$		$\times$	$\times$	$\times$		$\times$
ω_{79}	0.0069	$\times$		$\times$	$\times$			$\times$			$\times$
ω_{80}	0.0017									$\times$	
ω_{81}	0.0110	$\times$		$\times$	$\times$			$\times$	$\times$	$\times$	

ω_{82}	0.0091			$\times$	$\times$			$\times$			$\times$
ω_{83}	0.0031	$\times$	$\times$	$\times$			$\times$	$\times$	$\times$		
ω_{84}	0.0077	$\times$							$\times$	$\times$	$\times$

Bibliography

[1] F. Behnamfar, F. Alajaji, and T. Linder. Tight error bounds for space-time orthogonal block codes under slow Rayleigh flat fading. *IEEE Transactions on Communications*, 53(6):952–956, 2005.

[2] F. Behnamfar, F. Alajaji, and T. Linder. An efficient algorithmic lower bound for the error rate of linear block codes. *IEEE Transactions on Communications*, 55(6):1093–1098, 2007.

[3] D. Bertsimas and J. Tsitsiklis. *Introduction to Linear Optimization*. Athena Scientific, 1997.

[4] E. Boros, A. Scozzari, F. Tardella, and P. Veneziani. Polynomially computable bounds for the probability of the union of events. *Mathematics of Operations Research*, 2014.

[5] J. T. Chen and E. Seneta. A Frechet-optimal strengthening of the Dawson-Sankoff lower bound. *Methodology and Computing in Applied Probability*, 8(2):255–264, 2006.

[6] A. Cohen and N. Merhav. Lower bounds on the error probability of block codes based on improvements on de caen's inequality. *IEEE Transactions on Information Theory*, 50(2):290–310, 2004.

[7] D. Dawson and D. Sankoff. An inequality for probabilities. *Proceedings of the American Mathematical Society*, 18(3):504–507, 1967.

[8] D. De Caen. A lower bound on the probability of a union. *Discrete Mathematics*, 169(1):217–220, 1997.

[9] A. Dembo. Unpublished material. unpublished.

[10] C. Feng and L. Li. On the Móri-Székely conjectures for the Borel-Cantelli lemma. *Studia Scientiarum Mathematicarum Hungarica*, 50(2):280–285, 2013.

[11] C. Feng, L. Li, and J. Shen. Some inequalities in functional analysis, combinatorics, and probability theory. *The Electronic Journal of Combinatorics*, 17(R58):1, 2010.

[12] J. Galambos and I. Simonelli. *Bonferroni-type inequalities with applications.* Springer series in statistics: Probability and its applications. Springer, 1996.

[13] S. Gallot. A bound for the maximum of a number of random variables. *Journal of Applied Probability*, 3(2):556–558, 1966.

[14] F. M. Hoppe. Improving probability bounds by optimization over subsets. *Discrete Mathematics*, 306(5):526–530, 2006.

[15] F. M. Hoppe. The effect of redundancy on probability bounds. *Discrete Mathematics*, 309(1):123–127, 2009.

[16] R. A. Horn and C. R. Johnson, editors. *Matrix Analysis.* Cambridge University Press, New York, NY, USA, 1986.

[17] E. G. Kounias. Bounds for the probability of a union, with applications. *The Annals of Mathematical Statistics*, 39(6):2154–2158, 1968.

[18] H. Kuai. Tight Bounds on The Probability of a Union with Applications to Non-uniform Signaling over AWGN Channels. Master's thesis, Department of Mathematics and Statistics, Queen's University, 1999.

[19] H. Kuai, F. Alajaji, and G. Takahara. A lower bound on the probability of a finite union of events. *Discrete Mathematics*, 215(1-3):147–158, 2000.

[20] H. Kuai, F. Alajaji, and G. Takahara. Tight error bounds for nonuniform signaling over AWGN channels. *IEEE Transactions on Information Theory*, 46(7):2712–2718, 2000.

[21] O. Mangasarian. Uniqueness of solution in linear programming. *Linear Algebra and its Applications*, 25:151 – 162, 1979.

[22] Z. Mao, J. Cheng, and J. Shen. A new lower bound on error probability for nonuniform signals over AWGN channels. In *Wireless Communications and Networking Conference (WCNC)*, pages 3005–3009. IEEE, 2013.

[23] A. Prékopa and L. Gao. Bounding the probability of the union of events by aggregation and disaggregation in linear programs. *Discrete Applied Mathematics*, 145(3):444–454, 2005.

[24] V. V. Vazirani. *Approximation Algorithms.* Springer-Verlag New York, Inc., New York, NY, USA, 2001.

[25] B. Vizvári. New upper bounds on the probability of events based on graph structures. *RUTCOR Research Report (Sept. 2004)*.

[26] J. Yang, F. Alajaji, and G. Takahara. Lower bounds on the probability of a finite union of events. submitted, 2014.

[27] J. Yang, F. Alajaji, and G. Takahara. New bounds on the probability of a finite union of events. In *2014 IEEE International Symposium on Information Theory (ISIT)*, pages 1271–1275, June 2014.