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Towards Tightness with Pairwise Independence, Extremal Dependence and Robust Satisficing Using Linear and Conic Duality

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Abstract

Optimization under uncertainty as an area of research has seen remarkable progress over the past few decades, under the headings of stochastic programming, robust and distributionally robust optimization. Duality in its various forms has been at the heart of these advances. This dissertation addresses two classes of problems at the interface of optimization and uncertainty which harness the power of linear and conic duality. Firstly, we focus on distributional uncertainty where the goal is to find the best possible bounds on tail probability and expected value functions of sums of Bernoulli random variables, attained by an extremal probability distribution from a set of distributions consistent with the given marginal probability and correlation information. We primarily consider two types of correlation structure among the variables, *i.e.*, pairwise independence (where the variables are uncorrelated) and extremal dependence (where the correlation between the variables is unknown). The tail probability function we consider is the right tail or the probability of occurrence of at least k out of n Bernoulli events, where $k \in [0, n]$ is an integer while the expected value function is the expected value of a stop-loss type function.

For pairwise independent variables, while some useful bounds on the tail probability function have been proposed in the literature, none of these bounds are tight in general. We provide several results towards finding tight probability bounds for this class of problems. When the individual and bivariate probabilities are known, even verifying if a joint distribution consistent with the given information exists, is known to be an NP-complete problem. Surprisingly however, we show that it is possible to capture the tightest upper bound on the probability of the union of n pairwise independent events ($k = 1$) in a closed-form expression for any input marginal probability vector $\mathbf{p} \in [0, 1]^n$. The proof involves showing the existence of a positively correlated Bernoulli random vector for any $\mathbf{p} \in [0, 1]^n$, which is of independent interest in itself, since feasibility is typically not guaranteed for arbitrary correlation structures. Applications in correlation gap analysis, where pairwise independence provides better bounds (than extremal dependence) in some instances are discussed. For two random variables, we show that the correlation gap is upper bounded by $4/3$ for any non-negative, non-decreasing, submodular function. We also prove that the Bonferroni lower bounds on the union of pairwise independent events are tight for small probabilities. Secondly, for $k \geq 2$ and any input marginal probability vector $\mathbf{p} \in [0, 1]^n$, new upper bounds are derived exploiting ordering of probabilities. Numerical examples are provided to illustrate when the bounds provide significant improvement over existing bounds. Thirdly, while the existing and new bounds are not always tight, we provide special instances when they are shown to be tight. Specifically, when the marginals are identical, we show that for any $k \in [0, n]$, the bound derived in Boros and Prékopa (1989) is always tight and this result can be easily extended to identical t -wise independent variables. Further, we identify conditions under which this result provides useful small deviation bounds while other existing bounds are trivial. For the expected stop-loss function, in the special case when all the pairwise independent variables are identical, we provide an alternative proof to derive the tightest bound in a known closed-form expression, along with extremal distributions that attain the bound.

With extremal dependence, we show that the tightest bounds on a weighted tail probability function can be computed as the optimal value of a compact linear program. Useful applications in a *limited dependency* system where only some of the variables are extremally dependent while the rest are mutually independent and these two sets of

variables are independent of each other are explored. As a special case of the weighted tail probability function, we derive an earlier known closed-form bound (Rüger, 1978) on the probability that at least k out of n Bernoulli events occur. The usefulness of the closed-form bounds is subsequently demonstrated in solving *star-shaped* marginal systems. The results from the Bernoulli case are extended to derive useful upper bounds on the tail probability function of sums of random variables with discrete support. Numerical illustrations show that these bounds are tight in many randomly generated instances with identical and non-identical probabilities. For expected stop-loss functions, we prove that the comonotonic distribution attains the tightest upper bound while the Jensen (1906) bound is the tightest lower bound by similarly deriving a compact linear program.

cWe propose an alternative model inspired by the principle of satisficing but based on a constraint function that evaluates to the optimal objective value of a standard conic optimization problem, that can be used to model a wide range of constraint functions that are convex in the decision variables but can be either convex or concave in the uncertain parameters. As a result, our model provides a unifying framework that generalizes and encompasses a wide variety of similar problems considered in recent papers. We derive an exact semidefinite optimization formulation when the constraint is biconvex quadratic with quadratic penalty and the support set is ellipsoidal. For more general conic uncertain problems with polyhedral support sets and penalty functions, we show the equivalence between the robust satisficing problems and the classical adaptive robust linear optimization models with conic uncertainty sets, where the latter can be solved approximately using affine recourse adaptation. More importantly, under the stated assumptions, we show that the exact reformulation and safe approximations do not lead to infeasible problems if the chosen target is above the optimum objective of the nominal problem. For the special case of a non-negative orthant cone, we prove that despite being simpler, the affine recourse approximation of the dual reformulation is closer to the original problem when compared to a specific non-affine recourse approximation of the original problem itself. Finally, we extend our framework to the data-driven setting and showcase the modeling and the computational benefits of the robust satisficing framework over classical robust optimization with three numerical examples: growth optimal portfolio selection, log-sum-exp optimization and adaptive lot-sizing problem.

Keywords: Bernoulli random variables, tail probability, tight bounds, pairwise independence, extremal dependence, linear programming, linear duality, bivariate feasibility, correlation gap, small deviation bounds, submodular functions, expected stop-loss functions, robust optimization, robust satisficing, biconvex constraints, conic optimization, conic duality, affine recourse adaptation, data-driven optimization

Preprints

i) **Tight Probability Bounds with Pairwise Independence**

-This paper is the outcome of research conducted with Karthik Natarajan at the Singapore University of Technology and Design during the first half of my doctoral candidature and is included in Chapter 2 of this dissertation.

ii) **Robust Conic Satisficing**

-This paper is the outcome of research conducted with Napat Rujeerapaiboon and Melvyn Sim at the National University of Singapore during the second half of my doctoral candidature and is included in Chapter 4 of this dissertation.

iii) **Extremal probability bounds in combinatorial optimization**

-This paper is the outcome of joint research conducted with Divya Padmanabhan, Selin Damla Ahipasaoglu and Karthik Natarajan and Section 3.3 of this dissertation is included in this work.

Conferences

	Conference name	Location	Month and Year	Work presented
1.	ESD summer conference	SUTD, Singapore	September, 2018	Section 3.1.1
2.	Production and operations management society (POMS)	Hongkong	September, 2019	Section 3.1.2
3.	ESD summer conference	SUTD, Singapore	September, 2019	Sections 2.3, 2.4.1, 2.4.2
4.	INFORMS	Seattle	October, 2019	Sections 2.3, 2.4.1, 2.4.2
5.	Robust optimization webinar (ROW)	Virtual	October, 2020	Tight probability bounds with pairwise independence
6.	Global young scientists summit (GYSS)	Virtual	January, 2021	Sections 2.2, 2.2.3
7.	Analytics for X	NUS, Singapore	July, 2021	Robust conic satisficing

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Symbols and Description , Part I

The following tables are meant to be quick reference for the symbols used in this dissertation. The symbols along with their interpretation will be clearly defined as and when encountered in their specific context.

Description	Symbol	Expression/Interpretation
Set of real numbers	\mathbb{R}	$\mathbb{R} = (-\infty, \infty)$
Set of integers and positive integers	\mathbb{Z}, \mathbb{Z}_+	$\mathbb{Z} = \{\dots, -1, 0, 1, \dots\}, \mathbb{Z}_+ = \{1, 2, \dots\}$
Set of rational numbers	\mathbb{Q}	$\mathbb{Q} = \{p/q \mid p, q \in \mathbb{Z}, q \neq 0\}$
Floor and ceiling functions	$\lfloor x \rfloor, \lceil x \rceil$	$\lfloor x \rfloor = \{y \in \mathbb{Z} \mid y \leq x < y + 1\}, \lceil x \rceil = \{y \in \mathbb{Z} \mid y - 1 < x \leq y\}$
Positive and fractional part of a real number	$x^+, \{x\}$	$x^+ = \max(x, 0), x \in \mathbb{R}, \{x\} = x - \lfloor x \rfloor, x \in \mathbb{R}$
Binomial coefficient	$\binom{r}{s}$	$\binom{r}{s} = \frac{r!}{(s!(r-s)!)}, r \geq s \geq 0, r, s \in \mathbb{Z}_+$
Number of random variables	n	$n \in \mathbb{Z}_+$
Running index	$[n]$	$\{1, 2, \dots, n\}$
Closed interval of integers	$[i, j]$	$[i, j] = \{i, i + 1, \dots, j - 1, j\}, i, j \in \mathbb{Z}^+, i < j$
Set of pairwise indices	K_n	$K_n = \{(i, j) : 1 \leq i < j \leq n\}$
Indicator Function	$\mathbb{1}_A$	$\mathbb{1}_A(x) = \begin{cases} 1, & \text{if } x \in A \\ 0, & \text{otherwise} \end{cases}$
Random vector	\tilde{c}	$\tilde{c} = (\tilde{c}_i), i \in [n]$
Sum of random variables	$\tilde{\xi}$	$\tilde{\xi} = \sum_{i=1}^n \tilde{c}_i$
Number of support points (discrete)	m	$\tilde{c}_i \in \{0, 1, \dots, m - 1\}, \forall i \in [n]$
Set of realizations of c	$\mathcal{C}, \mathcal{C}_d$	$\mathcal{C} = \{0, 1\}^n, \mathcal{C}_d = \{0, 1, 2, \dots, m - 1\}^n$
Univariate marginal vector	\mathbf{p}	$\mathbf{p} = (p_i), i \in [n]$
Bivariate Marginals	p_{ij}	$p_{ij} = P(\tilde{c}_i = 1, \tilde{c}_j = 1), (i, j) \in K_n$
Univariate ambiguity set	Θ_u	$\Theta_u = \{\theta(\{0, 1\}^n) : \mathbb{P}_\theta(\tilde{c}_i = 1) = p_i, \forall i \in [n]\}$
Pairwise independence ambiguity set	Θ_{pw}	$\Theta_{pw} = \{\theta(\{0, 1\}^n) : \mathbb{P}_\theta(\tilde{c}_i = 1, \tilde{c}_j = 1) = p_i p_j \forall (i, j) \in K_n, \mathbb{P}_\theta(\tilde{c}_i = 1) = p_i, \forall i \in [n]\}$
Discrete variables ambiguity set	Θ_d	$\Theta_d = \{\theta(\{0, 1, \dots, m - 1\}^n) : \mathbb{P}_\theta(\tilde{c}_i = j) = p_{ij}, i \in [n], j \in [0, m - 1]\}$
Extremal tail probability and expectation upper bounds (lower bounds denoted with $\underline{P}, \underline{E}$)	$\bar{P}_u(n, k, \mathbf{p}), \bar{E}_u(n, k, \mathbf{p})$ (univariate)	$\bar{P}_u(n, k, \mathbf{p}) = \max_{\theta \in \Theta_u} \mathbb{P}_\theta(\sum_{i=1}^n \tilde{c}_i \geq k), k \in [n]$ $\bar{E}_u(n, k, \mathbf{p}) = \max_{\theta \in \Theta_u} \mathbb{E}_\theta \left[\left(\sum_{j=1}^n \tilde{c}_j - k \right)^+ \right], k \in [n]$
	$\bar{P}(n, k, \mathbf{p}), \bar{E}(n, k, \mathbf{p})$ (pairwise independence)	$\bar{P}(n, k, \mathbf{p}) = \max_{\theta \in \Theta_{pw}} \mathbb{P}_\theta(\sum_{i=1}^n \tilde{c}_i \geq k), k \in [n]$ $\bar{E}(n, k, \mathbf{p}) = \max_{\theta \in \Theta_{pw}} \mathbb{E}_\theta \left[\left(\sum_{j=1}^n \tilde{c}_j - k \right)^+ \right], k \in [n]$
Extremal weighted tail probability bounds	$\bar{P}_{uw}(n, \mathbf{w}, \mathbf{p})$ $\mathbf{w} = (w_i), w_i \in \mathbb{R}, \forall i \in [n]$	$\bar{P}_{uw}(n, \mathbf{w}, \mathbf{p}) = \max_{\theta \in \Theta_u} \sum_{l=0}^n w_l \mathbb{P}_\theta(\sum_{i=1}^n \tilde{c}_i = l)$
Extremal discrete variables tail probability bounds (univariate)	$\bar{P}_d(n, k, \mathbf{p})$	$\bar{P}_d(n, k, \mathbf{p}) = \max_{\theta \in \Theta_d} \mathbb{P}_\theta(\sum_{i=1}^n \tilde{c}_i \geq k), k \in [n(m - 1)]$
Multilinear polynomials	$S_j(\mathbf{c}), j \in [n]$	$S_j(\mathbf{c}) = \sum_{1 \leq i_1 < i_2 < \dots < i_j \leq n} c_{i_1} c_{i_2} \dots c_{i_j}$
Binomial Moments	$S_r, r \leq n$	$S_r = \mathbb{E}[S_r(\mathbf{c})]$
First and second partial binomial moments (pairwise independence)	S_{1r}, S_{2r}	$S_{1r} = \sum_{i=1}^{n-r} p_i, r \in [0, n - 1],$ $S_{2r} = \sum_{(i,j) \in K_{n-r}} p_i p_j, r \in [0, n - 2],$ $0 \leq p_1 \leq p_2 \leq \dots \leq p_n \leq 1$

Symbols and Description , Part II

Description	Symbol	Expression / Interpretation
Set of non-negative and strictly positive reals	$\mathbb{R}_+, \mathbb{R}_{++}$	$\mathbb{R}_+ = \{x \mid x \in \mathbb{R}, x \geq 0\}$ $\mathbb{R}_{++} = \{x \mid x \in \mathbb{R}, x > 0\}$
Space of n dimensional reals	\mathbb{R}^n	$\mathbb{R}^n = \{(x_1, x_2, \dots, x_n) \mid x_i \in \mathbb{R}, \forall i \in [n]\}$
Set of $m \times n$ real matrices	$\mathbb{R}^{m \times n}$	$\mathbf{A} \in \mathbb{R}^{m \times n}$ iff $\mathbf{A} = [a_{ij}]$, $a_{ij} \in \mathbb{R}$, $\forall i \in [m], \forall j \in [n]$
Set of positive semidefinite matrices	\mathbb{S}_+^n	$\mathbb{S}_+^n = \{\mathbf{M} \in \mathbb{S}^n \mid \mathbf{M} \succeq \mathbf{0}\}$, where $\mathbb{S}^n = \{\mathbf{A} \in \mathbb{R}^{n \times n} \mid \mathbf{A} = \mathbf{A}^\top\}$
Vector of zeros and ones (of appropriate dimension)	$\mathbf{0}, \mathbf{1}$	$\mathbf{0} = (0, 0, \dots, 0)^\top$, $\mathbf{1} = (1, 1, \dots, 1)^\top$
Identity matrix	\mathbf{I}_n	$\mathbf{I}_n = \{\mathbf{A} \in \mathbb{R}^{n \times n} \mid \mathbf{A}_{ij} = \mathbb{1}_{i=j}, \forall i, j \in [n]\}$
Proper cone	\mathcal{K}	$\mathcal{K} = \{\mathbf{x} \in \mathbb{R}^n \mid \mathbf{x} \in \mathcal{K} \implies \lambda \mathbf{x} \in \mathcal{K}, \forall \lambda \geq 0\}$
Dual cone	\mathcal{K}^*	$\mathcal{K}^* = \{\mathbf{y} \in \mathbb{R}^n \mid \mathbf{y}^\top \mathbf{x} \geq 0, \forall \mathbf{x} \in \mathcal{K}\}$
Conic inequality	$\mathbf{B}\mathbf{y} \succeq_{\mathcal{K}} \mathbf{v}$	$\mathbf{B}\mathbf{y} - \mathbf{v} \in \mathcal{K}$
Superscript indexing	$\mathbf{w}^i, \mathbf{A}^i$	i^{th} vector (matrix) among a countable set of vectors (matrices) $\{\mathbf{w}^i\}, \{\mathbf{A}^i\}$
Subscript indexing	\mathbf{A}_i	i^{th} row of a matrix \mathbf{A}
Dual norm	$\ \cdot\ ^*$	$\ \mathbf{x}\ ^* = \sup_{\ \mathbf{y}\ \leq 1} \mathbf{x}^\top \mathbf{y}$
Compact and convex sets	$\mathcal{X}, \mathcal{Z}, \mathcal{P}$	Feasible set (decision variables) : $\mathcal{X} \subseteq \mathbb{R}^{n_x}$, Uncertainty support set : $\mathcal{Z} \subseteq \mathbb{R}^{n_z}$ Dual uncertainty support set : $\mathcal{P} \subseteq \mathbb{R}^{n_h}$
Decision variables vector	\mathbf{x}	$\mathbf{x} \in \mathcal{X}$
Uncertain parameter vector	\mathbf{z}	$\mathbf{z} \in \mathcal{Z}$
Dual uncertain parameter	$\boldsymbol{\rho}$	$\boldsymbol{\rho} \in \mathcal{P}$
Penalty function	$p(\mathbf{z})$	$p(\mathbf{z}) : \mathbb{R}^n \mapsto \mathbb{R}_+$
Uncertainty set of radius r	\mathcal{U}_r	$\mathcal{U}_r = \{\mathbf{z} \in \mathcal{Z} \mid p(\mathbf{z} - \hat{\mathbf{z}}) \leq r\}$
Polyhedral uncertainty set	\mathcal{Z}	$\mathcal{Z} = \{\mathbf{z} \in \mathbb{R}^{n_z} \mid \mathbf{H}\mathbf{z} \leq \mathbf{h}\}$, $\mathbf{H} \in \mathbb{R}^{n_h \times n_z}$, $\mathbf{h} \in \mathbb{R}_+^{n_h}$
Robust satisficing parameter	k	$k \in \mathbb{R}_+$
Target	τ	$\tau > Z_0$
Deterministic nominal value	$\hat{\mathbf{z}}$	$\hat{\mathbf{z}} \in \mathcal{Z}$
Conic representable function	$g(\mathbf{x}, \mathbf{z})$	$g(\mathbf{x}, \mathbf{z}) = \min \mathbf{d}^\top \mathbf{y}$ s.t. $\mathbf{B}\mathbf{y} \succeq_{\mathcal{K}} \mathbf{f}(\mathbf{x}) + \mathbf{F}(\mathbf{x})\mathbf{z}$ $\mathbf{y} \in \mathbb{R}^{n_y}$, $\mathbf{f} : \mathbb{R}^{n_x} \mapsto \mathbb{R}^{n_f}$, $\mathbf{F} : \mathbb{R}^{n_x} \mapsto \mathbb{R}^{n_f \times n_z}$
Recourse matrix	\mathbf{B}	$\mathbf{B} : \mathbb{R}^{n_f} \mapsto \mathbb{R}^{n_y}$
Recourse variable	\mathbf{y}	$\mathbf{y} \in \mathbb{R}^{n_y}$
Dual recourse variables	$\boldsymbol{\beta}, \boldsymbol{\mu}, \eta$	$\boldsymbol{\beta} \in \mathbb{R}_+^{n_h}$, $\boldsymbol{\mu} \in \mathbb{R}^{n_\mu}$, $\eta \in \mathbb{R}$
Nominal optimal objective	Z_0	$Z_0 = \min \mathbf{c}^\top \mathbf{x}$ s.t. $g(\mathbf{x}, \hat{\mathbf{z}}) \leq 0$ $\mathbf{x} \in \mathcal{X}$
Robust optimal objective	Z_r	$Z_r = \min \mathbf{c}^\top \mathbf{x}$ s.t. $g(\mathbf{x}, \mathbf{z}) \leq 0 \quad \forall \mathbf{z} \in \mathcal{U}_r$, $\mathbf{x} \in \mathcal{X}$
Family of functions	$\mathcal{R}^{m,n}$	$\mathcal{R}^{m,n} = \{\mathbf{y} \mid \mathbf{y} : \mathbb{R}^m \mapsto \mathbb{R}^n\}$
Class of affine recourse functions	$\mathcal{L}^{m,n}$	$\mathcal{L}^{m,n} = \{\mathbf{y} \in \mathcal{R}^{m,n} \mid \exists \boldsymbol{\pi} \in \mathbb{R}^n, \boldsymbol{\Pi} \in \mathbb{R}^{n \times m} : \mathbf{y}(\mathbf{z}) = \boldsymbol{\pi} + \boldsymbol{\Pi}\mathbf{z} \}$.

Dedicated to:

My dearest parents Shrimati Vani Ramachandra and Shri KS Ramachandra,

My beloved, most admirable, awe-inspiring preceptor and ever well-wisher,

A.C. Bhaktivedanta Swami,

on his 125th birth anniversary

and

to so many other selfless souls who have inspired and shaped my very life.

Chapter 1

Introduction

1.1 Origins of linear programming and optimization under uncertainty

Operations research as a scientific discipline has contributed immensely to a holistic understanding of the mathematics behind optimization. What began as a wartime initiative to facilitate military planning and logistics has today expanded to include sophisticated mathematical models that address problems of a vast variety of industries in the civilian sector. The tremendous progress over the past half century and more has made a remarkable impact on society by finding applications in sectors ranging from oil refineries to insurance and banking to civil aviation. Traditionally, operations research has been concerned with optimization techniques that help determine optimal solutions to some real-world objective function while satisfying a given set of constraints. While breakthroughs in linear programming happened in the 1940's with the development of the simplex algorithm by George Dantzig (also attributed to Leonid Kantorovich¹), subsequent efforts focused on more complex constraints and objectives which led to the development of integer, quadratic, second-order cone, semidefinite, geometric, conic and non-convex programming techniques. While classical optimization methods were developed to solve deterministic planning problems, stochastic models independently evolved to address problems involving uncertainty. More recently, over the past few decades, an integrated approach combining optimization with uncertainty has gained huge traction under the headings of stochastic programming, robust and distributionally robust optimization. In the words of George Dantzig, who is considered to be the father of linear optimization, "Planning under uncertainty. This, I feel, is the real field we should all be working on"². Given the ubiquitous presence of uncertainty in real-world optimization problems, this unified approach is more practical, yet poses new computational challenges due to the increased complexity.

1.2 Role of uncertainty and duality in this dissertation

This dissertation broadly discusses two classes of problems at the intersection of optimization and uncertainty. Part I focuses on distributional uncertainty where the goal is to find the best possible bounds on functions of sums of random variables, attained by an extremal probability distribution from a set of distributions consistent with the given marginal probability information. Sums of random variables are part of a larger

¹<https://www.informs.org/Explore/History-of-O.R.-Excellence/Biographical-Profiles/Kantorovich-Leonid-V>

²<https://www.informs.org/Explore/History-of-O.R.-Excellence/Biographical-Profiles/Dantzig-George-B#oral>

class of problems considered in the literature which involve optimizing linear functions of random variables over a given feasible region (Natarajan, 2021). Within this subclass, Bernoulli random variables are a special case which is the focus of the majority of this work. Part II deals with robust uncertainty where the uncertain parameters of the optimization problem vary within a prescribed support set and their probability distribution is assumed to be unknown. The key intention is to achieve an ideal combination of flexibility and tractability by which the models considered can accommodate a broad class of robust optimization problems considered in the literature and yet provide efficiently computable optimal solutions or approximations, where “efficient computability” refers to polynomial time solvability in the input representation.

At the heart of all these optimization techniques is the concept of duality whose discovery, in the context of linear programming, is attributed to John von Neumann by George Dantzig himself³. Rigorous proofs were subsequently provided by Karush (1939) and Kuhn and Tucker (1951) with extensions to convex non-linear programming. The theory of linear duality suggests that for any given linear optimization problem, there exists another optimization problem in a different dimension which attains the same optimal objective function value, if it exists. Theoretical advances in non-linear optimization have given rise to more general versions of duality such as conic duality. While even a finite dimensional optimization problem in its primal form may be intractable (where tractability refers to polynomial time solvability using current available solvers) due to a large number of variables or constraints, the dual program, which reverses the number of variables and constraints may help reformulate the original problem to provide efficiently computable solutions or at the very least provide bounds on the objective function value while offering deeper insights into the structure of the problem responsible for the hardness. It would not be an exaggeration to say that the concept of duality has and continues to help address many challenging problems in mathematical optimization such as the assignment, shortest-path, max flow-min cut problems or existence of equilibria in zero-sum games to mention a few.

This dissertation also demonstrates the power of harnessing duality in providing efficiently computable solutions to otherwise challenging uncertain optimization problems. Part I of the dissertation consisting of Chapters 2 and 3 exploits linear duality to solve uncertain linear programs. More specifically, we consider computing tight bounds on tail probability and expected stop-loss functions of sums of Bernoulli random variables as the optimal value of a compact linear program. “Tight” here refers to a bound that is always attained by a joint probability distribution consistent with the given input information, *i.e.*, marginal probabilities and correlation, while “tail” refers to the right tail or the probability that at least k out of n variables are one, where $k \in [0, n]$ is an integer. One of the crucial factors that affects tractability of such bounds is the dependence structure among the variables. Assuming that the variables are mutually independent has been the predominant assumption in the literature, in part due to the convenience it affords in not requiring additional information about the joint probabilities. However, this is often not practical, since, in reality, the variables are likely to be correlated to varying degrees. For example, the individual risks in an insurance portfolio would not typically exhibit independence since they are influenced by common economic or environmental factors such as recessions or pandemics. At the other end of the spectrum, we have extremally dependent variables where the only information available is the univariate marginal probabilities, *i.e.*, no information

³Reminiscences About the Origins of Linear Programming (Dantzig, 1982)

about the correlation structure is specified. Introducing a small degree of independence into the extremally dependent model gives rise to pairwise independence, which is a weaker notion of complete independence, although pairwise independent variables are also uncorrelated like mutually independent variables. Our focus in Part I is to compute bounds on functions of sums of pairwise independent and extremally dependent variables, which are referred to as the pairwise independent and univariate bounds respectively throughout the dissertation.

Firstly, in Chapter 2, we consider pairwise independent variables which admit low cardinality joint distributions. Despite this advantage, computing bounds on the tail probability and expected value functions appears to be computationally challenging, even though formal hardness results, to the best of our knowledge, have not been established in the literature. The hardness in the problem primarily appears to stem from the quadratic nature of the constraints in the dual separation problem, which does not seem to admit compact reformulations as in the univariate case. Interestingly however, in some special cases, such as when the union probability is considered or when the variables are identical, we prove that the best bounds can be computed in closed-form by leveraging standard linear programming and duality theory, while in more general cases, new improved bounds are derived by suitable construction of dual feasible solutions. While some of these bounds are previously established in the literature, their tightness with pairwise independent variables does not appear to be known. Additionally, in the earlier mentioned special cases, our proof deploys a constructive approach, wherein we explicitly provide the extremal distributions that attain the closed-form bounds. With tail probability bounds, useful applications such as correlation gap analysis show that pairwise independence can improve the gap (as compared to the univariate bounds) with bounds derived from mutual independence. For two random variables, we show that the correlation gap is upper bounded by $4/3$ for any non-negative, non-decreasing, submodular function and that the bound is attained. Applications in analysis of small deviation bounds show that with Bernoulli variables, pairwise independence is sufficient to generate non-trivial bounds in contrast to more general random variables where 4-wise independence is known to be necessary. All these results and their extensions are the direct outcome of exploiting linear duality.

Next, in Chapter 3, we consider similar bounds for extremally dependent variables, where only the univariate marginal probabilities are known. Due to fewer restrictions, this class of problems offer more flexibility than the pairwise independent class and are thus amenable to tractable reformulations. While the number of primal variables in the large-sized linear program formulation that computes this bound grows exponentially in the input size, we prove the polynomial-time solvability of the dual separation problem (which is an integer linear program) by suitably leveraging duality to transform it into a compact linear program with an integer polytope. The equivalence of separation and optimization (Grötschel, Lovász, and Schrijver, 2012) then shows that the original optimization problem is efficiently solvable. This result is then extended to derive tight bounds on more general weighted tail probability functions as the optimal value of a compact linear program. These bounds find application in useful settings such as *limited dependency*, where some of the variables are extremally dependent while the rest are mutually independent. In special cases, these compact linear program formulations admit closed-form solutions. While some of these closed-form bounds are well known, we not only provide alternative optimization-based proofs of these results, but the derived compact linear programs employ far less constraints and decision variables than

existing compact formulations.

In Part II of this dissertation, we address conic uncertain problems with quadratic and polyhedral uncertainty sets in the context of a recently proposed framework known as *robust satisficing* (Long, Sim, and Zhou, 2021), where nature can adversarially choose the uncertain parameters from a pre-defined support set. Instead of sizing the uncertainty set as in robust optimization, the robust satisficing model is specified by a target objective with the aim of delivering a solution that is least impacted by uncertainty while achieving the target. At the heart of this framework, we minimize the level of constraint violation under all possible realizations within the support set, where the constraint function evaluates to the optimal objective value of a standard conic optimization problem and the violation is proportional to a pre-specified convex penalty function. The optimization model thus considered is very generic and encompasses a wide range of constraints including those convex in both the decision variables and the uncertain parameters, that cannot be handled by classical robust optimization techniques. With quadratic constraints, uncertainty support and penalty function, we derive an exact semidefinite program formulation. For more general conic uncertain problems with polyhedral support sets and penalty functions such exact reformulations may not be available. Conic duality once again plays a critical role in overcoming this challenge, albeit with necessary complete recourse assumptions. By successive dualization over the *wait-and-see* decisions and uncertain parameters, the original conic optimization problem is transformed into a classical adaptive robust linear program with a conic uncertainty set. This equivalent problem can not only be efficiently approximated using affine recourse adaptation, but also admits trivial feasible solutions. Unlike the primal problem where the structure of the feasible solution is difficult to ascertain, the dual reformulation always admits a feasible solution in which the recourse variables are affine functions of the uncertain parameters. Three numerical examples of growth optimal portfolio selection, log-sum-exp optimization and adaptive lot-sizing demonstrate the improved performance of the robust satisficing framework over classical robust optimization. Specifically, the lot-sizing numerical example demonstrates that with the non-negative orthant cone, the dual formulation shows a remarkable improvement in computational speed over the primal model. Thus, the dual formulation provides *tractability*, *feasibility* and *computational* benefits over the original primal problem.

1.3 Summary and contributions

In summary, this dissertation addresses uncertain optimization problems by harnessing the power of linear and conic duality to:

- i) Derive compact linear programming formulations that employ less constraints and decision variables than existing compact formulations to compute bounds on tail probability and expected stop-loss functions of sums of random variables.
- ii) Derive tight bounds on such functions in a closed-form expression where possible.
- iii) Demonstrate the usefulness of the derived tight bounds with interesting applications.
- iv) Construct extremal distributions that attain these tight bounds in special cases.

- v) Derive improved bounds on such functions when the tight bounds are not computable using existing techniques.
- vi) Illustrate the improved performance of these bounds over existing bounds with numerical examples.
- vii) Provide *tractability*, *feasibility* and *computational* advantages over classical robust models for conic optimization problems.
- viii) Provide better affine recourse approximations to two-stage adaptive linear optimization problems than specific non-affine recourse approximations of the original problem.

1.4 Dissertation structure

The presentation structure of this dissertation is as follows:

- Each part broadly covers themes under the banner of optimization under uncertainty.
- Every chapter in a part covers topics in line with the part theme, under specific assumptions on the input information to the problem.
- In every chapter, the most important results are segregated into sections while numerical illustrations and extensions are provided in sub-sections.
- At the beginning of each section, we provide a brief high-level introduction and literature survey of the topic being covered. Additionally, in Part I, after each result is presented, we provide a more detailed literature survey in a "Connection to earlier work" segment. This serves to guide the reader to more specific references related to the particular result derived, with alternative proofs or applications, after reading through the derived proofs.
- Symbols and notations are defined as and when necessary throughout the document and kept unique to retain their interpretation to the extent possible. In case of overlap, the interpretation will be clear from the specific context in which they are used.
- Dense equations, tables and figures are sometimes intentionally scaled to extend beyond the page margins so as to allow for easy readability and clarity of view.
- All proofs but one are provided in the main body of the dissertation. The appendix contains a single but lengthy proof of a result in Chapter 2. When similar ideas from earlier proofs are used, the proof or a part of it is omitted for the sake of brevity.
- References in the bibliography section are categorized chapter-wise and alphabetically ordered within each category.
- All numerical results in Part I were obtained using Gurobi 9.1.1 solver with Python 3.7.7 while the results in Part II were obtained using Mosek 9.2.38 together with YALMIP modeling language (Löfberg, 2004) and MATLAB R2020a, Gurobi 9.1.1 with RSOME (Robust Stochastic Optimization Made Easy) modeling language (Chen, Sim, and Xiong, 2020) and Python 3.7.7. All experiments were conducted on an Intel Core i7 2.7GHz MacBook with 16GB of RAM.

Part I

Bounds with Distributional Uncertainty

Chapter 2

Bounds with Pairwise Independence

Computing probability bounds on the occurrence of at least k of a finite number of Bernoulli events $\{E_1, E_2, \dots, E_n\}$, given their individual probabilities of occurrence, lies at the intersection of probability theory, computer science, financial risk management, reliability systems, stochastic programming and other allied topics and has thus received considerable attention from several authors across the spectrum over the past two centuries. We note that the problem can be expressed as finding probability bounds on Bernoulli random variables $c_i, i \in [n]$ adding up to at least a threshold k where $c_i = \mathbb{1}_{E_i}$ ($\mathbb{1}$ being the indicator function) and $k \in [n]$. Specifically, when $k = 1$, the problem of finding bounds on the probability of the union of n events has been extensively studied in the literature and popularly referred to as the union bounds.

In this chapter, our focus is on computing tail probability bounds on sums of pairwise independent Bernoulli random variables. Unlike with mutually independent Bernoulli variables, where the tail probability is efficiently computable using the Poisson Binomial distribution, efficient computation of extremal tail probability bounds for pairwise independent Bernoulli variables remains an open question, even though pairwise independence is a weaker notion of mutual independence. This chapter provides partial answers to this question by showing that in special cases such as when the union probability is considered or when the marginals are identical, the tightest bound can be captured in a closed-form expression. Other than these special cases, improved bounds exploiting ordering of the probabilities are derived in this chapter. Sections 2.1 - 2.4.2 in this chapter are primarily derived from our paper Ramachandra and Natarajan (2021), while the subsequent sections provide auxiliary results and generalizations of some results in these sections.

2.1 Motivation

It is well known that while mutually independent random variables are pairwise independent, the reverse is not true. Feller (1968) attributes Bernstein (1946) with identifying one of the earliest examples with $n = 3$ random variables which are pairwise independent, but not mutually independent. For general n , constructions of pairwise independent Bernoulli random variables can be found in the works of Geisser and Mantel (1962), Karloff and Mansour (1994), and Koller and Meggido (1994), pairwise independent discrete random variables in Feller (1959), Lancaster (1965), Joffe (1974), and O'Brien (1980) and pairwise independent normal random variables in Geisser and Mantel (1962). One of the motivations for studying constructions of pairwise independent random variables particularly in the computer science community is that the joint distribution can have a low cardinality support (polynomial in the number of random variables) in comparison to mutually independent random variables (exponential

in the number of random variables). The reader is referred to Lancaster (1965) and more recent papers of Babai (2013) and Gavinsky and Pudlák (2016) who have developed lower bounds on the entropy of the joint distribution of pairwise independent random variables which are shown to grow logarithmically with the number of random variables. The low cardinality of these distributions have important ramifications in efficiently derandomizing algorithms for NP-hard combinatorial optimization problems (see the review article of Luby and Wigderson, 2005, and the references therein for results on pairwise independent and more generally t -wise independent random variables).

Preliminaries:

Given an integer $n \geq 2$, denote by $[n]$, the set of indices $\{1, 2, \dots, n\}$ and by $K_n = \{(i, j) : 1 \leq i < j \leq n\}$, the set of all pairwise indices in $[n]$ (it can be viewed as a complete graph on n nodes). Given integers $i < j$, let $[i, j] = \{i, i + 1, \dots, j - 1, j\}$. Consider a Bernoulli random vector $\tilde{c} = (\tilde{c}_1, \dots, \tilde{c}_n)$ with marginal probabilities given by $p_i = \mathbb{P}(\tilde{c}_i = 1)$ for $i \in [n]$. Denote by $\mathbf{p} = (p_1, \dots, p_n) \in [0, 1]^n$, the univariate marginal vector, by $\mathcal{C} = \{0, 1\}^n$, the set of realizations of \tilde{c} and by $\Theta(\{0, 1\}^n)$, the set of all probability distributions supported on \mathcal{C} . Consider the set of joint probability distributions of Bernoulli random variables consistent with the given marginal probabilities and pairwise independence:

$$\Theta_{pw} = \left\{ \theta \in \Theta(\{0, 1\}^n) \mid \mathbb{P}_\theta(\tilde{c}_i = 1) = p_i, \forall i \in [n], \mathbb{P}_\theta(\tilde{c}_i = 1, \tilde{c}_j = 1) = p_i p_j, \forall (i, j) \in K_n \right\}$$

This set of distributions is clearly nonempty for any $\mathbf{p} \in [0, 1]^n$, since the mutually independent distribution lies in the set. Our problem of interest is to compute the maximum probability that n random variables add up to at least an integer $k \in [n]$ for distributions in this set. Denote the tightest upper bound by $\bar{P}(n, k, \mathbf{p})$ (observe that the bivariate probabilities here are simply given by the product of the univariate probabilities). Then,

$$\bar{P}(n, k, \mathbf{p}) = \max_{\theta \in \Theta_{pw}} \mathbb{P}_\theta \left(\sum_{i=1}^n \tilde{c}_i \geq k \right) \quad (2.1)$$

Two useful upper bounds that have been proposed for this problem are the following:

- (a) Chebyshev (1867) bound: The one-sided version of the Chebyshev tail probability bound for any random variable uses only the mean and variance of the random variable. Since the Bernoulli random variables are assumed to be pairwise independent or equivalently uncorrelated, the variance of the sum is given by:

$$\text{Variance} \left(\sum_{i=1}^n \tilde{c}_i \right) = \sum_{i=1}^n p_i(1 - p_i).$$

Applying the classical Chebyshev bound then gives an upper bound:

$$\bar{P}(n, k, \mathbf{p}) \leq \begin{cases} 1, & k < \sum_{i=1}^n p_i, \\ \sum_{i=1}^n p_i(1-p_i) / \left(\sum_{i=1}^n p_i(1-p_i) + (k - \sum_{i=1}^n p_i)^2 \right), & \sum_{i=1}^n p_i \leq k \leq n. \end{cases} \quad (2.2)$$

- (b) Schmidt, Siegel, and Srinivasan (1995) bound: The Schmidt, Siegel and Srinivasan bound is derived by bounding the tail probability using the moments of multilinear polynomials. This is in contrast to the Chernoff-Hoeffding bound (see Chernoff, 1952; Hoeffding, 1963) which bounds the tail probability of the sum of independent random variables using the moment generating function. A multilinear polynomial of degree j in n variables is defined as:

$$S_j(\mathbf{c}) = \sum_{1 \leq i_1 < i_2 < \dots < i_j \leq n} c_{i_1} c_{i_2} \dots c_{i_j}.$$

At the crux of their analysis is the observation that all the higher moments of the sum of Bernoulli random variables can be generated from linear combinations of the expected values of multilinear polynomials of the random variables. The construction of the bound makes use of the equality:

$$\binom{\sum_{i \in [n]} c_i}{j} = S_j(\mathbf{c}), \quad \forall \mathbf{c} \in \mathcal{C}, \forall j \in [0, n], \quad (2.3)$$

where $S_0(\mathbf{c}) = 1$ and $\binom{r}{s} = r! / (s!(r-s)!)$ for any pair of integers $r \geq s \geq 0$. The bound derived in Schmidt, Siegel, and Srinivasan (1995) (see Theorem 7, part (II) on page 239) for pairwise independent random variables is given by¹:

$$\bar{P}(n, k, \mathbf{p}) \leq \min \left(1, \frac{\sum_{i \in [n]} p_i}{k}, \frac{\sum_{(i,j) \in K_n} p_i p_j}{\binom{k}{2}} \right). \quad (2.4)$$

While both the Chebyshev's bound and the Schmidt, Siegel, Srinivasan bound in (2.2) and (2.4) have been shown to be useful and are easy to use, neither of them is tight for general values of n , k and $\mathbf{p} \in [0, 1]^n$, although in special cases they can be shown to be tight. In this chapter, we work towards identifying instances for pairwise independent random variables when these bounds can be tightened (Section 2.3) or shown to be tight (see Section 2.4.1).

2.1.1 Other related bounds

Consider the set of joint probability distributions of Bernoulli random variables consistent with the marginal probability vector $\mathbf{p} \in [0, 1]^n$ and general bivariate probabilities given by $p_{ij} = \mathbb{P}(\tilde{c}_i = 1, \tilde{c}_j = 1)$ for $(i, j) \in K_n$:

$$\Theta_b = \left\{ \theta \in \Theta(\{0, 1\}^n) \mid \mathbb{P}_\theta(\tilde{c}_i = 1) = p_i, \forall i \in [n], \mathbb{P}_\theta(\tilde{c}_i = 1, \tilde{c}_j = 1) = p_{ij}, \forall (i, j) \in K_n \right\}$$

¹While the statement in the theorem in Schmidt, Siegel, and Srinivasan (1995) is for $k > \sum_i p_i$, it is straightforward to see that their analysis would lead to the form here for general k .

Unlike the pairwise independent case, verifying if this set of distributions is nonempty is already known to be a NP-complete problem (see Pitowsky, 1991). The tightest upper bound on the probability for distributions in this set is given by $\max_{\theta \in \Theta_b} \mathbb{P}_\theta (\sum_{i=1}^n \tilde{c}_i \geq k)$ where the bound is set to $-\infty$ if the set of feasible distributions is empty. The bound is given by the optimal value of the linear program (see Hailperin, 1965a):

$$\begin{aligned}
\max \quad & \sum_{\mathbf{c} \in \mathcal{C}: \sum_t c_t \geq k} \mathbb{P}(\mathbf{c}) \\
\text{s.t.} \quad & \sum_{\mathbf{c} \in \mathcal{C}: c_i=1} \mathbb{P}(\mathbf{c}) = p_i, \quad \forall i \in [n], \\
& \sum_{\mathbf{c} \in \mathcal{C}: c_i=1, c_j=1} \mathbb{P}(\mathbf{c}) = p_{ij}, \quad \forall (i, j) \in K_n, \\
& \sum_{\mathbf{c} \in \mathcal{C}} \mathbb{P}(\mathbf{c}) = 1, \\
& \mathbb{P}(\mathbf{c}) \geq 0, \quad \forall \mathbf{c} \in \mathcal{C}
\end{aligned} \tag{2.5}$$

where the decision variables are the joint probabilities $\mathbb{P}(\mathbf{c}) = \mathbb{P}(\tilde{\mathbf{c}} = \mathbf{c})$ for all $\mathbf{c} \in \mathcal{C}$. The number of decision variables in this formulation, however, grows exponentially in the number of random variables n . The dual linear program is given by:

$$\begin{aligned}
\min \quad & \sum_{(i,j) \in K_n} \lambda_{ij} p_{ij} + \sum_{i=1}^n \lambda_i p_i + \lambda_0 \\
\text{s.t.} \quad & \sum_{(i,j) \in K_n} \lambda_{ij} c_i c_j + \sum_{i=1}^n \lambda_i c_i + \lambda_0 \geq 0, \quad \forall \mathbf{c} \in \mathcal{C}, \\
& \sum_{(i,j) \in K_n} \lambda_{ij} c_i c_j + \sum_{i=1}^n \lambda_i c_i + \lambda_0 \geq 1, \quad \forall \mathbf{c} \in \mathcal{C} : \sum_t c_t \geq k.
\end{aligned} \tag{2.6}$$

The dual linear program in (2.6) has a polynomial number of decision variables, exponential number of constraints and is always feasible (set $\lambda_0 = 1$ and remaining dual variables to be zero). Strong duality thus holds. Given the large size of the primal and dual linear programs, two main approaches to tackle these problems have been studied in the literature:

i) The first approach is to find closed-form bounds by generating dual feasible solutions as illustrated in Kounias (1968), Kounias and Marin (1976), Sathe, Pradhan, and Shah (1980), Móri and Székely (1985), Dawson and Sankoff (1967), Galambos (1975) and Galambos (1977), Caen (1997), Kuai, Alajaji, and Takahara (2000), Dohmen and Tittmann (2007) and related graph-based bounds in Hunter (1976), Worsley (1982), Veneziani (2008a), Vizvári (2007). These bounds have shown to be tight in special instances (see Section 2.2.2 for examples).

ii) The second approach is to try and reduce the size of the linear programs using relaxations and to solve it numerically. Since the primal linear program in (2.5) quickly becomes intractable with an increase in the number of random variables n , many papers adopting this approach, aggregate the primal decision variables, thus obtaining weaker bounds as a trade-off for the reduced size. Formulations of linear programs

under assumptions of partially or fully aggregated univariate, bivariate or m -variate information for $2 \leq m < n$ have been proposed in Kwerel (1975b), Platz (1985), Prékopa (1988) and Prékopa (1990a), Boros and Prékopa (1989), Prékopa and Gao (2005), Qiu, Ahmed, and Dey (2016), Yang, Alajaji, and Takahara (2016), Yoda and Prékopa (2016). Techniques to solve the dual formulations by restricting the dual variables have been similarly been studied (see Boros et al., 2014).

Using the second approach, in some cases, closed-form bounds have been derived for the aggregated linear programs. One such bound which is of particular relevance to this chapter is constructed in Boros and Prékopa (1989) by identifying dual feasible bases and using optimality conditions when the first and second binomial moments are known. The tightest upper bound on $\mathbb{P}(\xi \geq k)$ is derived by considering all distributions ω of a integer random variable $\tilde{\xi}$ (supported on $[0, n]$), which are assumed to lie in a set of distributions is given by:

$$\left\{ \omega([0, n]) \mid \mathbb{E}_\omega \left[\binom{\tilde{\xi}}{j} \right] = S_j, j = 1, 2 \right\}.$$

Setting $\tilde{\xi} = \sum_i \tilde{c}_i$ with $S_1 = \mathbb{E}[S_1(\tilde{c})]$ and $S_2 = \mathbb{E}[S_2(\tilde{c})]$, the upper bound is a closed-form expression as follows:

$$\mathbb{P} \left(\sum_{i=1}^n \tilde{c}_i \geq k \right) \leq \begin{cases} 1, & k < \frac{(n-1)S_1 - 2S_2}{n - S_1} \\ \frac{(k+n-1)S_1 - 2S_2}{kn}, & \frac{(n-1)S_1 - 2S_2}{n - S_1} \leq k < 1 + \frac{2S_2}{S_1} \\ \frac{(i-1)(i-2S_1) + 2S_2}{(k-i)^2 + (k-i)}, & k \geq 1 + \frac{2S_2}{S_1}, i = \left\lceil \frac{(k-1)S_1 - 2S_2}{k - S_1} \right\rceil, \end{cases} \quad (2.7)$$

where the ceiling function $\lceil x \rceil$ maps x to the smallest integer greater than or equal to x . Similar to the Chebyshev's bound and the Schmidt, Siegel, Srinivasan bound, the Boros and Prekopa bound in (2.7) is not generally tight when the input marginals are known as in (2.1), since it is constructed with aggregated binomial moment information. In the rest of this chapter, we will refer to the three bounds in (2.2), (2.4) and (2.7) as the (a) Chebyshev, (b) Schmidt, Siegel and Srinivasan and (c) Boros and Prekopa bound respectively.

To the best of our knowledge, the connection of these bounds which assume general bivariate information with tight bounds for pairwise independent random variables have not been well-studied in the literature. Another upper bound derived under weaker assumptions is the Boole (1854) (see also Fréchet, 1935) union bound ($k = 1$) which is valid with extremal dependence among the Bernoulli random variables. Boole's union bound is given as:

$$\bar{P}_u(n, 1, \mathbf{p}) = \max_{\theta \in \Theta_u} \mathbb{P}_\theta \left(\sum_{i=1}^n \tilde{c}_i \geq 1 \right) = \min \left(\sum_{i=1}^n p_i, 1 \right), \quad (2.8)$$

where Θ_u is the set of joint distributions supported on \mathcal{C} while consistent with the given univariate information defined as:

$$\Theta_u = \{ \theta \in \Theta(\{0, 1\}^n) : \mathbb{P}_\theta(\tilde{c}_i = 1) = p_i, \forall i \in [n] \}.$$

Clearly, $\bar{P}(n, 1, \mathbf{p}) \leq \bar{P}_u(n, 1, \mathbf{p})$. Extensions of this bound for $k \geq 2$ is provided in Ruger (1978).

2.1.2 Contributions and structure

This brings us to the key contributions and the structure of the current chapter:

- (a) In Section 2.2, we first establish (see Lemma 1) that a positively correlated Bernoulli random vector $\tilde{\mathbf{c}}$ with arbitrary univariate probability vector $\mathbf{p} \in [0, 1]^n$ and transformed bivariate probabilities $p_i p_j / p$ where $p \in [\max_i p_i, 1]$, always exists. This feasibility problem is of independent interest in itself, since feasibility is typically not guaranteed for arbitrary correlation structures with Bernoulli random vectors.
- (b) We then provide the tightest upper bound on the probability on the union of n pairwise independent events $\bar{P}(n, 1, \mathbf{p})$ in closed form (see Theorem 2). The contributions of Theorem 2 lie in:
 - i) Establishing that when the random variables are pairwise independent, for any given marginal vector $\mathbf{p} \in [0, 1]^n$, the upper bound proposed in Hunter (1976) and Worsley (1982) is tight using techniques from linear optimization. These bounds were initially developed for the sum of dependent Bernoulli random variables with arbitrary bivariate probabilities (using tree structures from graph theory) and are not in general guaranteed to be tight (see Example 1 in Section 2.2.2). Interestingly for pairwise independent random variables, we prove that this bound is indeed tight by using the feasibility result from Lemma 1.
 - ii) Building on the result (see Proposition 1), we show that the ratio of Boole’s union bound and the pairwise independent bound is upper bounded by $4/3$ and this is attained. Applications of the result in correlation gap analysis for a specific non-decreasing, non-negative, submodular set function are discussed.
- (c) In Section 2.3, we focus on $k \geq 2$ and for general probabilities $\mathbf{p} \in [0, 1]^n$, we present new bounds exploiting the ordering of probabilities (see Theorem 3). These bounds improve on the existing closed-form bounds mentioned in Section 2.1 and numerical examples are provided to quantify the improvement of the ordered bounds over existing bounds.
- (d) In Section 2.4, we provide instances when the existing closed-form and new ordered bounds are tight:
 - i) First, we identify a special case when the existing closed-form bounds can be shown to be tight. When the marginals of the pairwise independent Bernoulli random variables are identical, in Section 2.4.1, we provide the tightest upper bound in closed form (see Theorem 4) for any $k \in [n]$. The proof is based on showing an equivalence with a linear programming formulation of an aggregated moment bound for which closed-form solutions have been derived by Boros and Prekopa (1989). While the tight closed-form bound is more complicated than the closed-form Chebyshev bound in (2.2) and the Schmidt, Siegel, Srinivasan bound in (2.4), it helps us identify conditions under which these relatively simpler bounds are guaranteed to be tight (see Proposition 2).
 - ii) Second, when $n - 1$ marginal probabilities are identical, Proposition 3 provides instances when the new ordered bounds proposed in Section 2.3 are tight. The usefulness of the ordered bounds is illustrated with a numerical example.

- (e) In Section 2.6, we show that the Bonferroni (1936) lower bound is tight for tail probability bounds on sums of pairwise independent Bernoulli variables with small probabilities.
- (f) In Section 2.5, the results from Section 2.2.3 are generalized to show that, with $n = 2$ random variables (when pairwise independence is equivalent to mutual independence), the upper bound on the correlation gap can be improved from $e/(e - 1)$ to $4/3$ for any non-decreasing, non-negative, submodular set function and this bound is attained. On the other hand, we show that the correlation gap can be arbitrarily large with supermodular set functions under similar assumptions.
- (g) Section 2.7 provides three additional results for identical pairwise independent variables. Firstly, in Section 2.7.1, we show that with identical marginals, the tightness of the Boros and Prekopa bounds proved in Section 2.4.1 can be extended to more general t -wise independent Bernoulli variables by solving a polynomial-sized aggregate linear program. Next, in Section 2.7.2, we identify instances when the Boros and Prekopa bound (which is always tight with identical marginals), provides non-trivial small deviation bounds while the Chebyshev and Schmidt, Siegel, Srinivasan bounds are trivial. Lastly, in Section 2.7.3, we provide tight upper and lower bounds on the expected stop-loss function $\mathbb{E} \left[\left(\sum_{j=1}^n \tilde{c}_j - k \right)^+ \right]$ (earlier considered in Section 3.4 in the context of univariates) for identical pairwise independent variables.
- (h) Finally, in Section 3.5, we summarize the results derived in Part I of this dissertation and identify some future research questions.

2.2 Tight upper bound for $k = 1$

The goal of this section is to provide the tightest upper bound on the probability of the union of pairwise independent events. Towards this, we start by generating the following feasible solution to the dual linear program in (2.6) where $k = 1$, $p_{ij} = p_i p_j$ and the probabilities are sorted in increasing value as $0 \leq p_1 \leq p_2 \leq \dots \leq p_n \leq 1$:

$$\lambda_0 = 0, \lambda_i = 1 \forall i \in [n], \lambda_{in} = -1 \forall i \in [n - 1] \text{ and } \lambda_{ij} = 0 \text{ otherwise.}$$

The left hand side of the dual constraints in (2.6) simplifies to:

$$\begin{aligned} \sum_{(i,j) \in K_n} \lambda_{ij} c_i c_j + \sum_{i=1}^n \lambda_i c_i + \lambda_0 &= - \sum_{i=1}^{n-1} c_i c_n + \sum_{i=1}^n c_i \\ &= c_n + \sum_{i=1}^{n-1} c_i (1 - c_n). \end{aligned}$$

To verify that this solution is dual feasible, observe that with all $c_i = 0$, $c_n + \sum_{i=1}^{n-1} c_i (1 - c_n) = 0$. When $c_n = 1$, regardless of the values of c_1, \dots, c_{n-1} , we have $c_n + \sum_{i=1}^{n-1} c_i (1 - c_n) = 1$. Lastly, when $c_n = 0$ and at least one $c_i = 1$ for $i \in [n - 1]$, we have $c_n + \sum_{i=1}^{n-1} c_i (1 - c_n) \geq 1$. This gives a dual feasible solution with the objective value $\sum_{i=1}^n p_i - p_n \left(\sum_{i=1}^{n-1} p_i \right)$. Another dual feasible solution for the linear program is given

by:

$$\lambda_0 = 1, \lambda_i = 0 \forall i \in [n], \lambda_{ij} = 0 \forall (i, j) \in K_n,$$

with a dual objective of 1. From weak duality, we then have:

$$\bar{P}(n, 1, \mathbf{p}) \leq \min \left(\sum_{i=1}^n p_i - p_n \left(\sum_{i=1}^{n-1} p_i \right), 1 \right).$$

It is useful to note that while this bound has been derived in Kounias (1968), it has not been shown to be tight for general bivariate probabilities. A simple construction of an extremal distribution that attains this bound appears to be tricky. The key result we show is that there is always a feasible distribution which attains this upper bound. The proof of tightness involves showing that this problem can be transformed to proving the existence of a distribution of a Bernoulli random vector $\tilde{\mathbf{c}}$ with univariate probabilities $\mathbb{P}(\tilde{c}_i = 1) = p_i$ and transformed bivariate probabilities $\mathbb{P}(\tilde{c}_i = 1, \tilde{c}_j = 1) = p_i p_j / p_n$, where p_n is the largest univariate probability. In the following lemma, we prove that a more general version of such a correlated distribution always exists.

2.2.1 Bivariate feasibility with positively correlated Bernoulli variables

Lemma 1. *Given a univariate probability vector $\mathbf{p} \in [0, 1]^n$ and bivariate probabilities $p_i p_j / p$ where $p \in [\max_i p_i, 1]$, a Bernoulli random vector $\tilde{\mathbf{c}}$ consistent with the given univariate and bivariate probabilities always exists.*

Proof. Sort the probabilities in increasing value as $0 \leq p_1 \leq p_2 \leq \dots \leq p_n \leq 1$. We want to prove that there always exists a distribution $\theta \in \Theta_b$ such that

$$\begin{aligned} \sum_{\mathbf{c} \in \{0,1\}^n} \mathbb{P}(\mathbf{c}) &= 1, \\ \sum_{\mathbf{c} \in \{0,1\}^n: c_i=1} \mathbb{P}(\mathbf{c}) &= p_i, \quad \forall i \in [n], \\ \sum_{\mathbf{c} \in \{0,1\}^n: c_i=1, c_j=1} \mathbb{P}(\mathbf{c}) &= p_{ij}, \quad \forall (i, j) \in K_n \end{aligned} \tag{2.9}$$

where $p_{ij} = p_i p_j / p$ and $p \in [p_n, 1]$. The proof is divided into two parts.

- (i) We first argue that it is sufficient to verify the existence of probabilities $\mathbb{P}(\mathbf{c})$ for n Bernoulli random variables such that:

$$\begin{aligned} \sum_{\mathbf{c} \in \{0,1\}^n} \mathbb{P}(\mathbf{c}) &= 1, \\ \sum_{\mathbf{c} \in \{0,1\}^n: c_i=1} \mathbb{P}(\mathbf{c}) &= p_i, \quad \forall i \in [n], \\ \sum_{\mathbf{c} \in \{0,1\}^n: c_i=1, c_j=1} \mathbb{P}(\mathbf{c}) &= \frac{p_i p_j}{p_n}, \quad \forall (i, j) \in K_n, \end{aligned} \tag{2.10}$$

where the bivariate probabilities are modified from $p_i p_j / p$ to $p_i p_j / p_n$. To see this, since $1 \leq 1/p \leq 1/p_n$, it is always possible to find a $\lambda \in [0, 1]$ such that:

$$\frac{1}{p} = \lambda \frac{1}{p_n} + (1 - \lambda)(1).$$

Then, consider a convex combination two distributions $\bar{\theta}$, $\underline{\theta}$ as follows:

$$\theta = \lambda \bar{\theta} + (1 - \lambda) \underline{\theta},$$

where $\bar{\theta}$ is a probability distribution which satisfies (2.10) and $\underline{\theta}$ is a pairwise independent joint distribution on n Bernoulli random variables with univariate probabilities given by p_i and bivariate probabilities given by $p_i p_j$. The distribution $\underline{\theta}$ always exists (simply choose the mutually independent distribution on n random variables with univariate probabilities p_i) while we will prove the existence of $\bar{\theta}$ in the next part of the proof. The convex combination above guarantees the existence of a distribution θ which satisfies (2.9).

- (ii) Next, to show that (2.10) is feasible, by conditioning on $c_n = 1$, we use the fact that there exists a feasible distribution on $n - 1$ Bernoulli random variables with probabilities $\mathbb{P}_{n-1}(\mathbf{c}) = \mathbb{P}(\tilde{\mathbf{c}} = \mathbf{c})$ for all $\mathbf{c} \in \{0, 1\}^{n-1}$ such that:

$$\begin{aligned} \sum_{\mathbf{c} \in \{0,1\}^{n-1}} \mathbb{P}_{n-1}(\mathbf{c}) &= 1, \\ \sum_{\mathbf{c} \in \{0,1\}^{n-1}: c_i=1} \mathbb{P}_{n-1}(\mathbf{c}) &= \frac{p_i}{p_n}, \quad \forall i \in [n-1], \\ \sum_{\mathbf{c} \in \{0,1\}^{n-1}: c_i=1, c_j=1} \mathbb{P}_{n-1}(\mathbf{c}) &= \frac{p_i p_j}{p_n^2}, \quad \forall (i, j) \in K_{n-1}. \end{aligned} \tag{2.11}$$

Such a pairwise independent joint distribution θ_{n-1} on $n - 1$ random variables specified by (2.11) with univariate probabilities given by p_i/p_n and bivariate probabilities given by $(p_i/p_n)(p_j/p_n)$ always exists (simply choose the mutually independent distribution on $n - 1$ random variables with univariate probabilities p_i/p_n). Then, by assigning a probability of $1 - p_n$ to the vector of all zeros ($\mathbf{c} = \mathbf{0}$) and scaling the probabilities when $c_n = 1$, we obtain a feasible distribution satisfying (2.10) as seen in the construction of Table 2.1.

Scenarios	c_1	c_2	...	c_n	Probability
2^{n-1} scenarios	0	0	...	0	$\mathbb{P}(\mathbf{c}) = 1 - p_n$
	1	0	...	0	0
	\vdots	\vdots		\ddots	
	1		...	1	0
2^{n-1} scenarios	0	0	...	1	$\mathbb{P}(\mathbf{c}) = p_n \mathbb{P}_{n-1}(\mathbf{c})$
	\vdots	\vdots		\vdots	
	1	1		1	$\mathbb{P}(\mathbf{c}) = p_n \mathbb{P}_{n-1}(\mathbf{c})$

TABLE 2.1: Probabilities of the scenarios to create a feasible distribution in (2.10).

This completes the proof by showing the existence of the distribution $\bar{\theta}$. \square

We note that Lemma 1 proves feasibility for positively correlated Bernoulli random variables. Feasibility is typically not guaranteed for arbitrary correlation structures with Bernoulli random vectors. While there are several results on finding specific correlation structures which are compatible with given Bernoulli random variables and simulating from these distributions (see Chaganty and Joe, 2006; Qaqish, 2003; Emrich and Piedmonte, 1991; Lunn and Davies, 1998), this result appears to be unknown to the best of our knowledge, and hence significant in itself. This brings us to the first theorem, which provides the tightest upper bound on the probability of the union of n pairwise independent events using Lemma 1.

Theorem 2. *Sort the probabilities in increasing value as $0 \leq p_1 \leq p_2 \leq \dots \leq p_n \leq 1$. Then,*

$$\bar{P}(n, 1, \mathbf{p}) = \min \left(\sum_{i=1}^n p_i - p_n \left(\sum_{i=1}^{n-1} p_i \right), 1 \right). \quad (2.12)$$

Proof. When $p_{ij} = p_i p_j$ and $k = 1$, the optimal value of the primal linear program in (2.5) is clearly bounded since feasibility is guaranteed and the objective function is a probability value. The optimality conditions of linear programming states that $\{\mathbb{P}(\mathbf{c}); \mathbf{c} \in \mathcal{C}\}$ is primal optimal and $\{\lambda_{ij}; (i, j) \in K_n, \lambda_i; i \in [n], \lambda_0\}$ is dual optimal if and only if they satisfy: (i) the primal feasibility conditions in (2.5), (ii) the dual feasibility conditions in (2.6) and (iii) the complementary slackness conditions given by:

$$\begin{aligned} \left(\sum_{(i,j) \in K_n} \lambda_{ij} c_i c_j + \sum_{i=1}^n \lambda_i c_i + \lambda_0 \right) \mathbb{P}(\mathbf{c}) &= 0, \quad \forall \mathbf{c} \in \mathcal{C} : \sum_t c_t = 0, \\ \left(\sum_{(i,j) \in K_n} \lambda_{ij} c_i c_j + \sum_{i=1}^n \lambda_i c_i + \lambda_0 - 1 \right) \mathbb{P}(\mathbf{c}) &= 0, \quad \forall \mathbf{c} \in \mathcal{C} : \sum_t c_t \geq 1. \end{aligned} \quad (2.13)$$

1) Proof of tightness of non-trivial bound in (2.12)

We now show that $\bar{P}(n, 1, \mathbf{p}) = \sum_{i=1}^n p_i - p_n \left(\sum_{i=1}^{n-1} p_i \right)$ which is the non-trivial part of the upper bound in (2.12) when $\sum_{i=1}^{n-1} p_i \leq 1$.

Step (1a): Show tightness by constructing a pairwise independent distribution

We verify the tightness of the bound, by showing there exists a primal solution (feasible distribution) which satisfies the complementary slackness conditions. Towards this, observe that from the complementary slackness condition in (2.13):

$$\forall \mathbf{c} \in \mathcal{C} : \sum_{t=1}^{n-1} c_t \geq 2, c_n = 0, \text{ we have } \left(c_n + \sum_{i=1}^{n-1} c_i(1 - c_n) - 1 \right) > 0 \implies \mathbb{P}(\mathbf{c}) = 0.$$

This forces a total of $2^{n-1} - n$ scenarios to have zero probability. Building on this, we set the probabilities of the 2^n possible scenarios of $\tilde{\mathbf{c}}$ as shown in Table 2.2. The probability of the vector of all zeros (one scenario) is set to $1 - \sum_{i=1}^n p_i + p_n \left(\sum_{i=1}^{n-1} p_i \right)$. To match the bivariate probabilities $\mathbb{P}(\tilde{c}_i = 1, \tilde{c}_n = 0) = p_i(1 - p_n)$, we have to then set the probability of the scenario where $c_i = 1, c_n = 0$ and all

remaining $c_j = 0$ to $p_i(1 - p_n)$. This corresponds to the $n - 1$ scenarios in Table 2.2. Hence, to ensure feasibility of the distribution, we need to show that there

Scenarios	c_1	c_2	\dots	c_{n-1}	c_n	Probability
1 scenario	0	0	\dots	0	0	$1 - \sum_{i=1}^n p_i + p_n \left(\sum_{i=1}^{n-1} p_i \right)$
$n - 1$ scenarios	1	0	\dots	0	0	$p_1(1 - p_n)$
	0	1	\dots	0	0	$p_2(1 - p_n)$
	\vdots	\vdots		\vdots	\vdots	
	0		\dots	1	0	$p_{n-1}(1 - p_n)$
$2^{n-1} - n$ scenarios	1	1	\dots	0	0	0
	\vdots	\vdots		\vdots	0	0
	1	1		1	0	0
2^{n-1} scenarios	0	0	\dots	0	1	$\mathbb{P}(\mathbf{c})$
	\vdots	\vdots		\vdots	1	
	1	1		1	1	$\mathbb{P}(\mathbf{c})$

TABLE 2.2: Probabilities of scenarios where the probabilities of the last 2^{n-1} scenarios need to be determined.

exist non-negative values of $\mathbb{P}(\mathbf{c})$ for the last 2^{n-1} scenarios such that:

$$\begin{aligned} \sum_{\mathbf{c} \in \mathcal{C}: c_n=1} \mathbb{P}(\mathbf{c}) &= p_n, \\ \sum_{\mathbf{c} \in \mathcal{C}: c_i=1, c_n=1} \mathbb{P}(\mathbf{c}) &= p_i p_n, \quad \forall i \in [n-1], \\ \sum_{\mathbf{c} \in \mathcal{C}: c_i=1, c_j=1, c_n=1} \mathbb{P}(\mathbf{c}) &= p_i p_j, \quad \forall (i, j) \in K_{n-1}. \end{aligned}$$

or equivalently, by conditioning on $c_n = 1$, we need to show that there exists non-negative joint probabilities $\mathbb{P}_{n-1}(\mathbf{c})$ where $\mathbb{P}_{n-1}(\mathbf{c}) = \mathbb{P}(\tilde{\mathbf{c}} = \mathbf{c})$ for all $\mathbf{c} \in \{0, 1\}^{n-1}$ such that:

$$\begin{aligned} \sum_{\mathbf{c} \in \{0,1\}^{n-1}} \mathbb{P}_{n-1}(\mathbf{c}) &= 1, \\ \sum_{\mathbf{c} \in \{0,1\}^{n-1}: c_i=1} \mathbb{P}_{n-1}(\mathbf{c}) &= p_i, \quad \forall i \in [n-1], \\ \sum_{\mathbf{c} \in \{0,1\}^{n-1}: c_i=1, c_j=1} \mathbb{P}_{n-1}(\mathbf{c}) &= \frac{p_i p_j}{p_n}, \quad \forall (i, j) \in K_{n-1}, \end{aligned} \tag{2.14}$$

This corresponds to verifying the existence of a probability distribution on $n - 1$ Bernoulli random variables with univariate probabilities p_i and bivariate probabilities $p_i p_j / p_n$ where $p_n \geq p_{n-1} \geq p_{n-2} \geq \dots \geq p_1$. Observe, that in (2.14), the univariate probabilities remain the same but the random variables are no longer pairwise independent. In the next step of the proof, we show that such a distribution always exists.

Step (1b): Show there exists a distribution that satisfies (2.14)

We make use of the Lemma 1 to prove that 2.14 is always satisfied. By considering $n - 1$ variables instead of n and setting $p = p_n \geq \max_{i \in [n-1]} p_i$, it is too easy to see from Lemma 1 that there exists a distribution which satisfies (2.14).

An outline of the different distributions used in the construction in steps (1a) and Lemma 1 is shown in Figure 2.1.

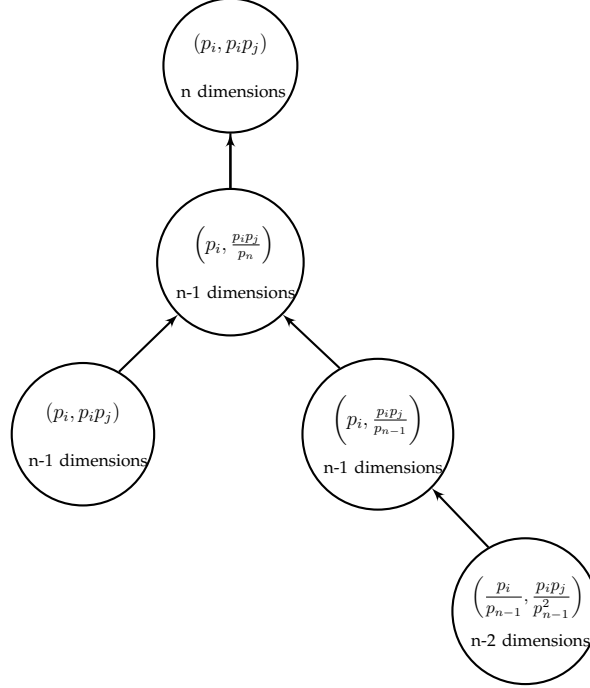


FIGURE 2.1: Construction of the pairwise independent extremal distribution

This completes the proof for the case where $\sum_{i=1}^{n-1} p_i \leq 1$ and the non-trivial tight bound is given by:

$$\bar{P}(n, 1, \mathbf{p}) = \sum_{i=1}^n p_i - p_n \left(\sum_{i=1}^{n-1} p_i \right).$$

2) Proof of the tightness of trivial part of the bound in (2.12)

To complete the proof, consider the case with $\sum_{i=1}^{n-1} p_i > 1$. Then, there exists an index $t \in [2, n - 1]$ such that $\sum_{i=1}^{t-1} p_i \leq 1$ and $\sum_{i=1}^t p_i > 1$. Let $\delta = 1 - \sum_{i=1}^{t-1} p_i$. Clearly $0 \leq \delta < p_t$. From steps (1)-(2) in the proof of the non-trivial bound, we know that there exists a distribution for $t + 1$ pairwise independent random variables with marginal probabilities $p_1, p_2, \dots, p_{t-1}, \delta, p_{t+1}$ such that the probability of the sum of the random variables being at least one is equal to one (since the sum of the first t probabilities in this case is equal to one). By increasing the marginal probability δ to p_t , we can only increase this probability. Hence, there exists a distribution for $t + 1$ pairwise independent random variables with probabilities $0 \leq p_1 \leq p_2 \leq \dots \leq p_t \leq p_{t+1} \leq 1$ such that there is a zero probability of these random variables to simultaneously take a value of 0. We can generate the remaining random variables $\tilde{c}_{t+2}, \dots, \tilde{c}_n$ independently with marginal probabilities p_{t+2}, \dots, p_n . This provides a feasible distribution that attains the bound of one, thus completing the proof. \square

2.2.2 Connection of Theorem 2 to existing results

The problem of bounding the probability that the sum of Bernoulli random variables is at least one has been extensively studied in the literature, under knowledge of general bivariate probabilities. Let A_i denote the event that $\tilde{c}_i = 1$ for each i , then, $k = 1$ simply corresponds to bounding the probability of the union of events. When the marginal probabilities $p_i = \mathbb{P}(A_i)$ for $i \in [n]$ and bivariate probabilities $p_{ij} = \mathbb{P}(A_i \cap A_j)$ for $(i, j) \in K_n$ are given, Hunter (1976) and Worsley (1982) derived the following bound by optimizing over the spanning trees $\tau \in T$:

$$\mathbb{P}(\cup_i A_i) \leq \sum_{i=1}^n p_i - \max_{\tau \in T} \sum_{(i,j) \in \tau} p_{ij}, \quad (2.15)$$

where T is the set of all spanning trees on the complete graph with n nodes (where the edge weights are given by p_{ij}). A special case of the Hunter (1976) bound was derived by Kounias (1968) as:

$$\mathbb{P}(\cup_i A_i) \leq \sum_{i=1}^n p_i - \max_{j \in [n]} \sum_{i \neq j} p_{ij}, \quad (2.16)$$

which subtracts the maximum weight of a star spanning tree on the complete graph from the sum of the marginal probabilities $\sum_i p_i$. Tree bounds have been shown to be tight, in some special cases as outlined below:

i) Zero bivariate probabilities for all pairs ($p_{ij} = 0, \forall (i, j) \in K_n$):

When all the probabilities p_{ij} are zero, the bound reduces to Boole's union bound which is tight.

ii) Zero bivariate probabilities outside a given tree:

Given a tree τ such that the bivariate probabilities p_{ij} are zero if and only if the edge $(i, j) \notin \tau$, Worsley (1982) proved that the bound is tight (see Veneziani, 2008b, for related results).

iii) Lower bounds on bivariate probabilities:

Boros et al. (2014) proved that by relaxing the equality of bivariate probabilities to lower bounds on bivariate probabilities as

$$\mathbb{P}(A_i \cap A_j) \geq p_{ij}, \quad \forall (i, j) \in K_n,$$

the tightest upper bound on the probability of the union is exactly the Hunter (1976) and Worsley (1982) bound (see Maurer, 1983, for related results).

iv) Pairwise independent variables (Theorem 2 in this chapter):

With pairwise independent random variables where $p_{ij} = p_i p_j$, the maximum weight spanning trees in (2.15) is exactly the star tree with the root at node n and edges (i, n) for all $i \in [n - 1]$. In this case, the Kounias (1968), Hunter (1976) and Worsley (1982) bound reduces to the bound in (2.12) which is shown to be tight in Theorem 2 in this chapter.

The next example illustrates that with general bivariate probabilities, even if a joint distribution exists, the Hunter (1976) and Worsley (1982) bound and thus the Kounias (1968) bound is not guaranteed to be tight.

Example 1. Consider $n = 4$ Bernoulli random variables with univariate marginal vector

$$\mathbf{p} = [0.35, 0.19, 0.13, 0.2],$$

and bivariate probabilities

$$p_{12} = 0.001, p_{13} = 0.022, p_{14} = 0.03, p_{23} = 0.017, p_{24} = 0.018, p_{34} = 0.019.$$

It can be verified that a joint distribution with these given univariate and bivariate probabilities exists. The tight upper bound on the probability by solving the linear program (2.5) is given by

$$\max_{\theta \in \Theta(\mathbf{p}, p_{ij}; (i,j) \in K_4)} \mathbb{P}_\theta (\tilde{c}_1 + \tilde{c}_2 + \tilde{c}_3 + \tilde{c}_4 \geq 1) = 0.784.$$

Figure 2.2 displays the star spanning tree chosen by the Kounias (1968) bound and spanning tree chosen by the Hunter (1976) and Worsley (1982) bound. It is clear that none of these bounds are tight in this given instance. Boros et al. (2014) also provide randomly generated instances (see Table 1 of Section 4 in their paper) when the Hunter (1976) bound is not tight though it is the best performing among the upper bounds considered there.

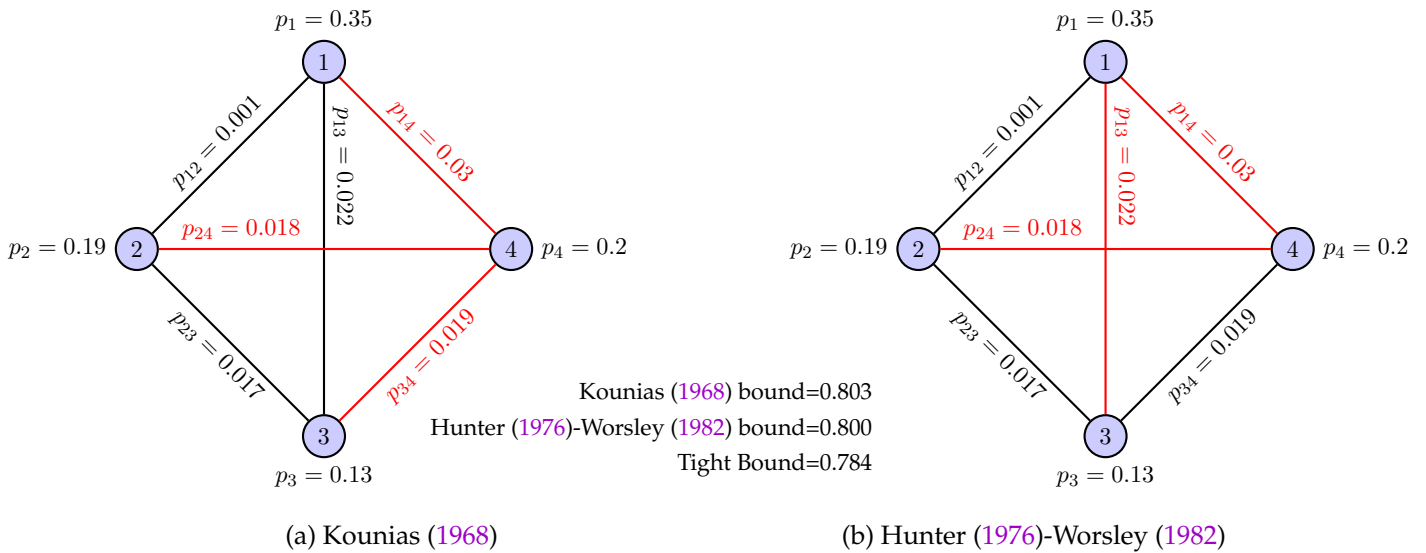


FIGURE 2.2: Spanning trees with general bivariate probabilities

Figure 2.3 demonstrates that with the same set of univariate marginals $\mathbf{p} = [0.35, 0.19, 0.13, 0.2]$, when pairwise independence is enforced, both the Kounias (1968) and Hunter (1976) and Worsley (1982) spanning trees are identical and the bounds in (2.16) and (2.15) equal the tight bound 0.688 (from Theorem 2).

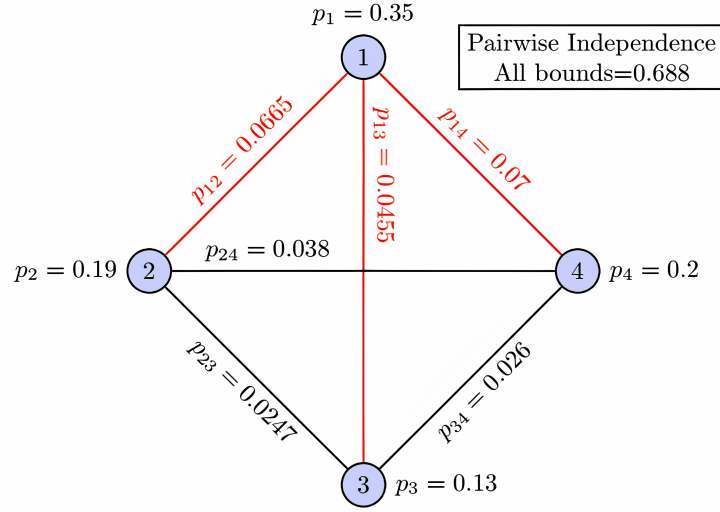


FIGURE 2.3: All spanning trees with pairwise independence

2.2.3 Comparison with the union bound and correlation gap analysis

The next proposition provides an upper bound on the ratio of Boole's union bound and the pairwise independent bound derived from Theorem 2.

Proposition 1. For all $\mathbf{p} \in [0, 1]^n$, we have:

$$\frac{\bar{P}_u(n, 1, \mathbf{p})}{\bar{P}(n, 1, \mathbf{p})} \leq \frac{4}{3}.$$

The ratio of $4/3$ is attained when $\sum_{i=1}^{n-1} p_i = 1/2$ and $p_n = 1/2$.

Proof. Assume the probabilities are sorted in increasing values as $0 \leq p_1 \leq p_2 \leq \dots \leq p_n \leq 1$. It is straightforward to see that if $\sum_{i=1}^{n-1} p_i > 1$, both the bounds take the value $\bar{P}(n, 1, \mathbf{p}) = \bar{P}_u(n, 1, \mathbf{p}) = 1$. Now assume, $\alpha = \sum_{i=1}^{n-1} p_i \leq 1$. The ratio is given as:

$$\begin{aligned} \frac{\bar{P}_u(n, 1, \mathbf{p})}{\bar{P}(n, 1, \mathbf{p})} &= \frac{\min(\sum_{i=1}^n p_i, 1)}{\sum_{i=1}^n p_i - p_n \left(\sum_{i=1}^{n-1} p_i\right)} \\ &= \frac{\min(\alpha + p_n, 1)}{\alpha + p_n - \alpha p_n}. \end{aligned}$$

If $\alpha + p_n \leq 1$, then we have:

$$\begin{aligned} \frac{\overline{P}_u(n, 1, \mathbf{p})}{\overline{P}(n, 1, \mathbf{p})} &= \frac{\alpha + p_n}{\alpha + p_n - \alpha p_n} \\ &= \frac{1}{1 - \frac{1}{\frac{1}{\alpha} + \frac{1}{p_n}}} \\ &\leq \frac{4}{3} \end{aligned} \tag{2.17}$$

where the maximum value is attained at $\alpha = 1 - p_n$, $p_n = 1/2$, while if $\alpha + p_n \geq 1$, then we have:

$$\begin{aligned} \frac{\overline{P}_u(n, 1, \mathbf{p})}{\overline{P}(n, 1, \mathbf{p})} &= \frac{1}{\alpha + p_n - \alpha p_n} \\ &= \frac{1}{\alpha(1 - p_n) + p_n} \\ &\leq \frac{4}{3} \end{aligned} \tag{2.18}$$

where the maximum value is again attained at $\alpha = 1 - p_n$, $p_n = 1/2$. This gives the bound of $4/3$ when $p_n = 1/2$ and $\alpha = 1/2$. \square

We now illustrate an application of Theorem 2 and Proposition 1 in comparing bounds with dependent and independent random variables in correlation gap analysis.

Example 2 (Correlation gap analysis). *The notion of a ‘‘correlation gap’’ was introduced by Agrawal et al. (2012). It is defined as the ratio of the worst-case expected cost for random variables with given univariate marginals to the expected cost when the random variables are independent. When $\tilde{\mathbf{c}}$ is a Bernoulli random vector and θ_{ind} denotes the independent distribution, the correlation gap is defined there as:*

$$\kappa_u(\mathbf{p}) = \sup_{\theta \in \Theta_u} \frac{\mathbb{E}_\theta[f(\tilde{\mathbf{c}})]}{\mathbb{E}_{\theta_{ind}}[f(\tilde{\mathbf{c}})]}. \tag{2.19}$$

A key result in this area is that for any non-negative, non-decreasing, submodular set function, $f(S)$, the correlation gap is always upper bounded by $e/(e - 1)$ (see Calinescu et al., 2007; Agrawal et al., 2012). The example constructed in these papers to show this bound is attained is for the maximum of binary variables:

$$f(\mathbf{c}) = \max \{c_i \mid i \in [n]\}.$$

This defines a non-negative, non-decreasing, submodular set function $f(S)$ which takes a value zero when $S = \emptyset$ and one when $S \neq \emptyset$. For a given marginal vector \mathbf{p} , the correlation gap in

(2.19) reduces to

$$\begin{aligned}
\kappa_u(\mathbf{p}) &= \frac{\max_{\theta \in \Theta_u} \mathbb{E}_\theta[\max(\tilde{c}_1, \tilde{c}_2, \dots, \tilde{c}_n)]}{1 - \prod_{i=1}^n (1 - p_i)} \\
&= \frac{\max_{\theta \in \Theta_u} \mathbb{P}_\theta(\sum_{i=1}^n \tilde{c}_i \geq 1)}{1 - \prod_{i=1}^n (1 - p_i)} \\
&= \frac{\min(\sum_{i=1}^n p_i, 1)}{1 - \prod_{i=1}^n (1 - p_i)}.
\end{aligned} \tag{2.20}$$

We now provide an extension of this definition by considering the ratio of the worst-case expected cost when the random variables are pairwise independent to the expected cost when the random variables are independent. This is given as:

$$\kappa(\mathbf{p}) = \sup_{\theta \in \Theta_{pw}} \frac{\mathbb{E}_\theta[f(\tilde{\mathbf{c}})]}{\mathbb{E}_{\theta_{ind}}[f(\tilde{\mathbf{c}})]},$$

which reduces in this specific case to:

$$\kappa(\mathbf{p}) = \frac{\min\left(\sum_{i=1}^n p_i - p_n \left(\sum_{i=1}^{n-1} p_i\right), 1\right)}{1 - \prod_{i=1}^n (1 - p_i)}.$$

Clearly $\kappa(\mathbf{p}) \leq \kappa_u(\mathbf{p})$. We now discuss the behaviour of these two ratios.

i) Worst case analysis:

Assume the marginal probability vector is given by $\mathbf{p} = (1/n, 1/n, \dots, 1/n)$. For the independent distribution, the probability is given by $1 - (1 - 1/n)^n$, while Boole's union bound is equal to one (attained by the distribution which assigns probability $1/n$ to each of n support points with $c_i = 1$, $c_j = 0, \forall j \neq i$ (for each $i \in [n]$) and zero otherwise). In this case the limit of the ratio as n goes to infinity is given by:

$$\lim_{n \rightarrow \infty} \kappa_u(\mathbf{p}) = \frac{1}{1 - (1 - 1/n)^n} \rightarrow \frac{e}{e - 1} \approx 1.5819.$$

Likewise it is easy to verify that with pairwise independence:

$$\lim_{n \rightarrow \infty} \kappa(\mathbf{p}) = \frac{1 - \frac{1}{n} \left(1 - \frac{1}{n}\right)}{1 - (1 - 1/n)^n} = \frac{e}{e - 1} \approx 1.5819.$$

Thus in the worst-case, both these bounds attain the ratio $e/(e - 1)$.

ii) Instances where correlation gap can be improved:

On the other hand, Proposition 1 illustrates that for the probabilities $p_n = 1/2$ and $\sum_{i=1}^{n-1} p_i = 1/2$, the pairwise independent bound is $3/4$ and Boole's union bound is one. For example with $n = 2$ where $\mathbf{p} = (1/2, 1/2)$, Boole's union bound is one, while both the pairwise independent and the independent probabilities are equal to $3/4$. Then, we have $\kappa_u((1/2, 1/2)) = 4/3$ while $\kappa((1/2, 1/2)) = 1$. Thus in specific instances, the correlation gap can be tightened by considering pairwise independent random variables.

2.3 Improved bounds with non-identical marginals for $k \geq 2$

In the previous section, we resolved the question of the tightest bound on the probability of the union of n pairwise independent events. We now shift attention to the more general case of at least two or more pairwise independent events occurring. With an arbitrary input marginal vector \mathbf{p} , deriving tight bounds appears to be challenging. However, we exploit the ordering of probabilities with pairwise independence to provide new upper bounds that are essentially feasible solutions to the dual linear program in (2.6). These bounds use the fact that in addition to the Boros and Prekopa bound in (2.7), the Chebyshev bound and Schmidt, Siegel, Srinivasan bound in (2.2) and (2.4) can be expressed in terms of the first two aggregated (or equivalently binomial) moments for the sum of pairwise independent random variables, $S_1 = \sum_i p_i$ and $S_2 = \sum_{(i,j) \in K_n} p_i p_j$. The new ordered bounds improve on the three existing closed-form bounds in (2.2), (2.4) and (2.7), which we will refer to as unordered bounds for the rest of the chapter. The next theorem provides new probability bounds for the sum of pairwise independent random variables with possibly non-identical marginals when $k \geq 2$.

Theorem 3. Sort the input probabilities in increasing order as $p_1 \leq p_2 \leq \dots \leq p_n$. Define the partial binomial moment $S_{1r} = \sum_{i=1}^{n-r} p_i$ for $r \in [0, n-1]$ and $S_{2r} = \sum_{(i,j) \in K_{n-r}} p_i p_j$ for $r \in [0, n-2]$.

(a) The ordered Schmidt, Siegel and Srinivasan bound is a valid upper bound on $\bar{P}(n, k, \mathbf{p})$:

$$\begin{aligned} \bar{P}(n, k, \mathbf{p}) &\leq \min \left(1, \min_{0 \leq r_1 \leq k-1} \left(\frac{S_{1r_1}}{k-r_1} \right), \min_{0 \leq r_2 \leq k-2} \left(\frac{S_{2r_2}}{\binom{k-r_2}{2}} \right) \right), \quad \forall k \in [2, n], \\ &= \min \left(1, \min_{0 \leq r_1 \leq k-1} \left(\frac{\sum_{i=1}^{n-r_1} p_i}{k-r_1} \right), \min_{0 \leq r_2 \leq k-2} \left(\frac{\sum_{(i,j) \in K_{n-r_2}} p_i p_j}{\binom{k-r_2}{2}} \right) \right), \quad \forall k \in [2, n]. \end{aligned} \quad (2.21)$$

(b) The ordered Boros and Prekopa bound is a valid upper bound on $\bar{P}(n, k, \mathbf{p})$:

$$\bar{P}(n, k, \mathbf{p}) \leq \min_{0 \leq r \leq k-1} BP(n-r, k-r, \mathbf{p}), \quad \forall k \in [2, n], \quad (2.22)$$

where:

$$BP(n-r, k-r, \mathbf{p}) = \begin{cases} 1, & k < \frac{(n-r-1)S_{1r} - 2S_{2r}}{n-r-S_{1r}} + r, \\ \frac{(k-r+n-r-1)S_{1r} - 2S_{2r}}{(k-r)(n-r)}, & \frac{(n-r-1)S_{1r} - 2S_{2r}}{n-r-S_{1r}} + r \leq k < 1 + \frac{2S_{2r}}{S_{1r}} + r, \\ \frac{(i-1)(i-2S_{1r}) + 2S_{2r}}{(k-r-i)^2 + (k-r-i)}, & k \geq 1 + \frac{2S_{2r}}{S_{1r}} + r, \quad i = \left\lceil \frac{(k-r-1)S_{1r} - 2S_{2r}}{k-r-S_{1r}} \right\rceil \end{cases}$$

(c) The ordered Chebyshev bound is a valid upper bound on $\bar{P}(n, k, \mathbf{p})$:

$$\bar{P}(n, k, \mathbf{p}) \leq \min_{0 \leq r \leq k-1} CH(n-r, k-r, \mathbf{p}), \quad \forall k \in [2, n], \quad (2.23)$$

where:

$$CH(n-r, k-r, \mathbf{p}) = \begin{cases} 1, & k < S_{1r} + r, \\ \frac{S_{1r} - (S_{1r}^2 - 2S_{2r})}{S_{1r} - (S_{1r}^2 - 2S_{2r}) + (k-r-S_{1r})^2}, & S_{1r} + r \leq k \leq n. \end{cases}$$

Proof.

- (a) We observe that for any $0 \leq r_1 \leq k-1$ and any subset $S \subseteq [n]$ of the random variables of cardinality $n-r_1$, an upper bound is given as:

$$\begin{aligned} \mathbb{P}\left(\sum_{i=1}^n \tilde{c}_i \geq k\right) &\leq \mathbb{P}\left(\sum_{i \in S} \tilde{c}_i \geq k-r_1\right) \\ &\quad [\text{since } \sum_{i=1}^n c_i \geq k \text{ for } \mathbf{c} \in \mathcal{C} \text{ implies } \sum_{i \in S} c_i \geq k-r_1 \text{ for } \mathbf{c} \in \mathcal{C}] \\ &\leq \frac{\mathbb{E}[\sum_{i \in S} \tilde{c}_i]}{k-r_1} \\ &\quad [\text{using Markov's inequality}] \\ &= \frac{\sum_{i \in S} p_i}{k-r_1}. \end{aligned}$$

The tightest upper bound of this form is obtained by minimizing over all $0 \leq r_1 \leq k-1$ and subsets $S \subseteq [n]$ with $|S| = n-r_1$, which gives:

$$\begin{aligned} \mathbb{P}\left(\sum_{i=1}^n \tilde{c}_i \geq k\right) &\leq \min_{0 \leq r_1 \leq k-1} \min_{S: |S|=n-r_1} \frac{\sum_{i \in S} p_i}{k-r_1} \\ &= \min_{0 \leq r_1 \leq k-1} \frac{\sum_{i=1}^{n-r_1} p_i}{k-r_1} \tag{2.24} \\ &\quad [\text{using the } n-r_1 \text{ smallest probabilities}]. \end{aligned}$$

We derive the next term in (2.21) using a similar approach while accounting for pairwise independence. For any $0 \leq r_2 \leq k-2$ and any subset $S \subseteq [n]$ of the

random variables of cardinality $n - r_2$, an upper bound is given by:

$$\begin{aligned}
\mathbb{P}\left(\sum_{i=1}^n \tilde{c}_i \geq k\right) &\leq \mathbb{P}\left(\sum_{i \in S} \tilde{c}_i \geq k - r_2\right) \\
&= \mathbb{P}\left(\binom{\sum_{i \in S} \tilde{c}_i}{2} \geq \binom{k - r_2}{2}\right) \\
&\leq \frac{\mathbb{E}\left[\sum_{i \in S} \sum_{j \in S: j > i} \tilde{c}_i \tilde{c}_j\right]}{\binom{k - r_2}{2}} \\
&\quad \text{[using equation (2.3) and Markov's inequality]} \\
&= \frac{\sum_{i \in S} \sum_{j \in S: j > i} \mathbb{E}[\tilde{c}_i] \mathbb{E}[\tilde{c}_j]}{\binom{k - r_2}{2}} \\
&\quad \text{[using pairwise independence]} \\
&= \frac{\sum_{i \in S} \sum_{j \in S: j > i} p_i p_j}{\binom{k - r_2}{2}}.
\end{aligned}$$

The tightest upper bound of this form is obtained by minimizing over $0 \leq r_2 \leq k - 2$ and all sets S of size $n - r_2$. This gives:

$$\begin{aligned}
\mathbb{P}\left(\sum_{i=1}^n \tilde{c}_i \geq k\right) &\leq \min_{0 \leq r_2 \leq k-2} \min_{S: |S|=n-r_2} \frac{\sum_{i \in S} \sum_{j \in S: j > i} p_i p_j}{\binom{k - r_2}{2}} \\
&= \min_{0 \leq r_2 \leq k-2} \left(\frac{\sum_{(i,j) \in K_{n-r_2}} p_i p_j}{\binom{k - r_2}{2}} \right) \tag{2.25} \\
&\quad \text{[using the } n - r_2 \text{ smallest probabilities].}
\end{aligned}$$

From the bounds (2.24) and (2.25), we get:

$$\bar{P}(n, k, \mathbf{p}) \leq \min \left(1, \min_{0 \leq r_1 \leq k-1} \left(\frac{S_{1r_1}}{k - r_1} \right), \min_{0 \leq r_2 \leq k-2} \left(\frac{S_{2r_2}}{\binom{k - r_2}{2}} \right) \right), \quad \forall k \in [2, n]$$

where $S_{1r_1} = \sum_{i=1}^{n-r_1} p_i$ for $r_1 \in [0, n - 1]$ and $S_{2r_2} = \sum_{(i,j) \in K_{n-r_2}} p_i p_j$ for $r_2 \in [0, n - 2]$. It is straightforward to see that this approach is essentially creating a set of dual feasible solutions and picking the best among it. The dual formulation is:

$$\begin{aligned}
\bar{P}(n, k, \mathbf{p}) = \min & \sum_{(i,j) \in K_n} \lambda_{ij} p_i p_j + \sum_{i=1}^n \lambda_i p_i + \lambda_0 \\
\text{s.t.} & \sum_{(i,j) \in K_n} \lambda_{ij} c_i c_j + \sum_{i=1}^n \lambda_i c_i + \lambda_0 \geq 0 \quad \forall \mathbf{c} \in \mathcal{C} \\
& \sum_{(i,j) \in K_n} \lambda_{ij} c_i c_j + \sum_{i=1}^n \lambda_i c_i + \lambda_0 \geq 1, \quad \forall \mathbf{c} \in \mathcal{C} : \sum_t c_t \geq k.
\end{aligned}$$

Each component of the second term is obtained by choosing dual feasible solutions with $\lambda_i = 1/(k - r_1)$ for $i \in [n - r_1]$ and setting all other dual variables to 0.

Similarly, each component of the third term is obtained by choosing dual feasible solutions with $\lambda_{ij} = 1/\binom{k-r_2}{2}$ for $(i, j) \in K_{n-r_2}$ and setting all other dual variables to 0.

(b) The bound in (2.22) is obtained by using the inequality:

$$\mathbb{P}\left(\sum_{i=1}^n \tilde{c}_i \geq k\right) \leq \mathbb{P}\left(\sum_{i=1}^{n-r} \tilde{c}_i \geq k-r\right), \quad \forall r \in [0, k-1].$$

Then, we compute an upper bound on $\mathbb{P}\left(\sum_{i=1}^{n-r} \tilde{c}_i \geq k-r\right)$ by using the aggregated moments S_{1r} and S_{2r} with the Boros and Prekopa bound from (2.7) as follows:

$$BP(n-r, k-r, \mathbf{p}) = \begin{cases} 1, & k < \frac{(n-r-1)S_{1r} - 2S_{2r}}{n-r-S_{1r}} + r \\ \frac{(k-r+n-r-1)S_{1r} - 2S_{2r}}{(k-r)(n-r)}, & \frac{(n-r-1)S_{1r} - 2S_{2r}}{n-r-S_{1r}} + r \leq k < 1 + \frac{2S_{2r}}{S_{1r}} + r \\ \frac{(i-1)(i-2S_{1r}) + 2S_{2r}}{(k-r-i)^2 + (k-r-i)}, & k \geq 1 + \frac{2S_{2r}}{S_{1r}} + r, \quad i = \left\lceil \frac{(k-r-1)S_{1r} - 2S_{2r}}{k-r-S_{1r}} \right\rceil \end{cases}$$

Since the relation $P(n, k, \mathbf{p}) \leq BP(n-r, k-r, \mathbf{p})$ is satisfied for every $0 \leq r \leq k-1$, the upper bound on $\bar{P}(n, k, \mathbf{p})$ is obtained by taking the minimum over all possible values of r :

$$\bar{P}(n, k, \mathbf{p}) \leq \min_{0 \leq r \leq k-1} BP(n-r, k-r, \mathbf{p}).$$

(c) Proceeding in a similar manner as in (b), by using the aggregated moments S_{1r} and S_{2r} with Chebyshev bound, the upper bound for a given r ($0 \leq r \leq k-1$) can be written as follows:

$$CH(n-r, k-r, \mathbf{p}) = \begin{cases} 1, & k < S_{1r} + r \\ \frac{S_{1r} - (S_{1r}^2 - 2S_{2r})}{S_{1r} - (S_{1r}^2 - 2S_{2r}) + (k-r-S_{1r})^2}, & S_{1r} + r \leq k \leq n. \end{cases}$$

The upper bound on $\bar{P}(n, k, \mathbf{p})$ is obtained by taking the minimum over all possible values of r :

$$\bar{P}(n, k, \mathbf{p}) \leq \min_{0 \leq r \leq k-1} CH(n-r, k-r, \mathbf{p}), \quad \forall k \in [2, n]$$

□

Connection to earlier work:

Prior work in Ruger (1978) shows that ordering of probabilities provides the tightest upper bound on the probability of the Bernoulli random variables adding up to at least k while allowing for extremal dependence. Specifically, the bound derived there is:

$$\min\left(1, \min_{0 \leq r \leq k-1} \left(\frac{S_{1r}}{k-r}\right)\right).$$

However, this bound does not use pairwise independence information. Part (a) of Theorem 3 tightens the analysis in Ruger (1978) for pairwise independent random variables. It is also straightforward to see that the ordered Schmidt, Siegel and Srinivasan bound in (2.21) is at least as good as the bound in (2.4) (simply plug in $r = 0$). Building on the ordering of probabilities, the bound in (2.22) uses aggregated binomial moments for k ordered sets of random variables of size $n - r$ where $0 \leq r \leq k - 1$. When $r = 0$, the bound in (2.22) reduces to the original aggregated moment bound of Boros and Prekopa in (2.7) and hence this bound is at least as tight. Further, the bounds in Theorem 3 are clearly efficiently computable. We next provide two numerical examples to illustrate the impact of ordering on the quality of the three bounds.

2.3.1 Numerical illustrations

Example 3 (Non-identical marginals). Consider an example with $n = 12$ random variables with the probabilities given by

$$\mathbf{p} = (0.0651, 0.0977, 0.1220, 0.1705, 0.3046, 0.4402, 0.4952, 0.6075, 0.6842, 0.8084, 0.9489, 0.9656).$$

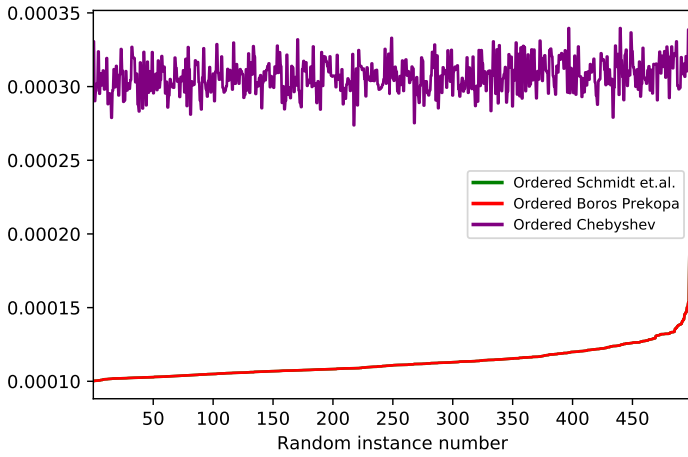
Table 2.3 compares the three ordered bounds with the three unordered bounds and the corresponding tight bound. Numerically, the ordered Boros and Prekopa bound is found to be tight in this example for $k = 7, 8, 9, 12$ while the ordered Schmidt, Siegel and Srinivasan bound is tight for $k = 12$. The Boros and Prekopa bound is uniformly the best performing of the three bounds, while among the other two bounds, none uniformly dominates the other. For example, comparing the ordered bounds when $7 \leq k \leq 9$, the Chebyshev bound outperforms the Schmidt, Siegel and Srinivasan bound, but when $k = 6$ or $10 \leq k \leq 12$, the Schmidt, Siegel and Srinivasan bound does better. Comparing the unordered bounds when $7 \leq k \leq 9$, the Schmidt, Siegel and Srinivasan bound outperforms the Chebyshev bound when $k = 6$ but for all $k \geq 7$, the Chebyshev bound does better. In terms of absolute difference between ordered and unordered bounds, ordering appears to provide the maximum improvement to the Schmidt, Siegel and Srinivasan bound, followed by the Boros, Prekopa and the Chebyshev bound.

Bounds	$k \in [1, 4]$	$k = 5$	$k = 6$	$k = 7$	$k = 8$	$k = 9$	$k = 10$	$k = 11$	$k = 12$
Chebyshev	1	1	0.9553	0.5192	0.2552	0.1424	0.0889	0.0603	0.0434
Ordered Chebyshev	1	1	0.9553	0.5192	0.2552	0.1424	0.0883	0.0549	0.0307
Schmidt, Siegel and Srinivasan	1	1	0.9517	0.6831	0.5123	0.3985	0.3188	0.2608	0.2173
Ordered Schmidt, Siegel and Srinivasan	1	1	0.9489	0.6162	0.3620	0.1827	0.0712	0.0250	<u>0.0064</u>
Boros and Prekopa	1	1	0.9497	<u>0.5018</u>	<u>0.2509</u>	0.1326	0.0795	0.0530	0.0379
Ordered Boros and Prekopa	1	1	0.9254	<u>0.5018</u>	<u>0.2509</u>	<u>0.1290</u>	0.0712	0.0249	<u>0.0064</u>
Tight bound	1	0.9957	0.8931	0.5018	0.2509	0.1290	0.0692	0.0230	0.0064

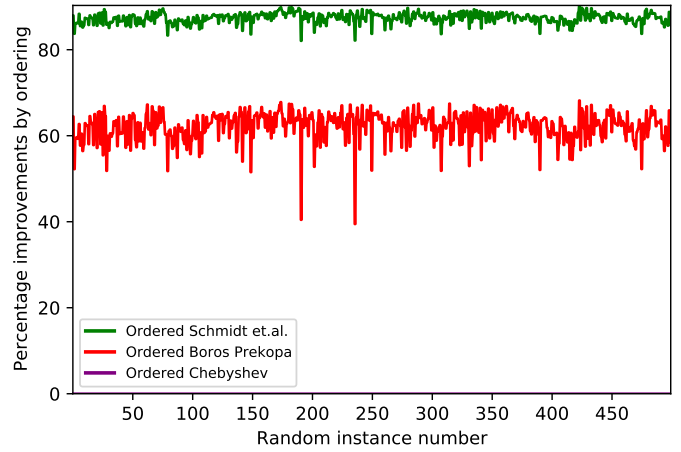
TABLE 2.3: Upper bounds on probability of sum of random variables for $n = 12$. For each value k , the bottom row provides the tightest bound which can be computed in this example as the optimal solution of an exponential-sized linear program. The underlined instances illustrate cases when the other upper bounds are tight.

Example 4 (Non-identical marginals). In this example, we numerically compute the improvement of the new ordered bounds over the unordered bounds for $n = 100$ variables by generating 500 instances of random probabilities $\mathbf{p} = (p_1, p_2, \dots, p_{100})$. First, we consider small marginal probabilities by uniformly and independently generating the entries of \mathbf{p} between 0.01 and 0.05. When $k = n$, Figure 2.4a plots the three ordered bounds while Figure 2.4b shows the

percentage improvement of the three bounds over their unordered counterparts. The percentage improvement is computed as $(\text{unordered} - \text{ordered}) / \text{unordered} \times 100\%$. In this example with small marginals, the ordered Schmidt, Siegel and Srinivasan bound is equal to the ordered Boros and Prekopa bound as seen in Figure 2.4a. Ordering tends to improve the Schmidt, Siegel and Srinivasan bound significantly for smaller probabilities, since both the partial binomial moment terms S_{1r} and S_{2r} are smaller with smaller marginal probabilities for all $r \in [0, k - 1]$.



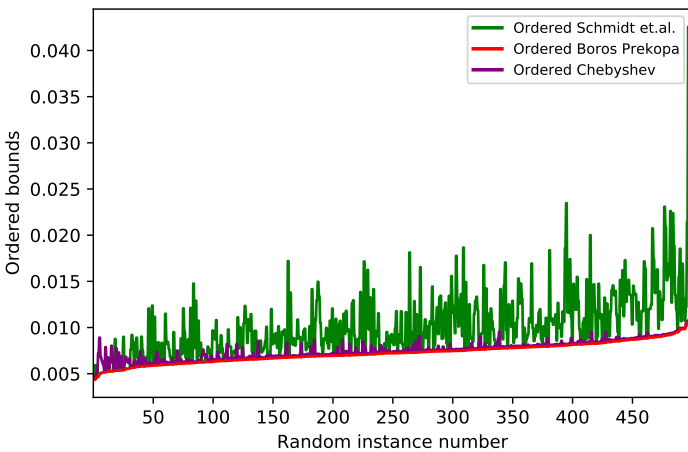
(a) Actual value of the ordered bounds



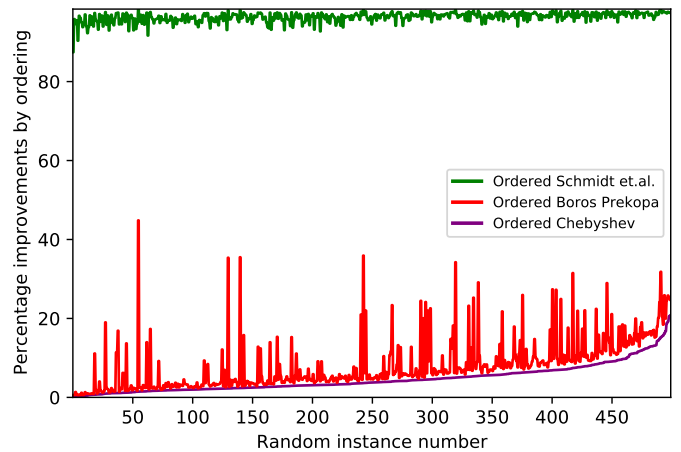
(b) Percentage improvement of ordered bounds

FIGURE 2.4: Smaller marginal probabilities p_i with $n = 100, k = 100$ and 500 instances.

The percentage improvement due to ordering in Figure 2.4b is consistently above 80% for the Schmidt, Siegel and Srinivasan bound, while that of the Boros and Prekopa bound hovers around 60%. The ordered Chebyshev bound shows an almost negligible improvement by ordering in this example.



(a) Actual value of the ordered bounds



(b) Percentage improvement of ordered bounds

FIGURE 2.5: Larger marginal probabilities p_i with $n = 100, k = 99$ and 500 instances.

Next, we consider similar plots when $k = n - 1$ with larger marginal probabilities. The entries of \mathbf{p} are generated uniformly and independently between 0.05 and 0.99. In Figure 2.5a, the ordered Chebyshev bound from (2.23) performs better than the ordered Schmidt, Siegel and Srinivasan bound from (2.21). In Figure 2.5b, the percentage improvement due to ordering is again most significant for the Schmidt, Siegel and Srinivasan bound, being consistently above 90% while that of the Boros and Prekopa bound is at most 45% and that of the Chebyshev bound is at most 20%. It is also clear from Figures 2.4 and 2.5 that the ordered Boros and Prekopa bound from (2.22) is the tightest of the three bounds across the instances, while among the other two bounds, none uniformly dominates the other. Note that the left plots in both figures 2.4 and 2.5 are shown with the bounds sorted according to the increasing value of the ordered Boros and Prekopa bound while the right plots in both figures are sorted according to the increasing percentage improvement of the ordered Chebyshev bound.

Comparison with Chernoff-Hoeffding bounds:

We next compare our ordered and unordered bounds with the Chernoff-Hoeffding bound (see Chernoff, 1952; Hoeffding, 1963) which are constructed for sums of mutually independent continuous random variables that range in $[0, 1]$. These bounds are typically used to provide right tail bounds when the sum deviates exceeds the mean by a positive quantity. More specifically, along the lines of Schmidt, Siegel, and Srinivasan (1995), we consider the Hoeffding estimate:

$$\mathbb{P}(\sum_{i=1}^n \tilde{c}_i \geq \mu(1 + \delta)) \leq F(n, \mu, \delta) = \frac{\left(1 + \frac{\mu\delta}{n - \mu(1 + \delta)}\right)^{n - \mu(1 + \delta)}}{(1 + \delta)^{\mu(1 + \delta)}}$$

where $\mu = \mathbb{E}[\sum_{i=1}^n \tilde{c}_i] = \sum_{i=1}^n p_i$ and $\delta > 0$ and $F(n, \mu, \delta)$ can be upper bounded as:

$$F(n, \mu, \delta) \leq G(\mu, \delta) = \left(\frac{e^\delta}{(1 + \delta)^{(1 + \delta)}}\right)^\mu$$

From Theorem 1 in Schmidt, Siegel, and Srinivasan (1995), the inequality

$$U_1(n, \mathbf{p}, \delta) \leq U_2(n, \mu, \delta) \leq F(n, \mu, \delta) \leq G(\mu, \delta) \quad (2.26)$$

holds for i^* -wise independent Bernoulli variables where:

$$U_1(n, \mathbf{p}, \delta) = \min_{0 \leq j \leq \mu(1 + \delta)} \frac{S_j(\mathbf{p})}{\binom{\mu(1 + \delta)}{j}}, \quad U_2(n, \mu, \delta) = \frac{\binom{n}{i^*} \left(\frac{\mu}{n}\right)^{i^*}}{\binom{\mu(1 + \delta)}{i^*}}, \quad i^* = \left\lceil \frac{\mu\delta}{1 - \mu/n} \right\rceil$$

and $S_j(\mathbf{p}) = \mathbb{E}[S_j(\mathbf{c})]$ is the expected value of the multilinear polynomial $S_j(\mathbf{c})$ defined in Section 2.1. Thus with pairwise independent variables and $\mu \leq k = \mu(1 + \delta) \leq 2$, the above inequality (2.26) will hold since $0 \leq i^* = \left\lceil \frac{k - \mu}{1 - \mu/n} \right\rceil \leq 2$ whenever $\mu \leq k \leq 2 + \mu(1 - 2/n)$. When the marginal probabilities are identical and equal p , we have $U_1 = U_2$, and $np \leq k \leq 2$ is sufficient to ensure that the inequality holds. Specifically when $k = 2$, the identical probability needs to satisfy $p \leq 2/n$. We next consider a numerical example to demonstrate instances for $k = 2$ when the unordered and ordered bounds considered in this section are tighter than the Chernoff-Hoeffding bounds.

Example 5 (Comparison with Chernoff-Hoeffding bounds). *In this example, we numerically compare the unordered and ordered bounds with the Chernoff-Hoeffding bounds for $n =$*

100 variables and $k = 2$. In Figure 2.6a, for 500 monotonically increasing instances of identical probabilities $p \in (0, 2/n)$, we plot the three unordered bounds with $F(n, \mu, \delta)$ and $G(\mu, \delta)$. The identical probability p is increased in equal step-sizes over the interval $(0, 2/n)$ for each instance. The unordered Schmidt, Siegel and Srinivasan bound (2.4) plotted here corresponds to both U_1 and U_2 (since $U_1 = U_2$ with identical probabilities) and almost coincides with the Boros and Prekopa bound (similar to the observation in Figure 2.4a with small heterogenous probabilities). The Chernoff-Hoeffding bounds perform better than the unordered Chebyshev bound for the first few instances, when the identical probabilities are small. However, the unordered Schmidt, Siegel, Srinivasan and Boros, Prekopa bounds are tighter than both estimates of the Chernoff-Hoeffding bounds across all the instances.

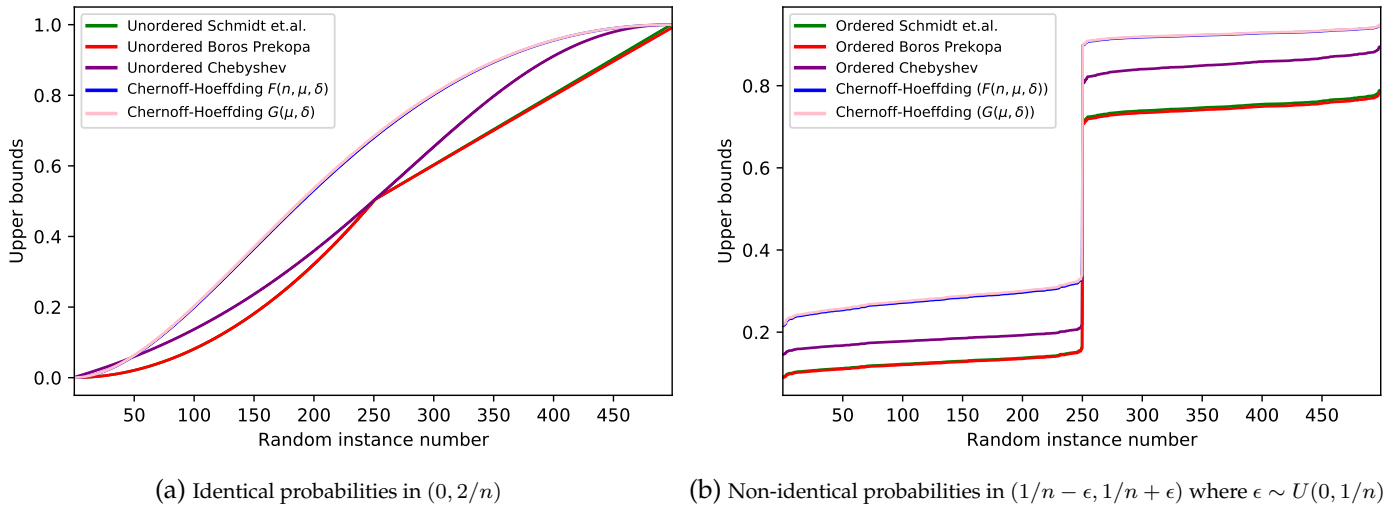


FIGURE 2.6: Comparison of unordered and ordered bounds with Chernoff-Hoeffding bounds with $n = 100, k = 2$ and 500 instances

In Figure 2.6b, we consider small heterogenous probabilities by perturbing the marginal probabilities around $1/n$. More specifically, we generate 500 random instances of marginal probabilities in the interval $(1/n - \epsilon, 1/n + \epsilon)$ where ϵ is uniformly and independently generated in $(0, 1/n)$ for each instance. The three ordered bounds are plotted with the Chernoff-Hoeffding bounds, where the bounds are sorted according to the increasing value of the ordered Boros and Prekopa bound. In this case, all the three ordered bounds are tighter than the Chernoff-Hoeffding bounds across all instances. However, when k is increased towards n , the Chernoff-Hoeffding bounds are increasingly likely to perform better than the ordered bounds. Specifically, the Chernoff-Hoeffding estimates $F(n, \mu, \delta)$ and $G(\mu, \delta)$ would likely overcome the unordered and ordered Schmidt, Siegel and Srinivasan bound U_1 , since the available information is only up to $j = 2$ while the minimization needs to be executed over $0 \leq j \leq k$.

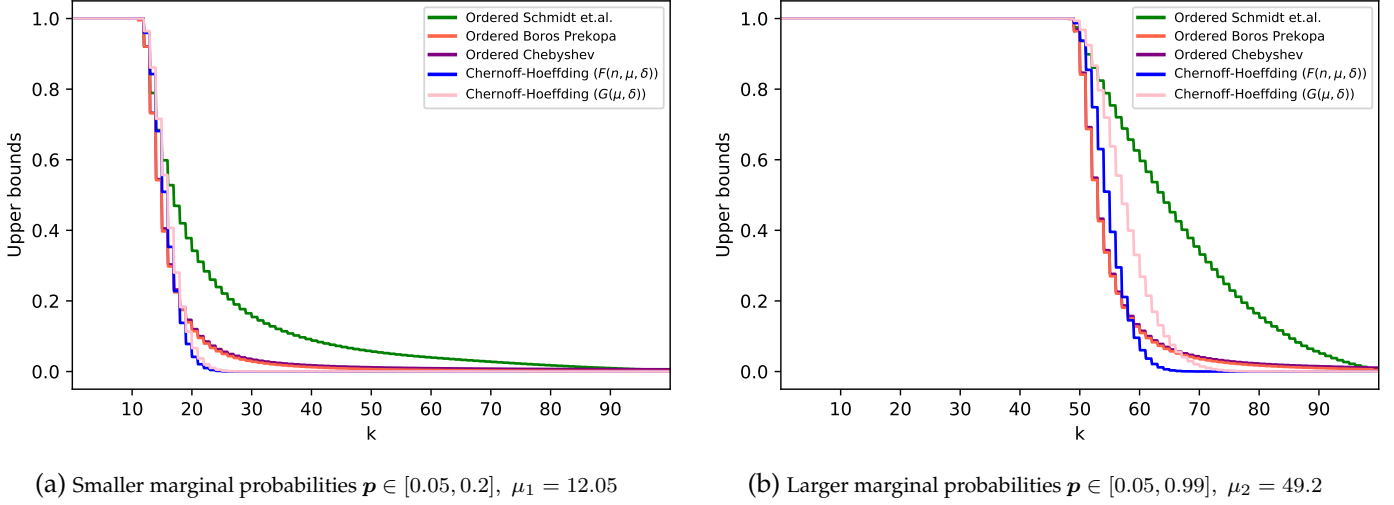


FIGURE 2.7: Comparison of unordered and ordered bounds with Chernoff-Hoeffding bounds with $n = 100$ for $k \in [n]$

This is demonstrated in Figure 2.7 where, for $n = 100$ random variables and for $k \in [n]$, we plot the three ordered bounds with the Chernoff-Hoeffding bounds for a single instance (each) of randomly generated small and large marginal probabilities. In Figure 2.7a, we consider small heterogenous probabilities generated uniformly and independently in $[0.05, 0.2]$ with mean $\mu_1 = 12.05$ while Figure 2.7b considers larger heterogenous probabilities uniformly and independently generated in $[0.05, 0.99]$ with $\mu_2 = 49.2$. When $k < \mu_1$ (μ_2), the ordered bounds and Chernoff-Hoeffding bounds are trivially one, while the ordered Schmidt, Siegel and Srinivasan bound is clearly dominated by the Chernoff-Hoeffding bounds for $k \geq \mu_1$ (μ_2) in both figures. The ordered Boros, Prekopa and Chebyshev bounds dominate the Chernoff-Hoeffding bounds in a small window $k \in [\mu_1, 17]$ and $k \in [\mu_2, 57]$ (in the left and right figures respectively), after which the Chernoff-Hoeffding bounds dominate in the right tail and quickly drop to zero. While the Chernoff-Hoeffding bounds restrict the random variables to be mutual independent and relax their support to $[0, 1]$, the improved bounds proposed in this section restrict the support to $\{0, 1\}$ and relax the independence assumption to pairwise independence. This example thus serves to demonstrate that the Chernoff-Hoeffding bounds in spite of their stronger assumptions of mutual independence are not necessarily tighter than the pairwise independent ordered and unordered bounds discussed in this section.

2.4 Tightness in special cases

In this section, we identify two tightness instances, one for the unordered Chebyshev, Schmidt, Siegel, Srinivasan and Boros, Prekopa bounds in (2.2), (2.4) and (2.7) and the other for the corresponding ordered bounds derived in Theorem 3 of the preceding section. Firstly, in Section 2.4.1, for identical variables, the symmetry in the problem allows for closed-form tight bounds for any $k \in [2, n]$. We prove this by showing an interesting equivalence of the exponential-sized linear program (2.5) which computes the exact bound with a polynomial sized linear program analyzed in computing the unordered Boros and Prekopa bound in (2.7). We further use this exact bound to identify instances when the other two unordered bounds are tight.

Secondly, in 2.4.2, we demonstrate the usefulness of the ordered bounds by identifying a special case when $n - 1$ marginals are identical (with additional conditions on the identical probability and k), when the ordered Schmidt, Siegel, Srinivasan and Boros, Prekopa bounds in (2.21) and (2.22) are tight.

2.4.1 Tightness of bounds with identical marginals

In this section, we provide probability bounds for n pairwise independent random variables adding up to at least $k \in [2, n]$ when their marginals are identical. The next theorem provides the tight bound with identical marginals, by applying the Boros and Prekopa bound in (2.7) to pairwise independent variables with $\xi = \sum_{i \in [n]} \tilde{c}_i$.

Theorem 4. Assume $p_i = p \in (0, 1)$ for $i \in [n]$. Let $\bar{P}(n, k, p)$ represent the tightest upper bound on the probability of n pairwise independent identical Bernoulli random variables adding up to at least an integer $k \in [n]$. Then,

$$\bar{P}(n, k, p) = \begin{cases} 1, & k < \eta, \text{ case (a)} \\ \frac{[(n-1)(1-p) + k]p}{k}, & k = \eta, \text{ case (b)} \\ \frac{n(n-1)p^2 + (i-1)(i-2np)}{(k-i)^2 + (k-i)}, & k > \eta, \text{ case (c)} \end{cases} \quad (2.27)$$

where $\eta = \lceil (n-1)p \rceil$ and $i = \left\lceil \frac{np(k-1 - (n-1)p)}{k-np} \right\rceil$.

Proof. The tightest upper bound $\bar{P}(n, k, p)$ is the optimal value of the linear program:

$$\begin{aligned} \bar{P}(n, k, p) = \max & \sum_{\mathbf{c} \in \mathcal{C}: \sum_i c_i \geq k} \mathbb{P}(\mathbf{c}) \\ \text{s.t.} & \sum_{\mathbf{c} \in \mathcal{C}: c_i = 1} \mathbb{P}(\mathbf{c}) = p, \quad \forall i \in [n], \\ & \sum_{\mathbf{c} \in \mathcal{C}: c_i = 1, c_j = 1} \mathbb{P}(\mathbf{c}) = p^2, \quad \forall (i, j) \in K_n, \\ & \sum_{\mathbf{c} \in \mathcal{C}} \mathbb{P}(\mathbf{c}) = 1 \\ & \mathbb{P}(\mathbf{c}) \geq 0, \quad \forall \mathbf{c} \in \mathcal{C}, \end{aligned} \quad (2.28)$$

where the decision variables are the joint probabilities $\mathbb{P}(\mathbf{c}) = \mathbb{P}(\tilde{\mathbf{c}} = \mathbf{c})$ for $\mathbf{c} \in \mathcal{C}$. Consider the following linear program in $n + 1$ variables which provides an upper

bound on $\bar{P}(n, k, p)$:

$$\begin{aligned}
 BP(n, k, p) = \max \quad & \sum_{\ell=k}^n v_\ell \\
 \text{s.t.} \quad & \sum_{\ell=0}^n v_\ell = 1 \\
 & \sum_{\ell=1}^n \ell v_\ell = np \\
 & \sum_{\ell=2}^n \binom{\ell}{2} v_\ell = \binom{n}{2} p^2 \\
 & v_\ell \geq 0, \quad \forall \ell \in [0, n],
 \end{aligned} \tag{2.29}$$

where the decision variables are the probabilities $v_\ell = \mathbb{P}(\sum_{i=1}^n \tilde{c}_i = \ell)$ for $\ell \in [0, n]$. Linear programs of the form (2.29) have been studied in Boros and Prékopa (1989) and Prékopa (1990a) in the context of aggregated binomial moment problems. As we shall see, these two formulations are equivalent with identical pairwise independent random variables.

Step (1): $\bar{P}(n, k, p) \leq BP(n, k, p)$

Given a feasible solution to (2.28) denoted by $\mathbb{P}(\mathbf{c})$, construct a feasible solution to the linear program (2.29) as:

$$v_\ell = \sum_{\mathbf{c} \in \mathcal{C}: \sum_i c_i = \ell} \mathbb{P}(\mathbf{c}), \quad \forall \ell \in [0, n].$$

By taking expectations on both sides of the equality (2.3), we get:

$$\sum_{l=j}^n \binom{l}{j} \mathbb{P} \left(\sum_{i=1}^n \tilde{c}_i = l \right) = \mathbb{E} [S_j(\tilde{\mathbf{c}})], \quad \forall j \in [0, n].$$

Applying it for $j = 0, 1, 2$, we get the three equality constraints in (2.29):

$$\begin{aligned}
 \sum_{\ell=0}^n v_\ell &= 1, \\
 \sum_{\ell=1}^n \ell v_\ell &= \mathbb{E} \left[\sum_{i=1}^n \tilde{c}_i \right] = np, \\
 \sum_{\ell=2}^n \binom{\ell}{2} v_\ell &= \mathbb{E} \left[\sum_{(i,j) \in K_n} \tilde{c}_i \tilde{c}_j \right] = n(n-1)p^2/2.
 \end{aligned}$$

Lastly, the objective function value of this feasible solution satisfies:

$$\begin{aligned} \sum_{\ell=k}^n v_{\ell} &= \sum_{\ell=k}^n \sum_{\mathbf{c} \in \mathcal{C}: \sum_i c_i = \ell} \mathbb{P}(\mathbf{c}) \\ &= \sum_{\mathbf{c} \in \mathcal{C}: \sum_i c_i \geq k} \mathbb{P}(\mathbf{c}). \end{aligned}$$

Hence, $\bar{P}(n, k, p) \leq BP(n, k, p)$.

Step (2): $\bar{P}(n, k, p) \geq BP(n, k, p)$

Given an optimal solution to (2.29) denoted by \mathbf{v} , construct a feasible solution to the linear program (2.28) by distributing v_{ℓ} equally among all the realizations in $\{0, 1\}^n$ with exactly ℓ ones:

$$\mathbb{P}(\mathbf{c}) = \frac{v_{\ell}}{\binom{n}{\ell}}, \quad \forall \mathbf{c} \in \mathcal{C} : \sum_{i=1}^n c_i = \ell, \forall \ell \in [0, n].$$

The first constraint in (2.28) is satisfied since:

$$\begin{aligned} \sum_{\mathbf{c} \in \mathcal{C}} \mathbb{P}(\mathbf{c}) &= \sum_{\ell=0}^n \sum_{\mathbf{c} \in \mathcal{C}: \sum_i c_i = \ell} \frac{v_{\ell}}{\binom{n}{\ell}} \\ &= \sum_{\ell=0}^n v_{\ell} \left[\text{since } |\{0, 1\}^n : \sum_{i=1}^n c_i = \ell| = \binom{n}{\ell} \right] \\ &= \sum_{\ell=0}^n v_{\ell} \\ &= 1. \end{aligned}$$

The second constraint in (2.28) is satisfied since:

$$\begin{aligned} \sum_{\mathbf{c} \in \mathcal{C}: c_j = 1} \mathbb{P}(\mathbf{c}) &= \sum_{\ell=1}^n \frac{v_{\ell}}{\binom{n}{\ell}} \binom{n-1}{\ell-1} \\ &= \sum_{\ell=1}^n \frac{\ell v_{\ell}}{n} \left[\text{since } |\{0, 1\}^n : \sum_{i=1}^n c_i = \ell, c_j = 1| = \binom{n-1}{\ell-1} \right] \\ &= \sum_{\ell=1}^n \frac{\ell v_{\ell}}{n} \\ &= p. \end{aligned}$$

The third constraint in (2.28) satisfied since:

$$\begin{aligned} \sum_{\mathbf{c} \in \mathcal{C}: c_i = 1, c_j = 1} \mathbb{P}(\mathbf{c}) &= \sum_{\ell=2}^n \frac{v_{\ell}}{\binom{n}{\ell}} \binom{n-2}{\ell-2} \\ &= \frac{2}{n(n-1)} \sum_{\ell=2}^n \binom{\ell}{2} v_{\ell} \left[\text{since } |\{0, 1\}^n : \sum_{t=1}^n c_t = \ell, c_i = 1, c_j = 1| = \binom{n-2}{\ell-2} \right] \\ &= \frac{2}{n(n-1)} \sum_{\ell=2}^n \binom{\ell}{2} v_{\ell} \\ &= p^2. \end{aligned}$$

The objective function value of the feasible solution is given by:

$$\begin{aligned} \sum_{\mathbf{c} \in \mathcal{C}: \sum_i c_i \geq k} \mathbb{P}(\mathbf{c}) &= \sum_{\ell=k}^n \sum_{\mathbf{c} \in \mathcal{C}: \sum_i c_i = \ell} \mathbb{P}(\mathbf{c}) \\ &= \sum_{\ell=k}^n v_\ell \\ &= BP(n, k, p). \end{aligned}$$

Hence, the optimal objective values of the two linear programs are equivalent. The formula for the tight bound in the theorem is then exactly the Boros and Prekopa bound in (2.7) (the bound $BP(n, k, p)$ is also derived in the work of Sathe, Pradhan, and Shah (1980), although tightness of the bound is not shown there). It is also straightforward to verify that the following distributions attain the bounds for each of the cases (a) – (c) in the statement of the theorem:

(a) The probabilities are given as:

$$\mathbb{P}(\mathbf{c}) = \begin{cases} \frac{(1-p)(j - (n-1)p)}{\binom{n-1}{j-1}}, & \text{if } \sum_{t=1}^n c_t = j-1, \\ \frac{(1-p)(1 + (n-1)p - j)}{\binom{n-1}{j}}, & \text{if } \sum_{t=1}^n c_t = j, \\ \frac{n(n-1)p^2 + (j-1)(j-2np)}{(n-j)^2 + (n-j)}, & \text{if } \sum_{t=1}^n c_t = n, \end{cases} \quad (2.30)$$

where $j = \lceil (n-1)p \rceil$ and all other support points have zero probability.

(b) The probabilities are given as:

$$\mathbb{P}(\mathbf{c}) = \begin{cases} \frac{1-p}{k}(k - (n-1)p), & \text{if } \sum_{t=1}^n c_t = 0, \\ \frac{p(1-p)}{\binom{n-2}{k-1}}, & \text{if } \sum_{t=1}^n c_t = k, \\ \frac{p((n-1)p - (k-1))}{n-k}, & \text{if } \sum_{t=1}^n c_t = n, \end{cases} \quad (2.31)$$

where all other support points have zero probability.

(c) The probabilities are given as:

$$\mathbb{P}(\mathbf{c}) = \begin{cases} \frac{np[(n-1)p - (k+i-1)] + ik}{\binom{n}{i-1}(k-i+1)}, & \text{if } \sum_{t=1}^n c_t = i-1, \\ \frac{np[(k+i-2) - (n-1)p] - k(i-1)}{\binom{n}{i}(k-i)}, & \text{if } \sum_{t=1}^n c_t = i, \\ \frac{n(n-1)p^2 + (i-1)(i-2np)}{\binom{n}{k}[(k-i)^2 + (k-i)]}, & \text{if } \sum_{t=1}^n c_t = k, \end{cases} \quad (2.32)$$

where all other support points have zero probability and the index i is evaluated as stated in equation (2.27)(c). It is straightforward to see that with identical marginals, the tight union bound in Theorem 2 reduces to the bound in case (b) of Theorem 4. \square

Connection of Theorem 4 to earlier work:

In related work, Benjamini, Gurel-Gurevich, and Peled (2012) and Peled, Yadin, and Yehudayoff (2011) derived probability bounds (not necessarily tight) for the sum of t -wise independent Bernoulli random variables with identical probabilities (as a special case, pairwise independent random variables are studied in these papers). For the specific case, where all the random variables take a value of one (this corresponds to $k = n$ in case (c)), the tight bound is provided in these works by making a connection with the Boros and Prekopa bound in (2.7). Recent work by Garnett (2020) provides the tight upper bound on the probability that the sum of pairwise independent Bernoulli random variables with identical marginals exceeds the mean by a small amount. This corresponds to case (b). Theorem 4, however, provides the equivalence for all values of (n, k, p) . The corresponding lower bound for identical pairwise independent random variables is derived in Section 2.6. Further, as we will show in Section 2.7.1, the analysis in Theorem 4 can be easily extended to more general t -wise independent variables ($t \geq 3$) from the symmetry assumptions.

Tightness of alternative bounds

We next discuss an application of Theorem 4. Since the marginals are identical, it is easy to see that the ordered bounds in Theorem 3 reduce to the unordered bounds corresponding to $r = 0$. While the unordered Boros and Prekopa bound provides the tightest upper bound with identical marginals, the formula is more involved than the unordered Chebyshev bound which reduces to:

$$\bar{P}(n, k, p) \leq \begin{cases} 1, & k < np, \\ np(1-p)/(np(1-p) + (k - np)^2), & np \leq k \leq n. \end{cases} \quad (2.33)$$

and the unordered Schmidt, Siegel and Srinivasan bound which reduces to:

$$\bar{P}(n, k, p) \leq \min \left(1, \frac{np}{k}, \frac{n(n-1)p^2}{k(k-1)} \right). \quad (2.34)$$

It is possible to then use Theorem 4 to identify conditions on the parameters (n, k, p) for which the bounds in (2.33) and (2.34) are tight. We only focus on the non-trivial cases where the tight bound is strictly less than one and $n \geq 3$. Henceforth, the Chebyshev and Schmidt, Siegel, Srinivasan bounds referred to in this section are the unordered bounds.

Proposition 2.

- (a) For $p = \alpha/(n-1)$ and any integer $\alpha \in [n-2]$, the Chebyshev bound in (2.33) is tight for the values of $k = \alpha + 1$ and $k = n$.
- (b) For $p \leq 1/(n-1)$, the Schmidt, Siegel and Srinivasan bound in (2.34) is tight for all $k \in [2, n]$ while for $p > 1/(n-1)$, the bound is tight for all $k \in [[1 + (n-1)p], \lfloor n(n-1)p^2/(np-1) \rfloor]$.

Proof. Since Theorem 4 provides the tight bound, we simply need to show the equivalence with the bounds in (2.33) and (2.34) for the instances in the proposition.

(a) Consider $p = \alpha/(n-1)$ for any integer $\alpha \in [n-2]$.

1. Set $k = \alpha + 1$. This corresponds to case (c) in Theorem 4. Plugging in the values, the index i which is required for finding the tight bound is given by:

$$\begin{aligned} i &= \left\lceil \frac{n\alpha(\alpha+1-1-\alpha)/(n-1)}{\alpha+1-n\alpha/(n-1)} \right\rceil \\ &= 0. \end{aligned}$$

The corresponding tight bound in (2.27) gives:

$$\bar{P}(n, k, p) = \frac{n\alpha}{(n-1)(\alpha+1)} = \frac{np}{np+1-p}.$$

It is straightforward to verify by plugging in the values that the Chebyshev bound is exactly the same.

2. Set $k = n$. This corresponds to case (c) in Theorem 4. Plugging in the values, the index i in the tight bound is given by:

$$\begin{aligned} i &= \left\lceil \frac{n\alpha(n-1-\alpha)/(n-1)}{n-n\alpha/(n-1)} \right\rceil \\ &= \alpha. \end{aligned}$$

The tight bound in (2.27) gives:

$$\bar{P}(n, k, p) = \frac{\alpha}{(n-1)(n-\alpha)} = \frac{p}{p+n(1-p)}.$$

It is straightforward to verify by plugging in the values that the Chebyshev bound is exactly the same in this case.

- (b) Observe that the last two terms in the Schmidt, Siegel and Srinivasan bound in (2.34) satisfy:

$$\frac{n(n-1)p^2}{k(k-1)} \leq \frac{np}{k} \text{ when } k \geq 1 + (n-1)p.$$

Since this implies $1 \geq np/k$, the bound in (2.34) reduces to $n(n-1)p^2/k(k-1)$. The range of $k \geq 1+(n-1)p$ corresponds to case (c) in Theorem 4. If $k = 1+(n-1)p$, the index $i = \left\lceil \frac{np(k - (1 + (n-1)p))}{k - np} \right\rceil = 0$ and the tight bound is:

$$\frac{np}{1 + (n-1)p},$$

which is exactly the Schmidt, Siegel and Srinivasan bound. We can also verify that when the index $i = 1$ in case (c), then the tight bound in Theorem 4 reduces to:

$$\begin{aligned} \bar{P}(n, k, p) &= \frac{n(n-1)p^2 + (1-1)(1-2np)}{(k-1)^2 + (k-1)} \\ &= \frac{n(n-1)p^2}{k(k-1)}. \end{aligned}$$

We now identify conditions when $k > 1 + (n - 1)p$ and the index i is equal to one.

1. Set $0 < p < 1/(n - 1)$. For the values of the p in this interval, the valid range of k in case (c) corresponds to all integer values of $k > 1 + (n - 1)p$ which means $k \geq 2$. For the probability $0 < p \leq 1/n$, the index i satisfies:

$$\begin{aligned} i &= \left\lceil \frac{np(k - np - (1 - p))}{k - np} \right\rceil \\ &= \left\lceil np \left(1 - \frac{1 - p}{k - np} \right) \right\rceil \\ &= 1 \\ &\quad [\text{since } 0 < np \leq 1 \text{ and } (1 - p) \in (0, 1) \text{ and } k - np \geq 1 - p]. \end{aligned}$$

For the probability $1/n < p < 1/(n - 1)$, let $(n - 1)p = 1 - \delta$ where $\delta < 1$. Then, since $np > 1$, we have $n \frac{(1 - \delta)}{n - 1} > 1$ or equivalently $n\delta < 1$. The index i satisfies:

$$\begin{aligned} i &= \left\lceil \frac{np((n - 1)p - (k - 1))}{np - k} \right\rceil \\ &< \left\lceil \frac{np(1 - \delta - (k - 1))}{1 - k} \right\rceil \\ &\quad [\text{since } np > 1 \text{ and } (n - 1)p = 1 - \delta] \\ &= \left\lceil \frac{np(k - 2 + \delta)}{k - 1} \right\rceil \\ &< \left\lceil \frac{n(k - 2 + \delta)}{(n - 1)(k - 1)} \right\rceil \\ &\quad [\text{since } p < 1/(n - 1)] \\ &= \left\lceil \frac{n(k - 2 + \delta)}{(nk - n - k + 1)} \right\rceil \\ &\leq \left\lceil \frac{n(k - 2 + \delta)}{nk - 2n + 1} \right\rceil \\ &\quad [\text{since } k \leq n] \\ &= \left\lceil \frac{n(k - 2) + n\delta}{n(k - 2) + 1} \right\rceil \\ &= 1 \\ &\quad [\text{since } k \geq 2 \text{ and } 0 < n\delta < 1] \end{aligned}$$

Hence, the bound in (2.34) is tight in this case for all integer values of $k \geq 2$.

2. For $p > 1/(n - 1)$, the index $i = 1$ when $k(np - 1) \leq n(n - 1)p^2$. This corresponds to all integer values $k \in [\lceil 1 + (n - 1)p \rceil, \lfloor n(n - 1)p^2 / (np - 1) \rfloor]$.

□

A specific instance to show the tightness of the Chebyshev bound is to set $p = 1/2$, $k = n$ and $n = 2^m - 1$ using m independent Bernoulli random variables to construct n pairwise independent Bernoulli random variables (see Tao, 2012; Goemans, 2015; Pass and Spektor, 2018, for this construction). Proposition 2(a) includes this instance (set $\alpha = (n - 1)/2$, $k = n$ and $n = 2^m - 1$). In addition, Proposition 2(a) identifies other values of p and k where the Chebyshev bound is tight. Proposition 2(b) also shows that the Schmidt, Siegel and Srinivasan bound is tight for identical marginals for small probability values ($p \leq 1/(n - 1)$), for all values of k , except $k = 1$. We now provide a numerical illustration of the results in Theorem 4 and Proposition 2.

Example 6 (Identical marginals). In Table 2.4, we provide a numerical comparison of the bounds for $n = 11$ for a set of values of p and k . The instances in Table 2.4 cover all the conditions identified in Proposition 2 when the Chebyshev and Schmidt, Siegel, Srinivasan bounds are tight. The instances when the Chebyshev bound is tight correspond to (i) $p = 0.1$ (here $\alpha = 1$ and the Chebyshev bound is tight for $k = 2$ and $k = 11$), (ii) $p = 0.2$ (here $\alpha = 2$ and the Chebyshev bound is tight for $k = 3$ and $k = 11$) and (iii) $p = 0.5$ (here $\alpha = 5$ and the Chebyshev bound is tight for $k = 6$ and $k = 11$). The Schmidt, Siegel and Srinivasan bound is tight for the small values of $p = 0.01, 0.05, 0.10$ (which are less than or equal to $1/(n - 1) = 0.1$) and for all values of k , except $k = 1$.

p/k	1	2	3	4	5	6	7	8	9	10	11
0.01	0.10900	0.00550	0.00184	0.00092	0.00055	0.00037	0.00027	0.00020	0.00016	0.00013	0.00010
	0.12087	0.02959	0.01288	0.00715	0.00454	0.00313	0.00229	0.00175	0.00138	0.00112	0.00092
	0.11000	0.00550	0.00184	0.00092	0.00055	0.00037	0.00027	0.00020	0.00016	0.00013	0.00010
0.05	0.52500	0.13750	0.04583	0.02292	0.01375	0.00917	0.00655	0.00491	0.00382	0.00306	0.00250
	0.72069	0.19905	0.08008	0.04205	0.02571	0.01729	0.01240	0.00933	0.00726	0.00582	0.00477
	0.55000	0.13750	0.04583	0.02292	0.01375	0.00917	0.00655	0.00491	0.00382	0.00306	0.00250
0.10	1	0.55000	0.18333	0.09167	0.05500	0.03667	0.02620	0.01965	0.01528	0.01223	0.01000
	1	0.55000	0.21522	0.10532	0.06112	0.03960	0.02766	0.02038	0.01562	0.01235	0.01000
	1	0.55000	0.18333	0.09167	0.05500	0.03667	0.02620	0.01965	0.01528	0.01223	0.01000
0.11	1	0.59950	0.22184	0.11092	0.06655	0.04437	0.03037	0.02170	0.01627	0.01266	0.01013
	1	0.63310	0.25156	0.12154	0.06975	0.04484	0.03113	0.02283	0.01744	0.01375	0.01112
	1	0.60500	0.22184	0.11092	0.06655	0.04437	0.03170	0.02377	0.01849	0.01479	0.01210
0.15	1	0.78750	0.41250	0.19584	0.09792	0.05875	0.039167	0.02798	0.020983	0.01632	0.01306
	1	0.91968	0.43489	0.20253	0.11109	0.06901	0.04672	0.03362	0.02531	0.01972	0.01579
	1	0.82500	0.41250	0.20625	0.12375	0.08250	0.05893	0.044197	0.034375	0.02750	0.02250
0.20	1	1	0.73334	0.33334	0.16667	0.10000	0.06667	0.04762	0.03572	0.02778	0.02223
	1	1	0.73334	0.35200	0.18334	0.10865	0.07097	0.04972	0.03667	0.02812	0.02223
	1	1	0.73334	0.36667	0.22000	0.14667	0.10477	0.07858	0.06112	0.04889	0.04000
0.50	1	1	1	1	1	0.91667	0.54167	0.29167	0.17500	0.11667	0.08334
	1	1	1	1	1	0.91667	0.55000	0.30556	0.18334	0.11957	0.08334
	1	1	1	1	1	0.91667	0.65477	0.49108	0.38195	0.30556	0.25000

TABLE 2.4: Upper bounds on probability of sum of random variables for $n = 11$. For each value of p and k , the table provides the tight bound in (2.27) followed by the Chebyshev bound (2.33) and the Schmidt, Siegel, Srinivasan bound (2.34). The underlined instances illustrate cases when the upper bounds in either (2.33) or (2.34) are tight.

It is also clear why the Schmidt, Siegel and Srinivasan bound is not tight for $k = 1$, since it just reduces to the Markov bound np and does not exploit the pairwise independence information. For $k = 1$, the tight bound from Theorem 4 is given by $np - (n - 1)p^2$ (see Theorem 2 which reduces to the same bound for $k = 1$). For larger values of p above 0.1, such as $p = 0.11$ in the table, from Proposition 2(b), the Schmidt, Siegel and Srinivasan bound is tight for $k \in [[2.1], [6.33]]$ which corresponds to $k \in [3, 6]$. This can be similarly verified for the other probabilities $p = 0.15, 0.2, 0.5$ in the table.

2.4.2 Tightness of ordered bounds in a special case

In this section, we provide an instance where two of the ordered bounds derived in Section 2.3 are shown to be tight. While the ordered bounds in Theorem 3 are not tight in general, the next proposition identifies a special case with almost identical marginals where the bounds of Schmidt, Siegel, Srinivasan in (2.21) and Boros, Prekopa in (2.22) are shown to be attained.

Proposition 3. *Suppose the marginal probabilities equal $p \in (0, 1/(n-1)]$ for $n-1$ random variables and $q \in (0, 1)$ for one random variable. Then, the ordered bounds in (2.21) and (2.22) are tight for the following three instances and given by the bound:*

$$\bar{P}(n, k, p, q) = \begin{cases} \frac{\binom{n-1}{2} p^2}{\binom{k-1}{2}}, & k \geq 3, q \geq (n-2)p & \text{case (a)} \\ \frac{\binom{n-1}{2} p^2}{\binom{k-1}{2}}, & k \in [2 + (n-2)p/q, n], p \leq q < (n-2)p & \text{case (b)} \\ pq, & k = n, 0 < q < p & \text{case (c)} \end{cases} \quad (2.35)$$

Proof. We first prove that the ordered bounds of Schmidt, Siegel, Srinivasan and Boros, Prekopa reduce to the bound in (2.35) in each of the three cases and then show that the bound is tight.

Step (1): Show reduction of ordered bounds to the bound in (2.35)

Let $\bar{P}(n, k, p, q)$ represent the tightest upper bound when $n-1$ probabilities are p and one is q . It can be observed that the bound in (2.35) is non-trivial for the three instances as follows:

$$\frac{\binom{n-1}{2} p^2}{\binom{k-1}{2}} = \frac{(n-1)p(n-2)p}{(k-1)(k-2)} < 1$$

for cases (a) and (b) since $(n-2)p < (n-1)p \leq 1$ and $k \geq 3$, and

$$pq < 1$$

for case (c) since $q < p < 1$. It is easy to verify that the ordered Schmidt, Siegel and Srinivasan bound in (2.21) reduces to the bound in (2.35) for a specific parameter r_2 in each of the three cases:

$$\begin{aligned} r_2 &= 1, & \text{cases (a) and (b)} \\ r_2 &= n-2, & \text{case (c)}. \end{aligned} \quad (2.36)$$

It can be similarly verified that the ordered Boros and Prekopa bound in (2.22) reduces to the bound in (2.35) with the following parameters r and i in each of the three cases:

$$\begin{aligned} r &= 1, i = 0, & \text{cases (a) and (b)} \\ r &= n-2, i = 0, & \text{case (c)}. \end{aligned} \quad (2.37)$$

The effectiveness of ordering is demonstrated by (2.36) and (2.37) in that the ordered bounds of Schmidt, Siegel, Srinivasan and Boros, Prekopa correspond to $r > 0$ while their unordered counterparts in (2.4) and (2.7) correspond to $r = 0$ (considering all n variables). The unordered bounds are thus strictly weaker than the ordered bounds

which in turn are tight as proved in the next step.

Step (2): Prove tightness of the bound in (2.35) by constructing extremal distributions

Consider the linear program to compute $\bar{P}(n, k, p, q)$ which can be written as:

$$\begin{aligned}
\bar{P}(n, k, p, q) = \max & \sum_{\mathbf{c} \in \mathcal{C}: \sum_t c_t \geq k} \mathbb{P}(\mathbf{c}) \\
\text{s.t.} & \sum_{\mathbf{c} \in \mathcal{C}: c_i = 1} \mathbb{P}(\mathbf{c}) = p, \quad \forall i \in [n] \\
& \sum_{\mathbf{c} \in \mathcal{C}: c_n = 1} \mathbb{P}(\mathbf{c}) = q \\
& \sum_{\mathbf{c} \in \mathcal{C}: c_i = 1, c_j = 1} \mathbb{P}(\mathbf{c}) = p^2, \quad \forall (i, j) \in K_{n-1} \\
& \sum_{\mathbf{c} \in \mathcal{C}: c_i = 1, c_n = 1} \mathbb{P}(\mathbf{c}) = pq, \quad \forall i \in [n-1] \\
& \sum_{\mathbf{c} \in \mathcal{C}} \mathbb{P}(\mathbf{c}) = 1 \\
& \mathbb{P}(\mathbf{c}) \geq 0, \quad \forall \mathbf{c} \in \mathcal{C}
\end{aligned} \tag{2.38}$$

We now proceed to prove tightness of the bound in (2.35) for each of the three instances of the (n, k, p, q) tuple by constructing feasible distributions of (2.38) which attain the bound.

(a) $\bar{P}(n, k, p, q) = \frac{\binom{n-1}{2} p^2}{\binom{k-1}{2}}$ (cases (a) and (b)):

The following distribution attains the tight bound:

$$\mathbb{P}(\mathbf{c}) = \begin{cases} (1-q)(1-(n-1)p), & \text{if } \sum_{t=1}^n c_t = 0 & (x) \\ p(1-q), & \text{if } \sum_{t=1}^{n-1} c_t = 1, c_n = 0 & (y) \\ q(1-(n-1)p) + \frac{(n-1)(n-2)p^2}{(k-1)}, & \text{if } \sum_{t=1}^{n-1} c_t = 0, c_n = 1 & (z) \\ p(q - \frac{n-2}{k-2}p), & \text{if } \sum_{t=1}^{n-1} c_t = 1, c_n = 1 & (u) \\ \frac{p^2}{\binom{n-3}{k-3}}, & \text{if } \sum_{t=1}^{n-1} \tilde{c}_t = k-1, c_n = 1 & (v) \end{cases} \tag{2.39}$$

We use symbols x, y, z, u, v to denote the probability of the associated scenarios in (2.39). The constraints in (2.38) reduce to:

$$\begin{aligned} \binom{n-2}{k-2}v + u + y &= p \\ \binom{n-1}{k-1}v + (n-1)u + z &= q \\ \binom{n-3}{k-3}v &= p^2 \\ \binom{n-2}{k-2}v + u &= pq \\ x + y + z + u + v &= 1 \end{aligned}$$

and using x, y, z, u, v from (2.39), it can be easily verified that all of the above constraints are satisfied. The non-negativity constraints for y, v are satisfied while $x \geq 0, z \geq 0$ is satisfied since $(n-1)p \leq 1$. For the remaining probability u , for which we have:

$$\begin{aligned} \text{case (a): } u &= p \left(q - \frac{n-2}{k-2}p \right) \\ &\geq y = p \left(q - \frac{n-2}{3-2}p \right) \\ &= p(q - (n-2)p) \\ &\geq 0 \end{aligned}$$

where the first inequality is due to $k \geq 3$ while the last inequality is due to $q > (n-2)p$ and

$$\begin{aligned} \text{case (b): } u &= p \left(q - \frac{n-2}{k-2}p \right) \\ &\geq p \left(q - \frac{k-2}{k-2}q \right) \\ &= 0. \end{aligned}$$

where the inequality is due to $k \geq 2 + (n-2)p/q$. The only support points contributing to the objective function are the first set of $\binom{n-1}{k-1}$ scenarios, and so we

$$\text{have } \bar{P}(n, k, p, q) = \binom{n-1}{k-1} \frac{p^2}{\binom{n-3}{k-3}} = \frac{\binom{n-1}{2}p^2}{\binom{k-1}{2}}.$$

(b) $\bar{P}(n, k, p, q) = pq$ (case (c)):

The following distribution attains the tight bound pq :

$$\mathbb{P}(\mathbf{c}) = \begin{cases} (1-p)(1-(n-2)p-q), & \text{if } \sum_{t=1}^n c_t = 0 & (x) \\ p(1-p), & \text{if } \sum_{t=1}^{n-1} c_t = 1, c_n = 0 & (y) \\ q(1-p), & \text{if } \sum_{t=1}^{n-1} c_t = 0, c_n = 1 & (z) \\ p(p-q), & \text{if } \sum_{t=1}^{n-1} c_t = n-1, c_n = 0 & (u) \\ pq, & \text{if } \sum_{t=1}^n c_t = n & (v) \end{cases} \quad (2.40)$$

The constraints in (2.38) reduce to:

$$\begin{aligned} y + u + v &= p \\ z + v &= q \\ u + v &= p^2 \\ v &= pq \\ x + y + z + u + v &= 1 \end{aligned}$$

and using x, y, z, u, v from (2.40), it can be easily verified that all of the above constraints are satisfied. The non-negativity constraints for y, z, u, v are satisfied by $0 < q \leq p \leq 1$ while for x , we have:

$$\begin{aligned} x &= (1-p)(1-(n-2)p-q) \\ &\geq (1-p)(1-(n-2)p-p) \\ &= (1-p)(1-(n-1)p) \\ &\geq 0 \end{aligned}$$

where the first inequality is due to $q < p$ while the last inequality is due to $(n-1)p \leq 1$. The distribution in (2.40) attains the bound pq . We have thus constructed two feasible probability distributions in (2.39) and (2.40) which attain the bound in (2.35) in each of the three instances defined by the (n, k, p, q) tuple. Hence the parameters r_2, r in (2.36) and (2.37) defined for each of the three cases must be the minimizers which exactly reduce the ordered bounds in (2.21) and (2.22) to the tight bound in (2.35). \square

Example 7. This example demonstrates the usefulness of Proposition 3 when $n = 100$ and $p = 0.01$ ($(n-1)p \leq 1$). It compares the tight bounds computed from (2.35) with the unordered bounds of Schmidt, Siegel, Srinivasan from (2.4) and that of Boros, Prekopa from (2.7).

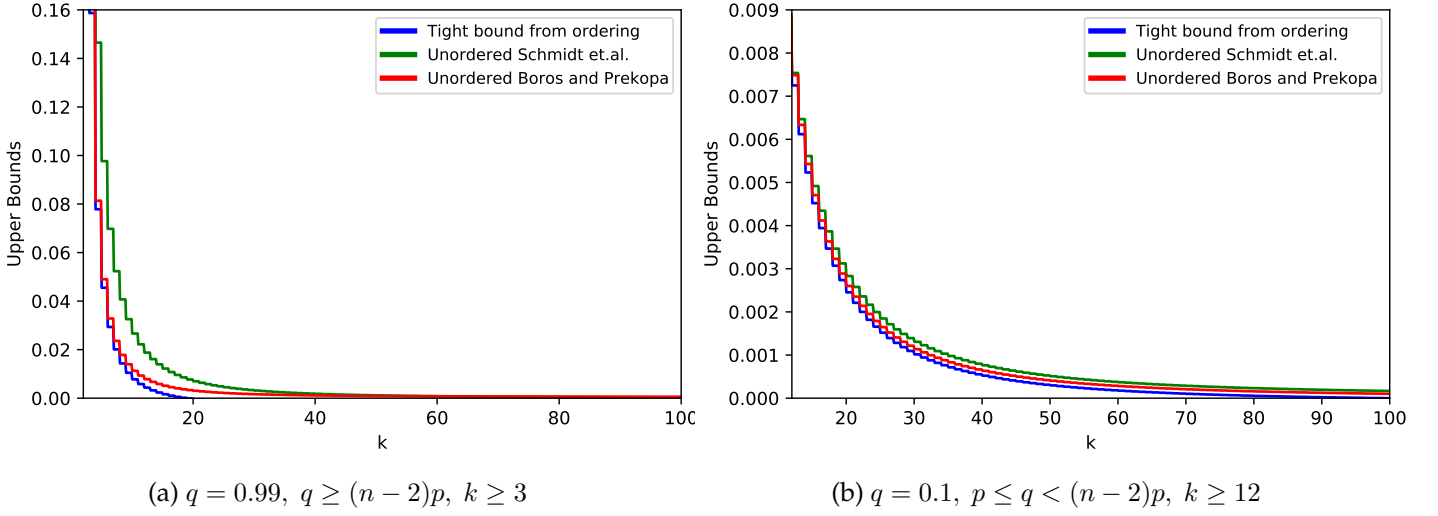
FIGURE 2.8: Comparison of unordered and tight bounds when $n = 100, p = 0.01$

Figure 2.8a plots the two unordered bounds along with the tight bound when $q = 0.99$ (case (a) of Proposition 3), where the tight bound is valid for all k in $[3, n]$, while Figure 2.8b compares the bounds when $q = 0.1$ (case (b) of Proposition 3) for $k \geq 12$ as the tight bound is valid when $k \geq \lceil 2 + (n - 2)p/q \rceil = \lceil 11.8 \rceil = 12$. The unordered Boros and Prekopa bound is much tighter than the unordered Schmidt, Siegel and Srinivasan bound in both figures. Hence, Figure 2.8 demonstrates that with ordering, the relative improvement of the Schmidt, Siegel and Srinivasan bound is much better than that of the Boros and Prekopa bound although both the ordered bounds reduce to the tight bound in (2.35).

2.5 Correlation gap improvements with general submodular functions for $n = 2$

In this section we extend the results from Section 2.2.3 to more general submodular functions to show that the upper bound on the correlation gap can be improved from $e/(e - 1)$ to $4/3$ for $n = 2$ random variables.

Theorem 5. Given $n = 2$ random variables with univariate marginal probabilities p_1, p_2 , the correlation gap $\kappa_u(\mathbf{p})$ for any nonnegative, nondecreasing, submodular set function, $f(S)$, is always upper bounded by $4/3$ and this bound is attained.

Proof. For $n = 2$ random variables, consider a nonnegative, nondecreasing, submodular set function $f : S \rightarrow \mathbb{R}_+$ whose domain $S \subseteq \{1, 2\}$ maps to the scenario set $\mathbf{c} \in \{0, 1\}^2$ through the relation:

$$c_i = \mathbb{1}_{i \in S}, \forall i = 1, 2, S \in \{\emptyset, \{1\}, \{2\}, \{1, 2\}\}$$

Recall from Section 2.2.3 that the correlation gap is defined as:

$$\kappa_u(\mathbf{p}) = \sup_{\theta \in \Theta_u} \frac{\mathbb{E}_\theta[f(S)]}{\mathbb{E}_{\theta_{\text{ind}}}[f(S)]}.$$

This theorem shows that the upper bound of $e/(e-1)$ on $\kappa_u(\mathbf{p})$ proved in Calinescu et al. (2007) and Agrawal et al. (2012) can be improved to $4/3$ in special cases such as $n = 2$ random variables. We note that for $n = 2$, the following conditions are satisfied if and only if f is a non-negative, non-decreasing, submodular set function:

Set function property	Condition satisfied by $f(S)$
Submodularity	$f(\{1\}) + f(\{2\}) \geq f(\{1, 2\}) + f(\emptyset)$
Non-decreasing, Non-negativity	$f(\{1, 2\}) \geq f(\{1\}) \geq f(\emptyset) \geq 0$ $f(\{1, 2\}) \geq f(\{2\}) \geq f(\emptyset) \geq 0$

TABLE 2.5: Conditions satisfied by assumed properties of set function for $n = 2$

Note that we consider a modified non-negative, non-decreasing submodular function

$$g_1(S) = f(S) - f(\emptyset), \quad S \subseteq \{1, 2\},$$

then, $g_1(\emptyset) = 0$ and the correlation gap $\kappa_u(\mathbf{p})$ can only increase by considering $g_1(S)$ instead of $f(S)$ since

$$\begin{aligned} \kappa_u(\mathbf{p}) &= \sup_{\theta \in \Theta_u} \frac{\mathbb{E}_\theta[g_1(S)]}{\mathbb{E}_{\theta_{ind}}[g_1(S)]} \\ &= \frac{\sup_{\theta \in \Theta_u} \mathbb{E}_\theta[f(S)] - f(\emptyset)}{\mathbb{E}_{\theta_{ind}}[f(S)] - f(\emptyset)} \\ &\geq \sup_{\theta \in \Theta_u} \frac{\mathbb{E}_\theta[f(S)]}{\mathbb{E}_{\theta_{ind}}[f(S)]} \end{aligned}$$

Similarly we can consider a normalized non-negative, non-decreasing submodular function by dividing f by its largest value $f(\{1, 2\})$, i.e.,

$$g_2(S) = \frac{f(S)}{f(\{1, 2\})}, \quad S \subseteq \{1, 2\},$$

where $f(\{1, 2\}) > 0$ (otherwise $f(S)$ is trivially zero everywhere) and the correlation gap $\kappa_u(\mathbf{p})$ would remain unchanged by considering $g_2(S)$ instead of $f(S)$. Since $g_1(\emptyset) = 0$ and $g_2(S) \in [0, 1]$, $\forall S \subseteq \{1, 2\}$, we can without loss of generality assume that

$$f(\emptyset) = 0, \quad f(\{1, 2\}) = 1$$

and the conditions in Table 2.5 reduce to:

$$0 \leq f(\{1\}) \leq 1, \quad 0 \leq f(\{2\}) \leq 1, \quad f(\{1\}) + f(\{2\}) \geq 1 \quad (2.41)$$

Next consider the primal-dual linear program pair which compute the numerator $\sup_{\theta \in \Theta_u} \mathbb{E}_\theta[f(S)]$ of $\kappa_u(\mathbf{p})$ as their optimal objective:

$$\begin{array}{l|l}
\max \sum_{S \subseteq [n]} f(S) \mathbb{P}(S) & \min \sum_{i=1}^n \lambda_i p_i + \lambda_0 \\
\text{s.t.} \sum_{S \subseteq [n]: i \in S} \mathbb{P}(S) = p_i, \quad i = 1, 2, & \text{s.t.} \quad \lambda_0 \geq f(\emptyset) \\
\sum_{S \subseteq [n]} \mathbb{P}(S) = 1, & \lambda_2 + \lambda_0 \geq f(\{2\}) \\
\mathbb{P}(S) \geq 0 & \lambda_1 + \lambda_0 \geq f(\{1\}) \\
& \lambda_1 + \lambda_2 + \lambda_0 \geq f(\{1, 2\}) \\
& \lambda_0, \lambda_1, \lambda_2 \text{ free}
\end{array} \tag{2.42} \tag{2.43}$$

For $n = 2$ random variables, the optimal objective of (2.42)-(2.43) pair can be shown to exist in a closed form attained by the following extremal distributions:

	Condition on $p_1 + p_2$	Extremal distribution (2.42)			Optimal dual solution (2.43)	Optimal objective attained	
		c_1	c_2	S			
Case 1	$p_1 + p_2 \leq 1$	0	0	\emptyset	$1 - p_1 - p_2$	$\lambda_0 = f(\emptyset)$ $\lambda_1 = f(\{1\}) - f(\emptyset)$ $\lambda_2 = f(\{2\}) - f(\emptyset)$	$f(\{1\})p_1 + f(\{2\})p_2$ $+ f(\emptyset)(1 - p_1 - p_2)$
		0	1	$\{2\}$	p_2		
		1	0	$\{1\}$	p_1		
		1	1	$\{1, 2\}$	0		
Case 2	$p_1 + p_2 > 1$	0	0	\emptyset	0	$\lambda_0 = f(\{1\}) + f(\{2\})$ $- f(\{1, 2\})$	$f(\{1\})(1 - p_2) + f(\{2\})(1 - p_1)$ $+ f(\{1, 2\})(p_1 + p_2 - 1)$
		0	1	$\{2\}$	$1 - p_1$	$\lambda_1 = f(\{1, 2\}) - f(\{2\})$	
		1	0	$\{1\}$	$1 - p_2$	$\lambda_2 = f(\{1, 2\}) - f(\{1\})$	
		1	1	$\{1, 2\}$	$p_1 + p_2 - 1$		

TABLE 2.6: Possible extremal distributions with extremal dependence for $n = 2$:

It is straightforward to verify using the conditions in Table 2.5 that the proposed optimal dual solutions are indeed feasible for the dual linear program (2.43) and attain the same objective value as the primal (2.42). We now proceed to prove that in both cases of Table 2.6, the correlation gap $\kappa_u(\mathbf{p}) \leq 4/3$.

Case 1:

Note that with $n = 2$, mutual independence is equivalent to pairwise independence, and thus when $p_1 + p_2 \leq 1$ we could directly use the analysis from (2.17) in Proposition 1 as follows:

$$\frac{p_1 + p_2}{p_1 + p_2 - p_1 p_2} = \frac{1}{1 - \frac{1}{\frac{1}{p_1} + \frac{1}{p_2}}} \leq \frac{4}{3} \quad \text{or} \quad p_1 + p_2 \geq 4p_1 p_2$$

The correlation gap can be written as:

$$\kappa_u(\mathbf{p}) = \frac{f(\{1\})p_1 + f(\{2\})p_2 + f(\emptyset)(1 - p_1 - p_2)}{f(\{1, 2\})p_1 p_2 + f(\{2\})p_2(1 - p_1) + f(\{1\})p_1(1 - p_2) + f(\emptyset)(1 - p_1)(1 - p_2)}$$

Using the simplified conditions in (2.41), we now need to prove that

$$\kappa_u(\mathbf{p}) = \frac{f(\{1\})p_1 + f(\{2\})p_2}{f(\{1\})p_1(1-p_2) + f(\{2\})p_2(1-p_1) + p_1p_2} \leq \frac{4}{3}$$

or

$$f(\{1\})p_1 + f(\{2\})p_2 - 4p_1p_2(f(\{1\}) + f(\{2\}) - 1) \geq 0 \quad (2.44)$$

The left hand side of the inequality (2.44) thus simplifies to:

$$\begin{aligned} f(\{1\})p_1 + f(\{2\})p_2 &\geq f(\{1\})p_1 + f(\{2\})p_2 \\ -4p_1p_2(f(\{1\}) + f(\{2\}) - 1) &- (p_1 + p_2)(f(\{1\}) + f(\{2\}) - 1) \\ &= p_2(1 - f(\{1\})) + p_1(1 - f(\{2\})) \\ &\geq 0 \end{aligned}$$

where the first inequality is due to the fact that $f(\{1\}) + f(\{2\}) - 1 \geq 0$ along with $p_1 + p_2 \geq 4p_1p_2$ while the last inequality is due to $f(\{1\}) \leq 1, f(\{2\}) \leq 1$.

Case 2:

When $p_1 + p_2 > 1$ we have:

$$(1-p_1)(1-p_2) < p_2(1-p_2) \leq \frac{1}{4} \quad \text{or} \quad p_1 + p_2 - p_1p_2 > \frac{3}{4}$$

Using the simplified conditions in (2.41), we need to prove that:

$$\kappa_u(\mathbf{p}) = \frac{f(\{1\})(1-p_2) + f(\{2\})(1-p_1) + (p_1 + p_2 - 1)}{f(\{1\})p_1(1-p_2) + f(\{2\})p_2(1-p_1) + p_1p_2} \leq \frac{4}{3}$$

or

$$[(1-p_1)(1-p_2) + \frac{1}{3}p_1p_2](f(\{1\}) + f(\{2\}) - 1) \leq \frac{1}{3}[f(\{1\})p_1 + f(\{2\})p_2] \quad (2.45)$$

The left hand side of the inequality (2.45) thus simplifies to:

$$\begin{aligned} \left[(1-p_1)(1-p_2) + \frac{1}{3}p_1p_2 \right] (f(\{1\}) + f(\{2\}) - 1) &< \left[\frac{1}{4} + \frac{1}{3}p_1p_2 \right] (f(\{1\}) + f(\{2\}) - 1) \\ &< \frac{1}{3}(p_1 + p_2)(f(\{1\}) + f(\{2\}) - 1) \\ &= \frac{1}{3}[f(\{1\})p_1 + f(\{2\})p_2] \\ &\quad - \frac{1}{3}[p_2(1 - f(\{1\})) + p_1(1 - f(\{2\}))] \\ &< \frac{1}{3}[f(\{1\})p_1 + f(\{2\})p_2] \end{aligned}$$

where the first two inequalities are due to the fact that $f(\{1\}) + f(\{2\}) - 1 \geq 0$ along with $(1 - p_1)(1 - p_2) < \frac{1}{4}$ while the last inequality is due to $f(\{1\}) \leq 1, f(\{2\}) \leq 1$. Finally we recall from the result in Proposition 1 that with $n = 2$, the ratio of the Boole's union bound and the pairwise independence union bound (which is the correlation gap $\kappa_u(p_1, p_2)$ with $f(S) = \mathbb{1}_{S \neq \emptyset}$) attains the 4/3 bound when $p_1 = 1/2$ and $p_2 = 1/2$. The proof is thus completed. \square

2.5.1 Correlation gap with supermodular functions for $n = 2$

Proposition 4. *Given $n = 2$ random variables with univariate marginal probabilities p_1, p_2 , the correlation gap $\kappa_u(\mathbf{p})$ can be arbitrarily large for any nonnegative, nondecreasing, supermodular set function, $f(S)$.*

Proof. Consider a nonnegative, nondecreasing, supermodular set function defined on $S \subseteq \{1, 2\}$ as follows:

$$f(\emptyset) = f(\{1\}) = f(\{2\}) = 0, f(\{1, 2\}) = 1$$

We now consider a simple instance when the correlation gap $\kappa_u(\mathbf{p})$ is arbitrarily large. Suppose the two variables have negligible marginal probabilities, *i.e.*,

$$p_1 = \epsilon_1, p_2 = \epsilon_2, \text{ where } \epsilon_2 \rightarrow 0^+, \epsilon_2 \geq \epsilon_1$$

Then with extremal dependence, it is well known that the comonotonic distribution is

c_1	c_2	S	$\mathbb{P}(S)$
0	0	\emptyset	$1 - \epsilon_2$
0	1	$\{2\}$	$\epsilon_2 - \epsilon_1$
1	0	$\{1\}$	0
1	1	$\{1, 2\}$	ϵ_1

TABLE 2.7: Comonotonic distribution θ_c^* for $n=2$ variables

the extremal distribution for supermodular functions (Tchen, 1980). It is the straightforward to see that the correlation gap is unbounded in the limit as follows:

$$\begin{aligned} \lim_{\epsilon_2 \rightarrow 0} \kappa_u(\mathbf{p}) &= \lim_{\epsilon_2 \rightarrow 0} \sup_{\theta \in \Theta_u} \frac{\mathbb{E}_\theta[f(S)]}{\mathbb{E}_{\theta_{ind}}[f(S)]} \\ &= \lim_{\epsilon_2 \rightarrow 0} \frac{\sum_{S \subseteq [n]} f(S) \mathbb{P}_{\theta_c^*}(S)}{\sum_{S \subseteq [n]} f(S) \mathbb{P}_{\theta_{ind}}(S)} \\ &= \lim_{\epsilon_2 \rightarrow 0} \frac{\epsilon_1}{\epsilon_1 \epsilon_2} \\ &= \infty \end{aligned}$$

\square

2.6 Lower bounds

In this section, we first derive tight lower bounds on the probability of the union of pairwise independent random variables. Further, we derive the tight lower bound corresponding to Theorem 4 on the tail probability of sums of identical pairwise independent random variables for any $k \in [0, n]$. While the tightest upper union bound $\overline{P}(n, 1, \mathbf{p})$ was shown in Section 2.2 to reduce to the Hunter (1976)-Worsley (1982) bound for any given marginal vector $\mathbf{p} \in [0, 1]^n$, we prove in this section that the corresponding lower bound reduces to the Bonferroni (1936) bound, albeit for a restricted region of the probability space where the probabilities are small. In the remaining region, the optimal lower bound increases with increasing probabilities, assuming multiple forms, unlike the Hunter (1976)-Worsley (1982) upper bound in (2.12), which only has a non-trivial and trivial part. Thus, the tight lower bounds, unlike the upper bound, do not appear to be computable in polynomial time for all $\mathbf{p} \in [0, 1]^n$. Denote by $\underline{P}(n, k, \mathbf{p})$ the tightest lower bound on the probability that n pairwise independent random variables add up to at least an integer $k \in [n]$ for distributions

$$\underline{P}(n, k, \mathbf{p}) = \min_{\theta \in \theta_{pw}} \mathbb{P}_{\theta} \left(\sum_{i=1}^n \tilde{c}_i \geq k \right).$$

Theorem 6. *Sort the probabilities in increasing value as $0 \leq p_1 \leq p_2 \leq \dots \leq p_n \leq 1$. Then, the tight lower bound $\underline{P}(n, 1, \mathbf{p})$ reduces to the Bonferroni bound $S_1 - S_2$ if the sum of the largest $n - 1$ probabilities is at most one, i.e., $\sum_{i=2}^n p_i \leq 1$, where $S_1 = \sum_i p_i$ and $S_2 = \sum_{(i,j) \in K_n} p_i p_j$ are the first two binomial moments for the sum of the pairwise independent random variables.*

Proof. The dual of the minimization version of the large-sized linear program (2.5) for $k = 1$ and $p_{ij} = p_i p_j$ which computes the tightest lower union bound $\underline{P}(n, 1, \mathbf{p})$ can be written as:

$$\begin{aligned} \underline{P}(n, 1, \mathbf{p}) &= \max \sum_{(i,j) \in K_n} \lambda_{ij} p_i p_j + \sum_{i=1}^n \lambda_i p_i + \lambda_0 \\ \text{s.t.} \quad &\sum_{(i,j) \in K_n} \lambda_{ij} c_i c_j + \sum_{i=1}^n \lambda_i c_i + \lambda_0 \leq \mathbb{1}_{\sum_t c_t \geq k}, \quad \forall \mathbf{c} \in \mathcal{C} \end{aligned} \tag{2.46}$$

Observe that the following solution is dual feasible

$$\lambda_0 = 0, \quad \lambda_i = 1 \quad \forall i \in [n], \quad \lambda_{ij} = -1 \quad \forall (i, j) \in K_n$$

since the left hand side of the indicator constraint in (2.46) reduces to:

$$\begin{aligned}
\sum_{(i,j) \in K_n} \lambda_{ij} c_i c_j + \sum_{i=1}^n \lambda_i c_i + \lambda_0 &= \sum_{i=1}^n c_i - \sum_{(i,j) \in K_n} c_i c_j \\
&= \sum_{i=1}^n c_i - \binom{\sum_{t=1}^n c_t}{2} \\
&= \left(\sum_{i=1}^n c_i \right) \left(\frac{3 - \sum_{i=1}^n c_i}{2} \right) \\
&= \begin{cases} 0, & \sum_{i=1}^n c_i = 0 \\ 1, & \sum_{i=1}^n c_i = 1 \text{ or } 2 \\ \leq 0, & \sum_{i=1}^n c_i \geq 3 \end{cases}
\end{aligned}$$

which satisfies the indicator function value on the right hand side. Note that the dual objective value attains the Bonferroni (1936) bound $S_1 - S_2$. We also observe that the indicator constraint in (2.46) is tight $\forall \mathbf{c} \in \mathcal{C} : \sum_{i=1}^n c_i = 0, 1, 2$ while it is not tight when $\sum_{i=1}^n c_i \geq 3$. Thus from the complementary slackness of the latter condition, any optimal primal distribution $\{\mathbb{P}(\mathbf{c}); \mathbf{c} \in \mathcal{C}\}$ must satisfy:

$$\mathbb{P}(\mathbf{c}) = 0 \quad \forall \mathbf{c} \in \mathcal{C} : \sum_{t=1}^n c_t \geq 3$$

This forces the entire mass of probability to be concentrated in the first $\binom{n}{2} + n + 1$ scenarios with $\sum_{t=1}^n c_t \leq 2$ as follows:

Scenarios	c_1	c_2	...	c_i	...	c_{n-1}	c_n	Probability
1 scenario	0	0	...	0	...	0	0	$1 - S_1 + S_2$
n scenarios	1	0	...	0	...	0	0	$p_1 \left(1 - \sum_{j=1, j \neq 1}^n p_j \right)$
	\vdots	\vdots		\vdots		\vdots	\vdots	
	0	0	...	1	...	0	0	$p_i \left(1 - \sum_{j=1, j \neq i}^n p_j \right)$
	\vdots	\vdots		\vdots		\vdots	\vdots	
$\binom{n}{2}$ scenarios	0	0	...	0	...	0	1	$p_n \left(1 - \sum_{j=1, j \neq n}^n p_j \right)$
	1	1	...	0	...	0	0	$p_1 p_2$
	\vdots	\vdots		\vdots		\vdots	\vdots	
	1	0	...	1	...	0	0	$p_1 p_i$
	\vdots	\vdots		\vdots		\vdots	\vdots	
	0	0	...	0	...	1	1	$p_{n-1} p_n$

TABLE 2.8: Probabilities of scenarios with $\sum_{t=1}^{n-1} c_t \leq 2$

Note that this is a feasible distribution for the primal problem since

$$0 \leq p_i \left(1 - \sum_{j=1, j \neq i}^n p_j\right) \leq 1, \quad \forall i \in [n]$$

is satisfied due to the condition $\sum_{i=2}^n p_i \leq 1$ and it attains the Bonferroni (1936) bound. It remains to be shown that the optimal objective value $S_1 - S_2$ lies in $(0, 1)$. Define the *disaggregated* binomial moment $S_2^i = p_i \left(\sum_{j=1, j \neq i}^n p_j\right) \leq p_i$, $i \in [n]$, then

$$\begin{aligned} \sum_{i=1}^n S_2^i &\leq \sum_{i=1}^n p_i \\ 2S_2 &\leq S_1 \\ S_1 - S_2 &\geq S_2 \\ &> 0 \end{aligned}$$

Let $a = \sum_{i=2}^n p_i \leq 1$, then $S_1 = p_1 + a$, and $S_2 = p_1 a + b$ where $b > 0$.

$$\begin{aligned} S_1 - S_2 &= p_1 + a - p_1 a - b \\ &= 1 - (1 - p_1)(1 - a) - b \\ &< 1 \end{aligned}$$

We have thus proved that the Bonferroni (1936) bound of the second degree is a tight lower bound on the probability of the union of n pairwise independent events when the sum of the probabilities of the $n - 1$ most likely events is at most one. \square

We next derive the tight lower bound corresponding to Theorem 4 on the tail probability for identical pairwise independent random variables.

Corollary 1. Let $\underline{P}(n, k, p)$ represent the tightest lower bound on the sum of n identical pairwise independent Bernoulli random variables (with probability $p \in (0, 1)$) adding up to at least an integer $k \in [0, n]$. Then,

$$\underline{P}(n, k, p) = \begin{cases} 1, & k = 0, \quad \text{case (a)} \\ \frac{2np(i-1) + (k-1)(k-2i) - n(n-1)p^2}{(k-i)^2 - (k-i)}, & 1 \leq k \leq \eta, \quad \text{case (b)} \\ \frac{[(n-1)p - (k-2)]p}{n - (k-1)}, & k = \eta + 1, \quad \text{case (c)} \\ 0, & k \geq \eta + 2, \quad \text{case (d)} \end{cases}$$

where $\eta = \lceil (n-1)p \rceil$ and $i = \left\lceil \frac{np[(n-1)p - (k-2)]}{np - (k-1)} \right\rceil$.

Proof. The proof is similar to that of Theorem 4 and can be derived from the closed-form lower bound derived in Boros and Prékopa (1989). We omit it here for the sake of brevity. \square

2.7 Additional results with identical marginals

In Theorem 4 of Section 2.4.1, we proved that with identical marginals, the Boros and Prekopa bound in (2.7) provides the tightest bound on the probability of n pairwise independent variables adding up to at least k . In this section we first extend this result to more general t -wise independent variables and then show how pairwise independence is sufficient to achieve non-trivial bounds when k is very close to the mean.

2.7.1 Tight bounds with t -wise independence

Proposition 5. *Consider identical t -wise independent Bernoulli random variables with probabilities $p \in (0, 1)$ where $t \in [2, n]$. Then, the tightest upper bound on the probability of n such variables adding up to at least $k \in [n]$, denoted by $\bar{P}(n, k, p, t)$, can be computed as the optimal value of the aggregated linear program proposed in Prékopa (1990a):*

$$\begin{aligned} \bar{P}(n, k, p, t) = \max \quad & \sum_{\ell=k}^n v_\ell \\ \text{s.t.} \quad & \sum_{\ell=m}^n \binom{\ell}{m} v_\ell = \binom{n}{m} p^m, \quad \forall m \in \{0, 1, \dots, t\} \\ & v_\ell \geq 0, \quad \forall \ell \in [0, n] \end{aligned} \quad (2.47)$$

where the decision variables are the probabilities $v_\ell = \mathbb{P}(\sum_{i=1}^n \tilde{c}_i = \ell)$ for $\ell \in [0, n]$.

Proof. The proof is straightforward from the proof of Theorem 4 which implies the equivalence of (2.47) with the large-sized linear program:

$$\begin{aligned} \bar{P}(n, k, p, t) = \max \quad & \sum_{\mathbf{c} \in \mathcal{C}: \sum_i c_i \geq k} \mathbb{P}(\mathbf{c}) \\ \text{s.t.} \quad & \sum_{\mathbf{c} \in \mathcal{C}} \mathbb{P}(\mathbf{c}) = 1 \\ & \sum_{\mathbf{c} \in \mathcal{C}: c_i=1, \forall i \in J} \mathbb{P}(\mathbf{c}) = p^m, \quad \forall J \in I_m, m \in [t] \\ & \mathbb{P}(\mathbf{c}) \geq 0, \quad \forall \mathbf{c} \in \mathcal{C}, \end{aligned} \quad (2.48)$$

where $I_m = \{I \subseteq [n] : |I| = m\}$. In particular for any given feasible solution of (2.47), we can distribute the probability mass v_ℓ evenly across the $\binom{n}{\ell}$ scenarios for every $\ell \in [0, n]$ and satisfy all the constraints in (2.48) while for any given feasible solution of (2.48), we can aggregate the probabilities $\mathbb{P}(\mathbf{c})$ as

$$v_\ell = \sum_{\mathbf{c} \in \mathcal{C}: \sum_i c_i = \ell} \mathbb{P}(\mathbf{c}), \quad \forall \ell \in [0, n].$$

and satisfy all constraints in (2.47). Lastly, we note that for 3-wise independent variables, a closed-form expression for the optimal objective in (2.47) using the first three binomial moments has been provided in Boros and Prékopa (1989). \square

The corresponding tight lower bound $\underline{P}(n, k, p, t)$ can be computed as the optimal value of the minimization version of the aggregated linear program (2.47).

2.7.2 Small deviation bounds

Small deviation bounds of the type $\mathbb{P}(\sum_{i=1}^n \tilde{x}_i \geq \mathbb{E}(\sum_{i=1}^n \tilde{x}_i) + \delta)$ for a small constant δ have been extensively studied in the literature. Classical tail bounds such as the Markov and Chebyshev inequalities provide small deviation bounds with extremal dependence and pairwise independence assumptions respectively while the Chernoff-Hoeffding bound (Chernoff, 1952; Hoeffding, 1963) assumes independence among the variables. With Bernoulli random variables, Schmidt, Siegel, and Srinivasan (1995) improved the Chernoff-Hoeffding bounds with the additional advantage of requiring only *limited independence* among the variables. In this section we look at small deviation bounds for sums of pairwise independent identical random variables. We next show the value of the Boros and Prekopa bound in (2.27) over the Chebyshev and Schmidt, Siegel, Srinivasan bounds in (2.33) and (2.34) respectively, in computing small deviation bounds for identical pairwise independent variables.

Proposition 6. *Consider n pairwise independent Bernoulli random variables with identical probabilities $p \in (0, 1)$. Then the Boros and Prekopa tight bound $\bar{P}(n, k, p)$ is strictly less than one while the Schmidt, Siegel, Srinivasan and Chebyshev bounds are trivially one in the following two cases:*

- (a) For $p = k/n$ and any integer $k \in [n - 1]$
- (b) For $k/n < p < k/(n - 1)$ and any integer $k \in [n - 2]$

Proof.

- (a) We note that in this case $k = np$ and hence computing $\bar{P}(n, k, p)$ is equivalent to computing tight small deviation bounds with $\delta = 0$. This corresponds to case (b) of the Boros and Prekopa bound in (2.27) which reduces to:

$$\begin{aligned} \bar{P}(n, k, p) &= \frac{[(n-1)(1-p) + k]p}{k} \\ &= \frac{[(n-1)(1-p) + np]p}{np} \\ &= 1 - \frac{(1-p)}{n} \\ &< 1 \end{aligned}$$

where the inequality is due to $p < 1$. When $k = np$, the Chebyshev bound in (2.33) reduces to one while the Schmidt, Siegel and Srinivasan bounds in (2.34) reduce to

$$\begin{aligned} \bar{P}(n, k, p) &\leq \min\left(1, \frac{np}{k}, \frac{n(n-1)p^2}{np(np-1)}\right) \\ &= \min\left(1, 1, \frac{np-p}{np-1}\right) \\ &= 1 \end{aligned}$$

- (b) We note that in this case

$$(n-1)p < k = \lfloor np \rfloor < np,$$

and hence computing $\bar{P}(n, k, p)$ is equivalent to computing tight small deviation bounds with $\delta = -\{np\}$ where $\{np\}$ is the fractional part of the mean. This again

corresponds to case (b) of Boros and Prekopa bound in (2.27) which reduces to:

$$\begin{aligned}\bar{P}(n, k, p) &= \left(\frac{(n-1)p}{\lfloor np \rfloor} \right) (1-p) + p \\ &< (1-p) + p \\ &= 1\end{aligned}\tag{2.49}$$

while the inequality is due to $\lfloor np \rfloor > (n-1)p$. The Chebyshev bound is trivially one when $k < np$ and the Schmidt, Siegel, Srinivasan bound reduces to:

$$\begin{aligned}\bar{P}(n, k, p) &\leq \min \left(1, \frac{np}{\lfloor np \rfloor}, \frac{np}{\lfloor np \rfloor} \frac{np-p}{(\lfloor np \rfloor - 1)} \right) \\ &= 1\end{aligned}$$

Hence in conclusion the Boros and Prekopa bound in (2.27) provides non-trivial small deviation bounds when $k = np$ or $k = \lfloor np \rfloor$ while the Chebyshev and Schmidt, Siegel, Srinivasan bounds are trivially one. \square

Corollary 2. Consider n identical pairwise independent Bernoulli random variables with symmetric probabilities $p = 1/2$ where n is even. Then the maximal probability that at least half the variables are one equals $\bar{P}(n, n/2, p) = 1 - (1/(2n))$ which is attained by the Boros and Prekopa bound while the Schmidt, Siegel, Srinivasan and Chebyshev bounds are trivially one.

Proof. The proof follows from case (a) of Proposition 6 with $k = n/2$. \square

Connection to earlier work: The result in Proposition 6 is interesting not only because of the non-triviality of the Boros and Prekopa bound when the other bounds are trivial, but also because this feature of Bernoulli random variables manifests from pairwise independence onwards. For more general random variables, Garnett (2020) proves that non-triviality of small deviation bounds shows up only with 4-wise independence and beyond. The fact that pairwise independence is sufficient for computing the best non-trivial small deviation bounds with identical Bernoulli random variables could be exploited in various applications using small deviation bounds in graph theory (Feige, 2006), inventory management (Wang and Zhang, 2015) and allied areas.

2.7.3 Bounds on expected stop-loss functions

In this section, we consider bounds on the expected value of a function of the Bernoulli random vector \tilde{c} and k instead of the tail probability function considered in the preceding sections of this chapter. In particular, we consider functions of the form:

$$\mathbb{E}_\theta \left[\left(\sum_{j=1}^n \tilde{c}_j - k \right)^+ \right] = \mathbb{E}_\theta \left[\max \left(\sum_{j=1}^n \tilde{c}_j, k \right) - k \right] = \mathbb{E}_\theta \left[\sum_{j=1}^n \tilde{c}_j - \min \left(\sum_{j=1}^n \tilde{c}_j, k \right) \right]$$

for some joint distribution θ of \tilde{c} , $k \in [n]$ and where $x^+ = \max(x, 0)$ is the positive part of a real number. These functions are commonly referred to as “stop-loss premiums” in the actuarial literature to denote the loss ceded by an insurer to the reinsurer beyond a retention point. If \tilde{c} represents the random claims from an insurance portfolio (where $c_i = 1$ if corresponding claim is made and 0 otherwise) and k denotes

the retention value, the insurer bears up to k claims, but transfers any excess claims $(\sum_{j=1}^n c_j - k)^+$ to the reinsurer. Hence, the expected value of this excess number denotes the average number of claims transferred to the reinsurer under given correlation assumptions. Alternatively, continuous random variables can be used to denote insurance claim amounts (instead of whether a claim was made) and in this case the expected value represents the average stop-loss premium paid by the insurer to the reinsurer in exchange for the risk undertaken.

More specifically, in our context, $\tilde{\xi} = \sum_{i=1}^n \tilde{c}_i$ is a discrete random variable which takes integer values in $[0, n]$. Problems involving $\tilde{\xi}$, popularly known as discrete moment problems (DMP), were introduced and extensively studied in the context of probability functions under assumptions of limited moment information by Prékopa (1988) and Prékopa (1990a). Prékopa (1990b) generalized the objective considered to linear functionals of the probabilities $\mathbb{P}(\tilde{\xi} = i)$, $i \in [0, n]$. As a special case, for expected stop-loss functions, useful applications were demonstrated in applied probability (Courtois and Denuit, 2009) and inventory control models (Ninh, Hu, and Allen, 2019).

In this section we focus on deriving the tight upper bound on such expected stop-loss functions for identical pairwise independent random variables (with probability of occurrence $p \in (0, 1)$), while in Section 3.4, we derive similar bounds for extremally dependent variables. Denote the tight upper bound on the expected stop-loss function computed over the set of distributions in the pairwise independent ambiguity set Θ_{pw} as:

$$\bar{E}(n, k, p) = \max_{\theta \in \Theta_{pw}} \mathbb{E}_{\theta} \left[\left(\sum_{j=1}^n \tilde{c}_j - k \right)^+ \right], \quad \forall k \in [0, n]$$

which can be computed as the optimal value of the following exponential-sized linear program:

$$\begin{aligned} \bar{E}(n, k, p) = \max \quad & \mathbb{E} \left[\left(\sum_{j=1}^n \tilde{c}_j - k \right)^+ \right] \\ \text{s.t.} \quad & \sum_{\mathbf{c} \in \mathcal{C}: c_i=1} \mathbb{P}(\mathbf{c}) = p, \quad \forall i \in [n], \\ & \sum_{\mathbf{c} \in \mathcal{C}: c_i=1, c_j=1} \mathbb{P}(\mathbf{c}) = p^2, \quad \forall i, j \in K_n, \\ & \sum_{\mathbf{c} \in \mathcal{C}} \mathbb{P}(\mathbf{c}) = 1, \\ & \mathbb{P}(\mathbf{c}) \geq 0 \quad \forall \mathbf{c} \in \mathcal{C} \end{aligned} \quad (2.50)$$

The next theorem provides the tight upper bound $\bar{E}(n, k, p)$ in closed-form.

Theorem 7. *Consider n pairwise independent Bernoulli random variables with identical probabilities $p \in (0, 1)$. Then, the tight upper bound $\bar{E}(n, k, p)$ admits the following closed-form expression:*

$$\bar{E}(n, k, p) = \begin{cases} np \left[1 - k \left(\frac{2j - (n-1)p}{j(j+1)} \right) \right], & k < \frac{1 + (n-1)p}{2}, j = \lceil (n-1)p \rceil, & \text{case (a)} \\ \frac{n(n-1)p^2 + (j-1)(j-2np)}{2(2(k-j) + 1)}, & \begin{cases} \frac{1 + (n-1)p}{2} \leq k \leq \frac{n + (n-1)p}{2}, \\ j = k - \lfloor \sqrt{(k-np)^2 + np(1-p)} \rfloor, \end{cases} & \text{case (b)} \\ \frac{(n-k)[n(n-1)p^2 + (j-1)(j-2np)]}{((n-j)^2 + (n-j))}, & k > \frac{n + (n-1)p}{2}, j = \lceil (n-1)p \rceil & \text{case (c)} \end{cases}$$

Proof. The proof of tightness along with the extremal distribution that attains this bound for any given (n, k, p) triplet is relegated to Appendix A. \square

Corollary 3. *The tight lower bound corresponding to the upper bound in Theorem 7 is given by:*

$$\underline{E}(n, k, p) = \begin{cases} np - k, & k < \eta, \text{ case (a)} \\ p[(n-1)p - (k-1)], & k = \eta, \text{ case (b)} \\ 0, & k > \eta, \text{ case (c)}. \end{cases} \quad (2.51)$$

where $\eta = \lceil (n-1)p \rceil$ and

$$\underline{E}(n, k, p) = \min_{\theta \in \Theta_{pw}} \mathbb{E}_{\theta} \left[\left(\sum_{j=1}^n \tilde{c}_j - k \right)^+ \right], \quad \forall k \in [0, n]$$

with n pairwise independent Bernoulli random variables having identical probabilities $p \in (0, 1)$.

Proof. The proof idea is similar to that of the upper bound in Theorem 7 and involves using the aggregated linear program formulation proposed by Boros and Prékopa (1989) and Prékopa (1990a) to identify primal and dual feasible bases consistent with the given assumptions and which attain the given bound. Although the proof is much simpler than that of the upper bound, we omit it here for the sake of brevity. \square

Note that the tight bound in (2.51) reduces to the Jensen (1906) bound $\max(S_1 - k, 0)$ (where $S_1 = np$) in cases (a) and (c) while providing better bounds close to the mean np in case (b). Recall that with univariate marginal information alone, we proved in Section 3.4.2 that the Jensen (1906) bound is the tightest lower bound for the expected stop-loss function. In other words, with identical marginals, while pairwise independence does not improve the univariate lower bounds in general, it adds value by tightening the bounds around the mean which could be of independent interest in itself.

Connection to earlier work: Expected stop-loss functions like that in (2.50) involving random variables with given univariate and bivariate probability information have been studied in the context of several applications in the literature. For example, such bounds can be used to compute the maximum expected mean absolute deviation of a symmetric random walk over n pairwise independent steps (Narayanan, 2019). Under

assumptions of limited moment information, Courtois and Denuit (2009) provide the best upper and lower bounds on expected stop-loss functions where the first and second moments $\mu_1 = S_1$, $\mu_2 = 2S_2 + S_1$ are known, with applications in ruin probability and stochastic modeling for dynamic mortality. More recently, Ninh, Hu, and Allen (2019) investigated discrete demand newsvendor problems under the same assumptions, where the minimum expected profit is related to maximizing an expected stop-loss function. While the proof of Courtois and Denuit (2009) uses algebraic techniques involving existence of quadratic polynomials, Ninh, Hu, and Allen (2019) first identify the optimal basis structure of the aggregated linear program in Boros and Prékopa (1989) for the stop-loss objective function and subsequently use quadratic polynomials to derive closed-form expressions (in terms of μ_1, μ_2) that exactly reduce to the bounds in Theorem 7 and Corollary 3 under assumption of identical pairwise independent variables. However, although the best upper and lower bounds under the given assumptions of univariate and bivariate aggregated information have been derived in these papers, their connection to pairwise independence and preservation of tightness with identical pairwise independent variables has not been established to the best of our knowledge. Our contribution also lies in providing extremal distributions that attain the bound for any input instance, *i.e.*, our proof of Theorem 7 identifies the exact conditions on n, k, p under which a particular basis becomes optimal.

Extension to t -wise independence: It is straightforward to extend Proposition 5 to expected stop-loss functions $\mathbb{E}\left[\left(\sum_{j=1}^n \tilde{c}_j - k\right)^+\right]$, and thus the tight upper and lower bounds are computable as the optimal value of the aggregated linear program (2.47) with the expected stop-loss objective function instead of the tail probability.

Chapter 3

Bounds with Extremal Dependence

In this chapter, we consider computation of bounds on the tail probability and expectation of sums of Bernoulli random variables under assumptions of extremal dependence among the variables. The only information known is the univariate marginal probabilities of each variable. The bounds are “extremal” since they are valid across all joint distributions with the given marginals. Compact linear programs are formulated to compute these bounds, the optimal solution to which, can be captured in a closed-form expression in some cases. While some of these results are previously established in the literature, we provide alternative proofs harnessing tools from linear programming and extend the results to variants of standard problems with useful applications. The results from the Bernoulli case are extended to random variables with discrete support where useful upper bounds on the tail probability are derived.

3.1 Tail probability bounds on sums of Bernoulli random variables

Sums of random variables have been interesting objects of study in probability and applied fields such as quantitative risk measurement in finance and insurance. A relevant problem is to determine tight bounds for the tail distribution function of sums of random variables and more specifically for sums of Bernoulli random variables given their marginal probabilities. For example, an insurer is interested to obtain tight bounds for the probability that the number of claims incurred is at least k out of n . In finance and risk management, a portfolio manager would be interested to compute the tail risk of the joint portfolio of a random risk vector given their marginal distribution functions (see Rüschendorf, Ludger, 2013; Wang, Peng, and Yang, 2013, and references therein). More recently Blanchet et al. (2021) provide bounds on quantiles of an aggregate risk with given marginal distributions but unspecified correlation structure which are directly related to the tail probability bounds. In the context of network reliability, it is of interest to compute the probability that at least k out of n components are functioning in a system (see Zemel, 1982). In inventory management applications, decision makers would like to hedge against extremal scenarios by computing the probability that at least k out of n outlets of a company experience stock-outs. Another interesting application is in hypothesis testing (Rüger, 1978; Rüger, 1981; Morgenstern, 1980). Given n tests, with level of significance α_i , $i \in [n]$, computing the level of significance of the combined test that at least k out of n tests are rejected, can be of practical value. The underlying random variables in all of the above and several other applications can naturally be represented as sums of Bernoulli random variables. Additionally, as we will see in Table 3.1, the tractability of bounds involving Bernoulli random variables makes them interesting objects of study. In this section we are interested in computing tail

probability bounds on sums of extremally dependent Bernoulli random variables, *i.e.*, with no specified correlation between the variables.

Preliminaries:

Throughout this chapter, $[n]$ denotes the set of indices $\{1, 2, \dots, n\}$ for $n \geq 2$ and $[i, j] = \{i, i+1, \dots, j-1, j\}$ for given integers $i < j$. Let \tilde{c} be an n dimensional multivariate Bernoulli random variable with a fixed univariate marginal vector \mathbf{p} where $\mathbb{P}(\tilde{c}_i = 1) = p_i$, $\forall i \in [n]$. Denote by $\mathcal{C} = \{0, 1\}^n$, the set of realizations of \tilde{c} , by $\Theta(\{0, 1\}^n)$, the set of all probability distributions supported on \mathcal{C} and by Θ_u the ambiguity set of joint distributions supported on \mathcal{C} while consistent with the given univariate information as defined in (2.1.1).

We denote the tight upper bound on the probability that at least k out of n Bernoulli events occur by:

$$\bar{P}_u(n, k, \mathbf{p}) = \max_{\theta \in \Theta_u} \mathbb{P}_\theta\left(\sum_{i=1}^n \tilde{c}_i \geq k\right), \quad \forall k \in [n]$$

Note that $\bar{P}_u(n, k, \mathbf{p})$ can be computed as the optimal value of the following exponential-sized linear program first proposed by Hailperin (1965b):

$$\begin{aligned} \bar{P}_u(n, k, \mathbf{p}) = \max \quad & \sum_{\mathbf{c} \in \mathcal{C}: \sum_{i=1}^n c_i \geq k} \mathbb{P}(\mathbf{c}) \\ \text{s.t.} \quad & \sum_{\mathbf{c} \in \mathcal{C}: c_i=1} \mathbb{P}(\mathbf{c}) = p_i, \quad \forall i \in [n], \\ & \sum_{\mathbf{c} \in \mathcal{C}} \mathbb{P}(\mathbf{c}) = 1, \\ & \mathbb{P}(\mathbf{c}) \geq 0 \quad \forall \mathbf{c} \in \mathcal{C} \end{aligned} \quad (3.1)$$

We next summarize some known hardness results for computing tail probabilities on sums of variables with arbitrary support, which shows that the Bernoulli nature of variables plays a significant role in efficiently computing tail probability bounds such as $\bar{P}_u(n, k, \mathbf{p})$.

Computational complexity: Table 3.1 displays the known complexity results of computing tail probability bounds on sums of random variables, for variables with different types of support and dependency conditions. When the variables c_i , $i \in [n]$ assume arbitrary support, it is known that computing the tail probability (with mutual independence) and tight bounds (with extremal dependence) are #P-hard (Kleinberg, Rabani, and Tardos, 2000) and NP-hard (Kleinberg, Rabani, and Tardos, 2000) respectively. In fact, even when each random variable c_i , $i \in [n]$ is restricted to assume just two possible values 0 and a_i , where a_i is rational, computing the tail probability and extremal tail bounds is #P-hard and NP-hard respectively (see Theorem 1.1.1 and 2.6.1 in Nataraian, 2021). However, when the variables are Bernoulli with fixed marginal probabilities, the independent tail probability (attained by the Poisson binomial distribution) is computable in polynomial time using dynamic programming recursion while the tightest bound with extremal dependence is efficiently computable in a closed-form (Rüger, 1978; Morgenstern, 1980) or by providing a polynomial time algorithm as in Zemel (1982).

Computational complexity	Independence (tail probability)	Dependence (extremal bounds)
Arbitrary Support	#P-hard (Kleinberg, Rabani, and Tardos, 2000)	NP-Hard (Kreinovich and Ferson, 2006)
Binary Support with $\mathbf{p} \in [0, 1]^n$	Easy Poisson Binomial (n, \mathbf{p})	Polynomial time solvable (Rüger, 1978; Morgenstern, 1980; Zemel, 1982)

TABLE 3.1: Computational complexity of computing tail probability bounds on sums of random variables

More general objective functions: It is interesting to note that for more involved objective functions, such as tail probability functions of linear combinations of extremally dependent Bernoulli random variables, tight bounds can be computed in polynomial time under special circumstances. More generally, tight upper bounds of the form

$$\max_{\theta \in \Theta_u} \mathbb{P}_\theta(Z(\tilde{\mathbf{c}}) \geq k), \quad \forall k \in [n]$$

where

$$\begin{aligned} Z(\tilde{\mathbf{c}}) = \max \quad & \tilde{\mathbf{c}}' \mathbf{x} \\ \text{s.t.} \quad & \mathbf{x} \in \mathcal{X} \subseteq \{0, 1\}^n, \end{aligned} \quad (3.2)$$

is the optimal value of a combinatorial optimization problem (that is assumed to be efficiently computable), have been considered in Padmanabhan et al., 2021. These bounds have been shown to be weakly NP-hard to compute by providing a pseudopolynomial time algorithm for compact 0/1 V-polytopes, *i.e.*, when the extreme points of the convex hull of the set \mathcal{X} are explicitly given as a set of finite points. Note that by setting $\mathcal{X} = \{\mathbf{1}_n\}$, where $\mathbf{1}_n$ is the vector of all ones, we retrieve the special case of sums of random variables. While these results hold for discrete random variables beyond Bernoulli variables, it is important to note that they cannot be generalized to arbitrary V-polytopes, since even with $x_i \in \{0, a_i\}$, $a_i \in \mathbb{Q}$, $\forall i \in [n]$ (where \mathbb{Q} is the set of rationals) and a Bernoulli random vector \mathbf{c} , $c_i x_i$ would be a two-point random variable with support $\{0, a_i\}$ and the earlier mentioned NP-hardness results of Kreinovich and Ferson, 2006 would apply. For pairwise independent Bernoulli random variables and compact 0/1 V-polytopes, to the best of our knowledge, it is not clear if these bounds are efficiently computable.

In this section, we first derive a compact linear program in Theorem 8, which efficiently computes the tightest bound $\bar{P}_u(n, k, \mathbf{p})$ and subsequently provide an alternate proof of the closed-form solution provided in Rüger (1978) using this compact linear program. Further, we extend our results to random variables with discrete support in Section 3.2 and weighted tail probability functions in Section 3.3.

Note that an optimal solution to the linear program (3.1) must exist since it cannot be unbounded (the objective is a tail probability function) and its feasible region is non-empty. It is evident that there are exponential number of decision variables ($\mathbb{P}(\mathbf{c})$, $\mathbf{c} \in \mathcal{C}$) in (3.1) and thus the linear program quickly becomes computationally intractable with

increase in number of random variables n . Ruger (1978) proves the equivalence of (3.1) to a smaller linear program maximizing $\mathbb{P}(\sum_{i=1}^n \tilde{c}_i = k)$ instead of $\mathbb{P}(\sum_{i=1}^n \tilde{c}_i \geq k)$ and relaxing the equality of univariate probabilities to upper bounds on the univariate probabilities, *i.e.*,

$$\mathbb{P}(\tilde{c}_i = 1) \leq p_i, \quad \forall i \in [n].$$

This reduced and relaxed linear formulation still has $\binom{n}{k}$ decision variables which could potentially be huge when k is close to $n/2$. The following theorem however, shows the equivalence of (3.1) to a much simpler compact linear program with $\mathcal{O}(n)$ variables and constraints, which can thus efficiently compute $\bar{P}_u(n, k, \mathbf{p})$.

3.1.1 Compact linear program and primal proof of correctness

Theorem 8. *The exponential size linear program in (3.1) is equivalent to the following compact linear program:*

$$\begin{aligned} \bar{P}_u(n, k, \mathbf{p}) = \max \quad & y_0 \\ \text{s.t.} \quad & 0 \leq y_0 - y_i \leq 1 - p_i, \quad \forall i \in [n], \\ & 0 \leq y_i \leq p_i, \quad \forall i \in [n], \\ & \sum_{i=1}^n y_i \geq ky_0 \end{aligned} \quad (3.3)$$

Proof. Consider the dual of the exponential-sized linear program (3.1)

$$\begin{aligned} \min \quad & \sum_{i=1}^n \lambda_i p_i + \lambda_0 \\ \text{s.t.} \quad & \sum_{i=1}^n \lambda_i c_i + \lambda_0 \geq \mathbb{1}_{\sum_{i=1}^n c_i \geq k}, \quad \forall \mathbf{c} \in \mathcal{C}, \\ & \lambda_i, \text{ free} \quad \forall i \in [n], \\ & \lambda_0 \text{ free} \end{aligned} \quad (3.4)$$

where $\mathbb{1}$ is the indicator function. The dual (3.4) has 2^n constraints, which can be split into two parts as follows:

$$\sum_{i=1}^n \lambda_i c_i + \lambda_0 \geq 0 \quad \forall \mathbf{c} \in \mathcal{C} \quad (3.5a)$$

$$\sum_{i=1}^n \lambda_i c_i + \lambda_0 \geq 1 \quad \forall \mathbf{c} \in \mathcal{C} : \sum_{i=1}^n c_i \geq k \quad (3.5b)$$

We now show how both the above constraint sets can be replaced by equivalent polynomial-sized constraint sets by converting them into optimization problems with $\{c_i, i \in [n]\}$ as decision variables for fixed $\{\lambda_0, \lambda_i, i \in [n]\}$.

The first constraint set (3.5a) can be written as:

$$\begin{aligned} & \lambda_0 + \underbrace{\left\{ \min \sum_{i=1}^n \lambda_i c_i : \mathbf{c} \in \mathcal{C} \right\}}_{Sep_1(\boldsymbol{\lambda})} \geq 0 \\ \equiv & \lambda_0 + \left\{ \min \sum_{i=1}^n \lambda_i c_i : 0 \leq c_i \leq 1, \forall i \in [n] \right\} \geq 0 \end{aligned} \quad (3.6)$$

where the equivalence follows from the fact that the linear program relaxation admits integer extreme points due to the totally unimodular structure of the constraint set.

The second constraint set (3.5b) can be similarly transformed as:

$$\begin{aligned} & \lambda_0 + \underbrace{\left\{ \min \sum_{i=1}^n \lambda_i c_i : \sum_{i=1}^n c_i \geq k, \mathbf{c} \in \mathcal{C} \right\}}_{Sep_2(\boldsymbol{\lambda})} \geq 0 \\ \equiv & \lambda_0 + \left\{ \min \sum_{i=1}^n \lambda_i c_i : \sum_{i=1}^n c_i \geq k, 0 \leq c_i \leq 1, \forall i \in [n] \right\} \geq 0 \end{aligned} \quad (3.7)$$

where the equivalence persists due to the totally unimodular structure of the constraint set. The two separation problems indicated by $Sep_1(\boldsymbol{\lambda})$, $Sep_2(\boldsymbol{\lambda})$ in (3.6) and (3.7) are thus transformed into efficiently solvable linear programs with integer polytopes. As a consequence of the equivalence of separation and optimization (Grötschel, Lovász, and Schrijver, 2012), the original large-sized dual problem (3.4) is also efficiently solvable. We now proceed to derive the precise compact linear programming formulation that is equivalent to the original large-sized primal problem (3.1).

Dualizing (3.6) gives us

$$\lambda_0 + \left\{ \max \sum_{i=1}^n w_i : w_i \leq 0, w_i \leq \lambda_i, \forall i \in [n] \right\} \geq 0 \quad (3.8)$$

Since we only need a single instance $\{w_i, i \in [n]\}$ to satisfy (3.8) by which (3.6) is automatically satisfied due to weak duality, we can replace the constraint set (3.5a) by:

$$\left\{ \lambda_0 + \sum_{i=1}^n w_i \geq 0, w_i \leq \lambda_i, w_i \leq 0, \forall i \in [n] \right\} \quad (3.9)$$

Dualizing (3.7) in a similar manner leads to

$$\lambda_0 + \left\{ \max kv_0 + \sum_{i=1}^n v_i : v_0 + v_i \leq \lambda_i, v_i \leq 0, v_0 \geq 0, \forall i \in [n] \right\} \geq 1 \quad (3.10)$$

and the constraint set (3.5b) can be replaced by

$$\left\{ \lambda_0 + kv_0 + \sum_{i=1}^n v_i - 1 \geq 0, v_0 + v_i \leq \lambda_i, v_i \leq 0, v_0 \geq 0, \forall i \in [n] \right\} \quad (3.11)$$

Replacing both constraint sets (3.5a) and (3.5b) by (3.9) and (3.11) respectively, the transformed polynomial-sized version of the dual (3.4) is:

$$\begin{aligned}
\min \quad & \sum_{i=1}^n \lambda_i p_i + \lambda_0 \\
\text{s.t.} \quad & \lambda_0 - \sum_{i=1}^n w_i \geq 0, \\
& \lambda_0 + kv_0 - \sum_{i=1}^n v_i - 1 \geq 0, \\
& \lambda_i + w_i \geq 0, \quad \forall i \in [n], \\
& \lambda_i + v_i - v_0 \geq 0, \quad \forall i \in [n], \\
& w_i \geq 0, \quad \forall i \in [n], \\
& v_i \geq 0, \quad \forall i \in [n], \\
& v_0 \geq 0
\end{aligned} \tag{3.12}$$

This transformed dual has $\mathcal{O}(n)$ constraints as opposed to $\mathcal{O}(2^n)$ constraints in the original dual. Finally, we dualize (3.12) to get a polynomial size primal equivalent of (3.1) as follows:

$$\begin{aligned}
\max \quad & y_0 \\
\text{s.t.} \quad & x_0 + y_0 = 1, \\
& x_i + y_i = p_i, \quad \forall i \in [n], \\
& x_0 - x_i \geq 0, \quad \forall i \in [n], \\
& y_0 - y_i \geq 0, \quad \forall i \in [n], \\
& \sum_{i=1}^n y_i \geq ky_0 \\
& x_i \geq 0, \quad \forall i \in [n], \\
& y_i \geq 0, \quad \forall i \in [n], \\
& x_0 \geq 0, \\
& y_0 \geq 0
\end{aligned} \tag{3.13}$$

where $x_i, y_i, i \in [n]$ are the primal variables corresponding to the constraint sets in (3.12), while x_0, y_0 are the primal variables corresponding to the first and second single constraints. It can be observed that by eliminating x_0, x_i , (3.13) can be reduced to the compact linear program (3.3) which has only $\mathcal{O}(n)$ decision variables and $\mathcal{O}(n)$ constraints and the result is proved. \square

Figure 3.1 summarizes the primal-dual transformations used in our proof. As noted earlier, an optimal solution to (3.1) must exist and thus by strong duality (3.4) also has an optimal solution. The duals (3.4) and (3.12) are equivalent since we have transformed the former into the latter by finding an equivalent facet defining constraint set of polynomial size without modifying the feasible region. Further, (3.12) and (3.3) have optimal solutions by strong duality and lastly the large-sized primal (3.3) and the compact primal (3.1) are equivalent and share the same optimal solution by dint of the previous steps.

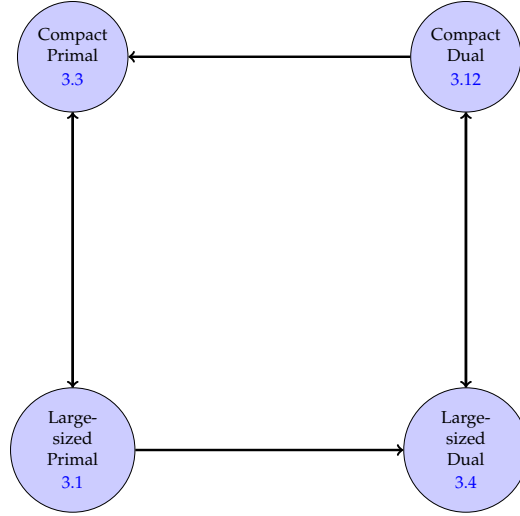


FIGURE 3.1: Equivalence of the large-sized and compact linear programs

Connection to earlier work: We note that other compact linear programming formulations to compute tail probability bounds on sums of Bernoulli random variables considered in this section have been proposed in the literature. These formulations are designed for *partially aggregated* information assumptions where the first m *partial* binomial moments of the form $S_m^j = \mathbb{E} \left[\tilde{c}_j \left(\sum_{\{i_1, i_2, \dots, i_{m-1}\} \in [n] \setminus j} \tilde{c}_{i_1} \tilde{c}_{i_2} \dots \tilde{c}_{i_{m-1}} \right) \right]$ ($\forall j \in [n]$, $m \leq n$) are assumed to be known. For example, Qiu, Ahmed, and Dey (2016) extend the work of Prékopa and Gao (2005) to compute $\max \mathbb{P}(\sum_{i=1}^n \tilde{c}_i \geq k)$ for any $k \in [n]$, assuming knowledge of first m *partial* binomial moments S_m^j by constructing a compact linear programming formulation. In parallel work, Yang, Alajaji, and Takahara (2016) provide the exact same compact formulation as Qiu, Ahmed, and Dey (2016) but only for $k = 1$ (union bound). Even though designed for *partially aggregated* probability information, both these formulations can be shown to achieve the tight bound $\bar{P}_u(n, k, \mathbf{p})$ for $m = 1$, when the first-order *partial* binomial moments S_1^j equal the univariate probabilities p_j ($\forall j \in [n]$). However, these formulations even though polynomial-sized, use $\mathcal{O}(n^2)$ variables and constraints as opposed to $\mathcal{O}(n)$ variables and constraints in our compact linear program (3.3). Thus, our compact formulation scales more efficiently with the number of variables n unlike other known compact formulations.

Primal proof of correctness

We next provide a direct proof of equivalence of the primal formulations in Figure 3.1, *i.e.*, the large-sized linear program (3.1) and the compact linear program (3.3) without going through the dual formulations and also interpret the decision variables of the compact primal formulation in terms of the probabilities from a feasible joint distribution of the large-sized primal formulation.

Proposition 7. *The large-sized primal linear program (3.1) is equivalent to the compact primal linear program (3.3), where for any extremal distribution $\theta^* \in \Theta_u$ of the large-sized linear program and any $k \in [n]$, the corresponding optimal solution (y_0, y_1, \dots, y_n) of the compact*

linear program satisfies

$$\begin{aligned} y_0 &= \mathbb{P}_{\theta^*} (\sum_{t=1}^n \tilde{c}_t \geq k) \\ y_i &= \mathbb{P}_{\theta^*} (\sum_{t=1}^n \tilde{c}_t \geq k, \tilde{c}_i = 1), \quad \forall i \in [n] \end{aligned} \quad (3.14)$$

Proof. Denote the optimal value of the compact linear program in (3.3) by $\bar{P}_u^c(n, k, \mathbf{p})$.

Step (1): $\bar{P}(n, k, \mathbf{p}) \leq \bar{P}_u^c(n, k, \mathbf{p})$ Given a feasible solution $\mathbb{P}_\theta(\mathbf{c})$, $\forall \mathbf{c} \in \mathcal{C}$ of the large-sized primal linear program (3.1) for some distribution $\theta \in \Theta_u$, construct a feasible solution of the compact linear program (3.3) by aggregating the probabilities as follows:

$$y_0 = \sum_{\mathbf{c} \in \mathcal{C}: \sum_{t=1}^n c_t \geq k} \mathbb{P}_\theta(\mathbf{c}), \quad y_i = \sum_{\mathbf{c} \in \mathcal{C}: \sum_{t=1}^n c_t \geq k, c_i=1} \mathbb{P}_\theta(\mathbf{c}) \quad (3.15)$$

Using the fact that $\mathbb{P}_\theta(\tilde{c}_i = 1) = p_i$, $\forall i \in [n]$, it is straightforward to see that the decision variables in (3.15) satisfy the first two constraint sets in (3.3), while the third constraint is satisfied as follows:

$$\sum_{i=1}^n \frac{y_i}{y_0} = \sum_{i=1}^n \mathbb{P}_\theta \left(\tilde{c}_i = 1 \mid \sum_{t=1}^n \tilde{c}_t \geq k \right) \geq k$$

which is true since given that the sum of n Bernoulli random variables is at least k , there must be at least k out of them that equal one. Lastly, from the interpretation of y_0 in (3.15), it is clear that the objective function values of the two linear programs coincide.

Step (2): $\bar{P}(n, k, \mathbf{p}) \geq \bar{P}_u^c(n, k, \mathbf{p})$

Given any feasible solution (y_0, y_1, \dots, y_n) of the compact linear program (3.3), the vector

$$\mathbf{y} = \left(\frac{y_1}{y_0}, \frac{y_2}{y_0}, \dots, \frac{y_n}{y_0} \right)$$

must lie in the n -dimensional hypercube since $y_i \leq y_0$, $\forall i \in [n]$. Additionally, from the last constraint in (3.3), we have $\sum_{i=1}^n (y_i/y_0) \geq k$ and hence \mathbf{y} can be written as a convex combination of the extreme points of the sliced hypercube $[0, 1]^n \cap (\sum_{i=1}^n c_i \geq k)$ as follows:

$$\mathbf{y} = \sum_{\mathbf{c} \in \mathcal{C}_k} \lambda_{\mathbf{c}} \mathbf{c}, \quad \text{where} \quad \sum_{\mathbf{c} \in \mathcal{C}_k} \lambda_{\mathbf{c}} = 1 \quad (3.16)$$

and $\mathcal{C}_k = \{\mathbf{c} \in \mathcal{C} : \sum_{i=1}^n c_i \geq k\} \subset \{0, 1\}^n$ is the set of realizations of \mathbf{c} where each realization adds up to at least k for all $k \in [n]$. We now construct a probability distribution supported on \mathcal{C}_k where

$$\mathbb{P}_\theta(\mathbf{c}) = \lambda_{\mathbf{c}} y_0 \quad \forall \mathbf{c} \in \mathcal{C}_k$$

such that the constraints in (3.1) are satisfied as follows:

$$\begin{aligned} \sum_{\mathbf{c} \in \mathcal{C}_k, c_i=1} \mathbb{P}_\theta(\mathbf{c}) &= y_0 \left(\sum_{\mathbf{c} \in \mathcal{C}_k, c_i=1} \lambda_{\mathbf{c}} \right) \quad \forall i \in [n] \\ &= y_i \quad \forall i \in [n] \\ \text{and} \quad \sum_{\mathbf{c} \in \mathcal{C}_k} \mathbb{P}_\theta(\mathbf{c}) &= y_0 \left(\sum_{\mathbf{c} \in \mathcal{C}_k} \lambda_{\mathbf{c}} \right) \\ &= y_0 \end{aligned} \tag{3.17}$$

where the second equality follows from (3.16) since:

$$\sum_{\mathbf{c} \in \mathcal{C}_k, c_i=1} \lambda_{\mathbf{c}} = \frac{y_i}{y_0}, \quad \forall i \in [n]$$

while the last inequality is due to the $\lambda_{\mathbf{c}}$, $\mathbf{c} \in \mathcal{C}_k$ being the coefficients of a convex combination. Note that from (3.17), we retrieve the same interpretation for (y_0, y_1, \dots, y_n) as in (3.15) and the objective function values of the two linear programs coincide. Since $y_i \leq p_i, \forall i \in [n]$ for any feasible solution to (3.3), the remaining mass $p_i - y_i$ can be distributed among the scenarios $\mathbf{c} : \sum_{t=1}^n c_t < k, c_i = 1$ for all $i \in [n]$ such that $\mathbb{P}_\theta(\tilde{c}_i = 1) = p_i, \forall i \in [n]$. Thus a feasible solution of the large-size linear program attaining the same objective as the compact formulation exists and the result is proved. \square

For the simple case of univariate tail probability bounds considered in this section, the tightest bound $\bar{P}_u(n, k, \mathbf{p})$ admits a closed-form expression that has been derived in Rügner (1978). However, we next provide an alternative proof of tightness of this closed-form bound using the compact linear program (3.3) derived in this section.

3.1.2 Closed-form expression for tight bounds

Theorem 9. (Rügner, 1978) Sort the probabilities in increasing value as $0 \leq p_1 \leq p_2 \leq \dots \leq p_n \leq 1$. Then,

$$\bar{P}_u(n, k, \mathbf{p}) = \min \left(\min_{1 \leq \ell \leq k} \frac{\sum_{i=1}^{n-k+\ell} p_i}{\ell}, 1 \right), \quad 1 \leq k \leq n \tag{3.18}$$

Proof. Consider the dual of the linear program (3.3)

$$\begin{aligned}
\bar{P}_u(n, k, \mathbf{p}) = \min & \sum_{i=1}^n w_i p_i + \sum_{i=1}^n v_i (1 - p_i) \\
\text{s.t.} & \sum_{i=1}^n v_i - \sum_{i=1}^n u_i + k\lambda - 1 \geq 0 \\
& u_i - v_i + w_i - \lambda \geq 0, \quad \forall i \in [n], \\
& u_i \geq 0, \quad \forall i \in [n], \\
& v_i \geq 0, \quad \forall i \in [n], \\
& w_i \geq 0, \quad \forall i \in [n], \\
& \lambda \geq 0
\end{aligned} \tag{3.19}$$

Let $q = \min_{1 \leq \ell \leq k} \frac{\sum_{i=1}^{n-k+\ell} p_i}{\ell}$ and $\ell^* = \operatorname{argmin}_{1 \leq \ell \leq k} \frac{\sum_{i=1}^{n-k+\ell} p_i}{\ell}$. We ignore the trivial case of $k = 0$

when the bound is one and consider $k \in [n]$ henceforth. We next consider two possible cases when the bound in (3.18) is either non-trivial or trivially one as follows:

i) **Non-trivial bound** ($q < 1$):

When $q < 1$, we consider two cases, *i.e.*, $1 \leq \ell^* < k$ and $\ell^* = k$.

(a) $1 \leq \ell^* < k$:

Consider the following dual feasible solution of (3.19):

$$\begin{aligned}
u_i &= \begin{cases} 0, & 1 \leq i \leq n - k + \ell^* \\ \frac{1}{\ell^*}, & n - k + \ell^* + 1 \leq i \leq n \end{cases}, \\
v_i &= 0, \quad \forall i \in [n] \\
w_i &= \begin{cases} \frac{1}{\ell^*}, & 1 \leq i \leq n - k + \ell^* \\ 0, & n - k + \ell^* + 1 \leq i \leq n \end{cases}, \\
\lambda &= \frac{1}{\ell^*}
\end{aligned} \tag{3.20}$$

By complementary slackness of w_i, u_i we have respectively

$$\begin{aligned}
y_i &= p_i, \quad 1 \leq i \leq n - k + \ell^* \\
y_i &= y_0, \quad n - k + \ell^* + 1 \leq i \leq n
\end{aligned} \tag{3.21}$$

By complementary slackness of λ , we have

$$\begin{aligned} \sum_{i=1}^n y_i &= ky_0 \\ \sum_{i=1}^{n-k+\ell^*} p_i &= ky_0 - \sum_{i=n-k+\ell^*+1}^n y_0 \\ y_0 &= \frac{\sum_{i=1}^{n-k+\ell^*} p_i}{\ell^*} \\ &= q < 1 \end{aligned}$$

Consequently, it can be observed that the proposed dual feasible solution in (3.20) satisfies the constraint set $y_0 - y_i \leq 1 - p_i$, $i \in [n]$ in the compact linear program (3.3). We will next show that the solution also satisfies the remaining two constraint sets in (3.3), i.e.,

$$\begin{aligned} y_0 - y_i &\geq 0, \quad \forall i \in [n] \\ 0 &\leq y_i \leq p_i, \quad \forall i \in [n] \end{aligned}$$

Using the solution from (3.21), we thus need to prove that:

$$\begin{aligned} y_0 &\geq p_i, \quad 1 \leq i \leq n - k + \ell^* \\ y_0 &\leq p_i, \quad n - k + \ell^* + 1 \leq i \leq n \end{aligned}$$

Since the marginal probabilities p_i , $i \in [n]$ are arranged in increasing order, it suffices to show that

$$p_{n-k+\ell^*} \leq y_0 \leq p_{n-k+\ell^*+1}$$

i) $y_0 \leq p_{n-k+\ell^*+1}$:

Since ℓ^* is the minimizer of q and $y_0 = q$, we have:

$$\begin{aligned} \frac{\sum_{i=1}^{n-k+\ell^*} p_i}{\ell^*} &\leq \frac{\sum_{i=1}^{n-k+\ell^*+1} p_i}{\ell^* + 1} \\ &= \frac{\sum_{i=1}^{n-k+\ell^*} p_i + p_{n-k+\ell^*+1}}{\ell^* + 1} \\ \frac{\sum_{i=1}^{n-k+\ell^*} p_i}{\ell^*} &\leq p_{n-k+\ell^*+1} \\ y_0 &\leq p_{n-k+\ell^*+1} \end{aligned}$$

ii) $y_0 \geq p_{n-k+\ell^*}$:

Firstly, if $\ell^* = 1$, we have

$$y_0 = \frac{\sum_{i=1}^{n-k+1} p_i}{1} = \sum_{i=1}^{n-k+1} p_i \geq p_{n-k+1}$$

If $1 < \ell^* < k$, since ℓ^* is the minimizer of q and $y_0 = q$, we have:

$$\begin{aligned} \frac{\sum_{i=1}^{n-k+\ell^*} p_i}{\ell^*} &\leq \frac{\sum_{i=1}^{n-k+\ell^*-1} p_i}{\ell^* - 1} \\ &= \frac{\sum_{i=1}^{n-k+\ell^*} p_i - p_{(n-k+\ell^*)}}{\ell^* - 1} \\ \frac{\sum_{i=1}^{n-k+\ell^*} p_i}{\ell^*} &\geq p_{(n-k+\ell^*)} \\ y_0 &\geq p_{n-k+\ell^*} \end{aligned}$$

Hence all constraints are satisfied and both the primal and dual attain the suggested optimal value q .

(b) **Special Case** ($\ell^* = k$):

Consider the following dual feasible solution:

$$u_i = v_i = 0, \quad \forall i \in [n], \quad w_i = \frac{1}{k}, \quad \forall i \in [n], \quad \lambda = \frac{1}{k}$$

By complementary slackness of w_i , $i \in [n]$ we have

$$y_i = p_i, \quad \forall i \in [n]$$

and by complementary slackness of λ , we have

$$\sum_{i=1}^n y_i = k y_0 \quad \text{or} \quad y_0 = \frac{\sum_{i=1}^n p_i}{k} = q < 1 \quad (3.22)$$

Consequently, the two constraint sets

$$\begin{aligned} y_0 - y_i &\leq 1 - p_i, \quad \forall i \in [n] \\ 0 &\leq y_i \leq p_i, \quad \forall i \in [n] \end{aligned}$$

are satisfied by the above feasible solution. It remains to show that

$$\begin{aligned} y_0 &\geq y_i, \quad \forall i \in [n] \\ \text{or} \quad y_0 &\geq p_i, \quad \forall i \in [n] \end{aligned}$$

It suffices to prove that $y_0 \geq p_n$. Since $\ell^* = k$, by definition of ℓ^* and y_0 from (3.22) we have:

$$\begin{aligned} \frac{\sum_{i=1}^n p_i}{k} &= \frac{\sum_{i=1}^{n-k+k} p_i}{k} \\ &\leq \frac{\sum_{i=1}^{n-k+k-1} p_i}{k-1} \\ &\leq \frac{\sum_{i=1}^n p_i - p_n}{k-1} \\ \text{or} \quad \frac{\sum_{i=1}^n p_i}{k} &\geq p_n \\ y_0 &\geq p_n \end{aligned}$$

Hence we have proved that when $q < 1$, there exist primal and dual feasible solutions for all possible values of ℓ^* ($1 \leq \ell^* \leq k$, $k \in [n]$) that attain the non-trivial bound q , which is thus optimal.

ii) **Trivial bound** ($q \geq 1$):

When $q > 1$, consider the following dual feasible solution:

$$u_i = 0, \forall i \in [n], \quad v_i = w_i = \frac{1}{n}, \forall i \in [n], \quad \lambda = 0$$

By complementary slackness of v_i, w_i we have

$$\begin{aligned} y_0 - y_i &= 1 - p_i, & \forall i \in [n] \\ y_i &= p_i, & \forall i \in [n] \end{aligned}$$

Then $y_0 = 1$ and since ℓ^* is the minimizer of q and $q \geq 1$, we have:

$$\begin{aligned} \sum_{i=1}^n y_i &= \sum_{i=1}^n p_i \\ &= k \frac{\sum_{i=1}^{n-k+k} p_i}{k} \\ &\geq k \frac{\sum_{i=1}^{n-k+\ell^*} p_i}{\ell^*} \\ &= kq \\ &\geq ky_0 \end{aligned}$$

Hence all constraints of the compact primal (3.3) are satisfied and both the primal and dual attain the bound of one which is thus optimal when $q \geq 1$.

Summarizing the results of the trivial and non-trivial bounds, we have

$$\bar{P}_u(n, k, \mathbf{p}) = \min(q, 1)$$

which is precisely the tight bound in (3.18). \square

Connection to earlier work: We note that the closed-form bound in (3.18) was first derived by Ruger (1978) in the context of hypothesis testing while Morgenstern (1980) subsequently provided a simpler proof of the result. However, it appears that these works are largely unknown to the academic community due to their being published in the German language journal *Metrika* (the only citations that we are aware of are in Ruschendorf (1991) and Ruschendorf, Ludger (2013)). Several other closed-form bounds on the tail probability of sums of random variables with known marginal distribution functions have been proposed in the literature. While Markov bounds are the earliest known, standard bounds and dual bounds have been more recently proposed (see chapter 4 of Ruschendorf, Ludger, 2013, and the references therein for a detailed review). While none of these bounds are tight in general, the dual bounds can be shown to reduce to the Ruger (1978) bound when the variables are Bernoulli. Note that Ruger (1978) bound reduces to the Markov bound with identical marginals and the Frechet (1935) union and intersection bounds when $k = 1$ and $k = n$ respectively.

3.1.3 Lower bounds on tail probability

We now extend the results of the previous section to provide closed-form lower bounds on the tail probability of sums of Bernoulli variables. Denote by $\underline{P}_u(n, k, \mathbf{p})$ the tight lower bound on the probability that at least k out of n Bernoulli events occur, i.e.,

$$\underline{P}_u(n, k, \mathbf{p}) = \min_{\theta \in \Theta_u} \mathbb{P}_\theta \left(\sum_{i=1}^n \tilde{c}_i \geq k \right), \quad \forall k \in [n]$$

Corollary 4. *The tight lower bound $\underline{P}_u(n, k, \mathbf{p})$ can be computed as the optimal value of the following compact linear program:*

$$\begin{aligned} \bar{P}_u(n, k, \mathbf{p}) = \min \quad & y_0 \\ \text{s.t.} \quad & 0 \leq y_0 - y_i \leq 1 - p_i, \quad \forall i \in [n], \\ & 0 \leq y_i \leq p_i, \quad \forall i \in [n], \\ & \sum_{i=1}^n y_i \geq k y_0 \end{aligned} \quad (3.23)$$

Proof. Note that except for the minimization instead of maximization, the compact linear program (3.23) is exactly identical to (3.3) which was used to compute the upper bound. The dual indicator constraint for the lower bound would be reversed and of the form:

$$\sum_{i=1}^n \lambda_i c_i + \lambda_0 \leq \mathbb{1}_{\sum_{i=1}^n c_i \geq k}, \quad \forall \mathbf{c} \in \mathcal{C},$$

which can be equivalently written as:

$$\sum_{i=1}^n \lambda_i c_i + \lambda_0 \leq 0 \quad \forall \mathbf{c} \in \mathcal{C} : \sum_{i=1}^n c_i \leq k \quad (3.24a)$$

$$\sum_{i=1}^n \lambda_i c_i + \lambda_0 \leq 1 \quad \forall \mathbf{c} \in \mathcal{C} \quad (3.24b)$$

The proof then easily follows by similar techniques used in the derivation of (3.3). We omit further details here for the sake of brevity. \square

Corollary 5. *Sort the probabilities in increasing value as $0 \leq p_1 \leq p_2 \leq \dots \leq p_n \leq 1$. Then,*

$$\underline{P}_u(n, k, \mathbf{p}) = \max \left(\max_{1 \leq \ell \leq n-k+1} \frac{\sum_{i=1}^{k-1+\ell} p_{n-i+1} - (k-1)}{\ell}, 0 \right), \quad \forall k \in [n] \quad (3.25)$$

Proof. We first define the tight upper bound on the probability of at most k out of n Bernoulli events occurring as

$$\bar{Q}_u(n, k, \mathbf{p}) = \max_{\theta \in \Theta_u} \mathbb{P}_\theta \left(\sum_{i=1}^n \tilde{c}_i \leq k \right), \quad \forall k \in [0, n]$$

Define a complementary Bernoulli random variable $d_i = 1 - c_i$, $i \in [n]$. Then for $k \in [0, n]$,

$$\begin{aligned}\bar{Q}_u(n, k, \mathbf{p}) &= \max_{\theta \in \Theta_u} \mathbb{P}_\theta(\sum_{i=1}^n \tilde{c}_i \leq k), \\ &= \max_{\theta \in \Theta_u^c} \mathbb{P}(\sum_{i=1}^n \tilde{d}_i \geq n - k) \\ &= \bar{P}_u(n, n - k, \mathbf{q})\end{aligned}$$

where Θ_u^c is the complementary ambiguity set of distributions such that

$$\Theta_u^c = \{\theta \in \Theta(\{0, 1\}^n) : \mathbb{P}_\theta(\mathbf{s}) = \mathbb{P}_{\theta_u}(\mathbf{s}^c), \forall \mathbf{s} \in \mathcal{C}, \forall \theta_u \in \Theta_u\}$$

and \mathbf{s}^c is the complementary scenario obtained by flipping the ones and zeros in \mathbf{s} which thus satisfies $\mathbb{P}_\theta(\tilde{d}_i = 1) = 1 - p_i$, $i \in [n]$ for any feasible distribution θ and \mathbf{q} is the marginal probability vector of the complementary Bernoulli random vector \mathbf{d} such that it is arranged in increasing order, i.e., $q_i = 1 - p_{n-i+1}$, $i \in [n]$. Now using the fact that

$$\begin{aligned}\underline{P}_u(n, k, \mathbf{p}) &= 1 - \bar{Q}_u(n, k - 1, \mathbf{p}), \quad \forall k \in [n], \\ &= 1 - \bar{P}_u(n, n - k + 1, \mathbf{q}), \quad \forall k \in [n]\end{aligned}$$

and the closed-form expression from (3.18), the tight lower bound in (3.25) follows. Note that this lower bound has been derived in Ruger (1981) as a follow-up to the upper bounds derived in Ruger (1978). \square

Similarly, the lower bound corresponding to $\bar{Q}_u(n, k, \mathbf{p})$ can be computed as

$$\begin{aligned}\underline{Q}_u(n, k, \mathbf{p}) &= \min_{\theta \in \Theta_u} \mathbb{P}_\theta(\sum_{i=1}^n \tilde{c}_i \leq k), \quad \forall k \in [0, n] \\ &= 1 - \bar{P}_u(n, k + 1, \mathbf{p}), \quad \forall k \in [0, n - 1],\end{aligned}$$

where we ignore $k = n$ since the bound is trivially one when $k = n$. We summarize the four tight bounds below (assuming the probabilities p_i are sorted in increasing order as before):

$$\begin{aligned}\bar{P}_u(n, k, \mathbf{p}) &= \begin{cases} \min \left(\min_{1 \leq \ell \leq k} \frac{\sum_{i=1}^{n-k+\ell} p_i}{\ell}, 1 \right), & 1 \leq k \leq n \\ 1, & k = 0 \end{cases} \\ \underline{P}_u(n, k, \mathbf{p}) &= \begin{cases} \max \left(\max_{1 \leq \ell \leq n-k+1} \frac{\sum_{i=1}^{k-1+\ell} p_{n-i+1} - k + 1}{\ell}, 0 \right), & 1 \leq k \leq n \\ 1, & k = 0 \end{cases} \\ \bar{Q}_u(n, k, \mathbf{p}) &= \begin{cases} \min \left(\min_{1 \leq \ell \leq n-k} \frac{\sum_{i=1}^{k+\ell} (1 - p_{n-i+1})}{\ell}, 1 \right), & 0 \leq k \leq n - 1 \\ 1, & k = n \end{cases} \\ \underline{Q}_u(n, k, \mathbf{p}) &= \begin{cases} \max \left(\max_{1 \leq \ell \leq k+1} \frac{\ell - (\sum_{i=1}^{n-k-1+\ell} p_i)}{\ell}, 0 \right), & 0 \leq k \leq n - 1 \\ 1, & k = n \end{cases}\end{aligned}$$

We next demonstrate an application of the closed-form expression derived in Theorem 9 to a special case of star-shaped marginals when the marginal information for only one *root* variable is known while the bivariate information of all other variables is known with respect to this *root* variable, forming a *star* structure.

3.1.4 Application to star-shaped system

Consider an $n + 1$ dimensional Bernoulli random vector $\tilde{\mathbf{c}} = [\tilde{c}_i]$, $i \in [0, n]$ for which we only know the univariate marginal distribution for one variable say \tilde{c}_0 (which we shall call as the *root* variable) *i.e.* $\mathbb{P}(\tilde{c}_0 = 1) = q_0 > 0$. Further suppose that for the remaining variables, we are given the bivariate probabilities with respect to the *root* variable *i.e.*

$$\begin{aligned}\mathbb{P}(\tilde{c}_i = 1, \tilde{c}_0 = 0) &= p_{i0}, \quad \forall i \in [n] \\ \mathbb{P}(\tilde{c}_i = 1, \tilde{c}_0 = 1) &= p_{i1}, \quad \forall i \in [n]\end{aligned}$$

This bivariate marginal structure resembles that of a *star-shaped* system which has been studied in the works of Rüschemdorf (1991), Embrechts and Puccetti (2010), and Puccetti and Rüschemdorf (2012).

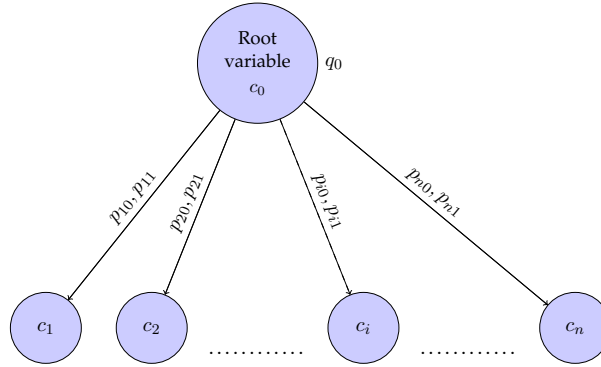


FIGURE 3.2: Star-shaped marginal structure

Let \mathbf{p}_0 and \mathbf{p}_1 be the vectors of bivariate probabilities p_{i0} and p_{i1} respectively for $i \in [n]$. Denote by $\mathcal{C}^* = \{0, 1\}^{n+1}$, the set of realizations of $\tilde{\mathbf{c}}$ and by $\bar{P}_b^*(n, k, q_0, \mathbf{p}_0, \mathbf{p}_1)$ the optimal value of the following exponential-sized star-structured linear program:

$$\begin{aligned}\bar{P}_b^*(n, k, q_0, \mathbf{p}_0, \mathbf{p}_1) &= \max \quad \mathbb{P}\left(\sum_{i=0}^n \tilde{c}_i \geq k\right) \\ \text{s.t.} \quad &\sum_{\mathbf{c} \in \mathcal{C}^*: c_0=1} \mathbb{P}(\mathbf{c}) = q_0 \\ &\sum_{\mathbf{c} \in \mathcal{C}^*: c_i=1} \mathbb{P}(\mathbf{c}) = p_{i0} + p_{i1} \quad \forall i \in [n] \\ &\sum_{\mathbf{c} \in \mathcal{C}^*: c_0=1, c_i=1} \mathbb{P}(\mathbf{c}) = p_{i1}, \quad \forall i \in [n] \\ &\sum_{\mathbf{c} \in \mathcal{C}^*} \mathbb{P}(\mathbf{c}) = 1 \\ &\mathbb{P}(\mathbf{c}) \geq 0 \quad \forall \mathbf{c} \in \mathcal{C}^*\end{aligned} \tag{3.26}$$

Define two sets of Bernoulli random variables $\{\alpha_i, i \in [n]\}$ and $\{\beta_i, i \in [n]\}$ such that

$$\begin{aligned}\mathbb{P}(\alpha_i = 1) &= q_{i0}, \quad \forall i \in [n] \\ \mathbb{P}(\beta_i = 1) &= q_{i1}, \quad \forall i \in [n]\end{aligned}$$

where q_{i0}, q_{i1} are the conditional probabilities

$$\begin{aligned}q_{i0} &= \mathbb{P}(\tilde{c}_i = 1 | \tilde{c}_0 = 0) = \frac{p_{i0}}{(1 - q_0)}, \quad \forall i \in [n] \\ q_{i1} &= \mathbb{P}(\tilde{c}_i = 1 | \tilde{c}_0 = 1) = \frac{p_{i1}}{q_0}, \quad \forall i \in [n]\end{aligned}$$

The correlation between the n variables α_i and β_i is unspecified and thus we consider the following two regular univariate linear programs (similar to (3.1)) with $\alpha_i, \beta_i, i \in [n]$ as random variables respectively:

$$\begin{aligned}\bar{P}_u(n, k, \mathbf{q}_0) &= \max_{\alpha \in \mathcal{C}: \sum_{i=1}^n \alpha_i \geq k} \sum \mathbb{P}(\alpha) \\ \text{s.t.} \quad &\sum_{\alpha \in \mathcal{C}: \alpha_i = 1} \mathbb{P}(\alpha) = q_{i0}, \quad \forall i \in [n], \\ &\sum_{\alpha \in \mathcal{C}} \mathbb{P}(\alpha) = 1, \\ &\mathbb{P}(\alpha) \geq 0\end{aligned} \tag{3.27}$$

and

$$\begin{aligned}\bar{P}_u(n, k, \mathbf{q}_1) &= \max_{\beta \in \mathcal{C}: \sum_{i=1}^n \beta_i \geq k} \sum \mathbb{P}(\beta) \\ \text{s.t.} \quad &\sum_{\beta \in \mathcal{C}: \beta_i = 1} \mathbb{P}(\beta) = q_{i1}, \quad \forall i \in [n], \\ &\sum_{\beta \in \mathcal{C}} \mathbb{P}(\beta) = 1, \\ &\mathbb{P}(\beta) \geq 0\end{aligned} \tag{3.28}$$

where $\mathbf{q}_0, \mathbf{q}_1$ are the n dimensional vectors of conditional probabilities q_{i0} and q_{i1} and $\mathcal{C} = \{0, 1\}^n$. The linear programs (3.27) and (3.28) can be treated as independent of the root variable c_0 and can be solved by using the compact linear program (3.3) derived earlier or the closed-form expression (3.18) directly. It has been shown in Rüschemdorf (1991) (see Proposition 8) that the optimal value of the star-structured linear program (3.26) can be expressed in terms of the optimal values of the regular univariate linear programs (3.27) and (3.28) as:

$$\bar{P}_b^*(n, k, q_0, \mathbf{p}_0, \mathbf{p}_1) = (1 - q_0) \bar{P}_u(n, k, \mathbf{q}_0) + q_0 \bar{P}_u(n, k - 1, \mathbf{q}_1)$$

Using the closed-form bound from Theorem 9, the above result can be concisely expressed as:

$$\bar{P}_b^*(n, k, q_0, \mathbf{p}_0, \mathbf{p}_1) = (1 - q_0) \min \left(\min_{1 \leq \ell \leq k} \frac{\sum_{i=1}^{n-k+\ell} q_{(i0)}}{\ell}, 1 \right) + q_0 \min \left(\min_{1 \leq \ell \leq k-1} \frac{\sum_{i=1}^{n-k+\ell+1} q_{(i1)}}{\ell}, 1 \right)$$

where $q_{(i0)}, q_{(i1)}$ represent the i^{th} order statistic of the conditional probabilities q_{i0}, q_{i1} respectively.

3.2 Extension to discrete marginals

In this section we consider a natural extension of Bernoulli random variables to variables with discrete support where we assume that all variables have identical discrete integer support points of the form $0, 1, 2, \dots, m - 1$ for some $m \in \mathbb{Z}_+$. This assumption is without loss of generality since we will later show in Corollary 7 that the results with identical integer support can be generalized to the case of non-identical rational discrete support points. Consider an n dimensional random vector $\tilde{\mathbf{c}} = [\tilde{c}_i], i \in [n]$ where each discrete random variable \tilde{c}_i can assume a value $0, 1, 2, \dots, m - 1$ for some integer $m \geq 2$. Further assume that the marginals are given as

$$\mathbb{P}(\tilde{c}_i = j) = p_{ij}, \quad \forall i \in [n], \forall j \in [0, m - 1],$$

$$\text{where } \sum_{j=0}^{m-1} p_{ij} = 1, \quad \forall i \in [n]$$

Denote by $\mathcal{C}_d = \{0, 1, 2, \dots, m - 1\}^n$ the set of realizations of $\tilde{\mathbf{c}}$ and by $\bar{P}_d(n, k, \mathbf{p})$ the tight upper bound on the probability that the sum of n discrete random variables at least equals k by:

$$\bar{P}_d(n, k, \mathbf{p}) = \max_{\theta \in \Theta_d} \mathbb{P}_\theta \left(\sum_{i=1}^n \tilde{c}_i \geq k \right), \quad \forall k \in [n(m - 1)]$$

where Θ_d denotes the ambiguity set of joint distributions supported on \mathcal{C}_d consistent with the given univariate information, *i.e.*,

$$\Theta_d = \{ \theta \in \Theta(\{0, 1, \dots, m - 1\}^n) : \mathbb{P}_\theta(\tilde{c}_i = j) = p_{ij}, \forall i \in [n], \forall j \in [0, m - 1] \}$$

$\bar{P}_d(n, k, \mathbf{p})$ can be computed as the optimal value of the following exponential-sized linear program:

$$\begin{aligned} \bar{P}_d(n, k, \mathbf{p}) = \max & \sum_{\mathbf{c} \in \mathcal{C}_d: \sum_{i=1}^n c_i \geq k} \mathbb{P}(\mathbf{c}) \\ \text{s.t.} & \sum_{\mathbf{c} \in \mathcal{C}_d: c_i = j} \mathbb{P}(\mathbf{c}) = p_{ij}, \quad \forall i \in [n], \forall j \in [0, m - 1] \\ & \sum_{\mathbf{c} \in \mathcal{C}_d} \mathbb{P}(\mathbf{c}) = 1 \\ & \mathbb{P}(\mathbf{c}) \geq 0 \quad \forall \mathbf{c} \in \mathcal{C}_d \end{aligned} \tag{3.29}$$

We next derive a compact linear programming formulation that provides valid upper bounds on $\bar{P}_d(n, k, \mathbf{p})$.

3.2.1 Compact linear program and primal proof of correctness

Theorem 10. *The optimum solution of the exponential-sized linear program in (3.29) is upper bounded by the optimal solution of the following compact linear program:*

$$\begin{aligned}
\bar{P}_d(n, k, \mathbf{p}) \leq \max \quad & z_0 \\
\text{s.t.} \quad & 0 \leq z_{ij} \leq p_{ij}, \quad \forall i \in [n], \forall j \in [0, m-1], \\
& \sum_{j=0}^{m-1} z_{ij} = z_0, \quad \forall i \in [n], \\
& \sum_{i=1}^n \sum_{j=0}^{m-1} j z_{ij} \geq k z_0
\end{aligned} \tag{3.30}$$

Proof. The proof broadly parallels that of Theorem 8 and thus we only preserve the most important steps and highlight differences for the purpose of exposition. Introduce an auxiliary binary random variable $y_{ij} = \mathbb{1}_{c_i=j}$, $i \in [n], j \in [0, m-1]$ which thus satisfies the constraints

$$\begin{aligned}
\sum_{j=0}^{m-1} y_{ij} &= 1, \quad \forall i \in [n] \\
\sum_{j=0}^{m-1} j y_{ij} &= c_i, \quad \forall i \in [n]
\end{aligned}$$

for any realization \mathbf{c} of the random vector $\tilde{\mathbf{c}}$. Next consider the dual of (3.29):

$$\begin{aligned}
\bar{P}_d(n, k, \mathbf{p}) = \min \quad & \sum_{i=1}^n \sum_{j=0}^{m-1} \lambda_{ij} p_{ij} + \lambda_0 \\
\text{s.t.} \quad & \sum_{i=1}^n \sum_{j=0}^{m-1} \lambda_{ij} y_{ij} + \lambda_0 \geq \mathbb{1}_{\sum c_i \geq k}(\mathbf{c}), \quad \forall \mathbf{c} \in \mathcal{C}_d, \\
& \sum_{j=0}^{m-1} y_{ij} = 1, \quad \forall i \in [n], \\
& y_{ij} \in \{0, 1\}, \quad \forall i \in [n], \forall j \in [0, m-1], \\
& \lambda_{ij} \text{ free}, \quad \forall i \in [n], \forall j \in [0, m-1], \\
& \lambda_0 \text{ free}
\end{aligned} \tag{3.31}$$

We use a similar approach as was used in Section 3.1 to derive the compact linear program (3.3) for the Bernoulli case, by splitting the indicator constraint set in (3.31)

into two sets

$$\begin{aligned} \sum_{i=1}^n \sum_{j=0}^{m-1} \lambda_{ij} y_{ij} + \lambda_0 &\geq 0 \quad \forall c \in \mathcal{C} \\ \sum_{i=1}^n \sum_{j=0}^{m-1} \lambda_{ij} y_{ij} + \lambda_0 &\geq 1 \quad \forall c \in \mathcal{C} : \sum_{i=1}^n c_i \geq k \end{aligned}$$

and subsequently converting them into optimization problems with the binary variables y_{ij} as decision variables (for fixed λ_{ij}, λ_0). Next, consider their respective linear program relaxations as follows:

$$\lambda_0 + \left\{ \begin{array}{l} \min \sum_{i=1}^n \sum_{j=0}^{m-1} \lambda_{ij} y_{ij} \\ \text{s.t.} \sum_{j=0}^{m-1} y_{ij} = 1, \quad \forall i \in [n], \\ 0 \leq y_{ij} \leq 1, \quad \forall i \in [n], \forall j \in [0, m-1] \end{array} \right\} \geq 0 \quad (3.33)$$

$$\lambda_0 + \left\{ \begin{array}{l} \min \sum_{i=1}^n \sum_{j=0}^{m-1} \lambda_{ij} y_{ij} \\ \text{s.t.} \sum_{j=0}^{m-1} y_{ij} = 1, \quad \forall i \in [n], \\ \sum_{i=1}^n \sum_{j=0}^{m-1} j y_{ij} \geq k, \\ 0 \leq y_{ij} \leq 1, \quad \forall i \in [n], \forall j \in [0, m-1] \end{array} \right\} \geq 1 \quad (3.34)$$

In the first relaxation (3.33), the constraint matrix is totally unimodular and thus guarantees integer extreme points. However, we note that in the second relaxation (3.34), the constraint matrix is *not* totally unimodular due to the coefficients j in the single constraint involving k and hence the linear program relaxation does not guarantee integer extreme points. Note that since (3.34) involves a minimization problem, the relaxation provides a lower bound on the integer separation problem which makes it harder to satisfy the ≥ 1 constraint, *i.e.*, it tightens the dual feasible region.

Dualizing (3.33) and (3.34) and forcing a single instance to satisfy the resulting dual as in (3.8) and (3.10), we can write the tightened compact dual version of (3.31) with

polyhedral-sized constraint sets as:

$$\begin{aligned}
\bar{P}_d^c(n, k, \mathbf{p}) = \min & \sum_{i=1}^n \sum_{j=0}^{m-1} \lambda_{ij} p_{ij} + \lambda_0 \\
\text{s.t.} & \lambda_0 - \sum_{i=1}^n \sum_{j=0}^{m-1} u_{ij} + \sum_{i=1}^n v_i \geq 0, \\
& \lambda_0 - \sum_{i=1}^n \sum_{j=0}^{m-1} w_{ij} + \sum_{i=1}^n t_i + kw_0 - 1 \geq 0, \\
& \lambda_{ij} + u_{ij} - v_i \geq 0, & \forall i \in [n], \forall j \in [0, m-1], \\
& \lambda_{ij} + w_{ij} - jw_0 - t_i \geq 0, & \forall i \in [n], \forall j \in [0, m-1], \\
& \lambda_{ij} \text{ free}, u_{ij} \geq 0, w_{ij} \geq 0, & \forall i \in [n], \forall j \in [0, m-1], \\
& v_i, t_i \text{ free}, & \forall i \in [n], \\
& w_0 \geq 0, \\
& \lambda_0 \text{ free}
\end{aligned} \tag{3.35}$$

Note that the compact dual (3.35) is not in general equivalent to, but rather a tightening of the large-sized dual (3.31) and thus the optimal value $\bar{P}_d^c(n, k, \mathbf{p})$ (where the superscript c indicates that it is the optimal value of a compact linear program) provides a valid upper bound on $\bar{P}_d(n, k, \mathbf{p})$. Finally, we dualize (3.35) and eliminate redundant variables as in (3.12) to obtain the following compact primal linear program:

$$\begin{aligned}
\bar{P}_d^c(n, k, \mathbf{p}) = \max & z_0 \\
\text{s.t.} & 0 \leq z_0 - z_{ij} \leq 1 - p_{ij}, \quad \forall i \in [n], \forall j \in [0, m-1], \\
& 0 \leq z_{ij} \leq p_{ij}, \quad \forall i \in [n], \forall j \in [0, m-1], \\
& \sum_{j=0}^{m-1} z_{ij} = z_0, \quad \forall i \in [n], \\
& \sum_{i=1}^n \sum_{j=0}^{m-1} j z_{ij} \geq kz_0
\end{aligned} \tag{3.36}$$

Note that the constraints in the compact linear programs (3.36) and (3.3) are similar except for the coefficients j in the single constraint involving k and the third set of constraints $\sum_{j=0}^{m-1} z_{ij} = z_0$, $i \in [n]$ which corresponds to the constraint on the auxiliary binary variables $\sum_{j=0}^{m-1} y_{ij} = 1$, $i \in [n]$. In fact we can show that the second and third sets of constraints in (3.36) are subsumed by the first set as follows:

$$\begin{aligned}
z_0 - z_{ij} &= \sum_{t=0}^{m-1} z_{it} - z_{ij} \quad \forall i \in [n], \forall j \in [0, m-1], \\
&= \sum_{t=0, t \neq j}^{m-1} z_{it} \quad \forall i \in [n], \forall j \in [0, m-1], \\
&\geq 0
\end{aligned}$$

where the last inequality follows from non-negativity of z_{ij} in the second constraint set. Further,

$$\begin{aligned} z_0 - z_{ij} &= \sum_{t=0, t \neq j}^{m-1} z_{it} \quad \forall i \in [n], \forall j \in [0, m-1], \\ &\leq \sum_{t=0, t \neq j}^{m-1} p_{it} \quad \forall i \in [n], \forall j \in [0, m-1], \\ &= 1 - p_{ij} \quad \forall i \in [n], \forall j \in [0, m-1], \end{aligned}$$

where the second inequality follows from $z_{ij} \leq p_{ij}$ of the second constraint set. We can thus eliminate the first set of constraints in (3.36) and only retain the *most compact* linear program formulation (3.30) with only $\mathcal{O}(nm)$ decision variables and constraints. Note that (3.30) is a relaxation of the large-sized linear program (3.29) and hence $\bar{P}_d(n, k, \mathbf{p}) \leq \bar{P}_d^c(n, k, \mathbf{p})$ and the proof is thus completed. \square

Connection to other work: We note that it has been shown that the tight upper bound $\bar{P}_d(n, k, \mathbf{p})$ is computable as the optimal value of a compact linear program (see Section 2.2 in Padmanabhan et al., 2021). This linear program involves reformulating the dual separation problem in (3.34) using dynamic programming recursions, which admits pseudo-polynomial time solutions. Although the tight bound $\bar{P}_d(n, k, \mathbf{p})$ is efficiently computable as the optimal solution of this compact linear program, the trade off is that the formulation is considerably more involved with $\mathcal{O}(n^2m^2)$ variables and constraints compared to our compact linear program in (3.30) with $\mathcal{O}(nm)$ decision variables and constraints. In spite of the simplicity of the compact formulation in (3.30), numerical examples in Section 3.2.3 demonstrate that the computed upper bounds $\bar{P}_d^c(n, k, \mathbf{p})$ are tight in many, if not most instances. More importantly, this simplified formulation admits closed-form solutions (see Section 3.2.2) when the discrete variables are identical. Numerical experiments in Example 9 show that the derived closed-form bound is tight in most randomly generated instances with identical discrete variables, while it appears to be almost always tight for symmetric and identical discrete variables.

Primal proof of correctness

We next provide a direct proof of Theorem 10 without going through the dual formulations and also interpret the decision variables of the compact linear program (3.30) in terms of the probabilities from a feasible joint distribution of the large-sized primal linear program (3.29).

Proposition 8. *The optimal value $\bar{P}_d^c(n, k, \mathbf{p})$ of the compact linear program in (3.30) provides a valid upper bound on the tight bound $\bar{P}_d(n, k, \mathbf{p})$. Further, for any feasible distribution $\theta \in \Theta_d$ of the large-sized linear program (3.29) and any $k \in [n(m-1)]$, there exists a feasible solution of the compact linear program that satisfies:*

$$\begin{aligned} z_0 &= \mathbb{P}_\theta \left(\sum_{t=1}^n \tilde{c}_t \geq k \right) \\ z_{ij} &= \mathbb{P}_\theta \left(\sum_{t=1}^n \tilde{c}_t \geq k, \tilde{c}_i = j \right), \quad \forall i \in [n], \forall j \in [0, m-1] \end{aligned} \quad (3.37)$$

Proof. Given a feasible solution $\mathbb{P}_\theta(\mathbf{c})$, $\forall \mathbf{c} \in \mathcal{C}_d$ of the large-sized primal linear program (3.29) for some distribution $\theta \in \Theta_d$, construct a feasible solution to (3.30) by aggregating the probabilities as follows:

$$z_0 = \sum_{\mathbf{c} \in \mathcal{C}_d: \sum_{t=1}^n c_t \geq k} \mathbb{P}_\theta(\mathbf{c}), \quad z_{ij} = \sum_{\mathbf{c} \in \mathcal{C}_d: \sum_{t=1}^n c_t \geq k, c_i = j} \mathbb{P}_\theta(\mathbf{c}) \quad \forall i \in [n], \forall j \in [0, m-1] \quad (3.38)$$

Using the fact that $\mathbb{P}_\theta(\tilde{c}_i = j) = p_{ij}$, $\forall i \in [n]$, $\forall j \in [0, m-1]$, it is straightforward to see that the interpretation in (3.38) satisfies the first two constraint sets in (3.30), while the third constraint is satisfied as follows:

$$\begin{aligned} \sum_{i=1}^n \sum_{j=0}^{m-1} \frac{jz_{ij}}{z_0} &= \sum_{i=1}^n \sum_{j=0}^{m-1} j \mathbb{P}_\theta \left(\tilde{c}_i = j \mid \sum_{t=1}^n \tilde{c}_t \geq k \right) \\ &= \sum_{i=1}^n \mathbb{E}_\theta \left(\tilde{c}_i \mid \sum_{t=1}^n \tilde{c}_t \geq k \right) \\ &= \mathbb{E}_\theta \left(\sum_{i=1}^n \tilde{c}_i \mid \sum_{t=1}^n \tilde{c}_t \geq k \right) \\ &\geq k \end{aligned}$$

where the last inequality is true since given that the sum of n non-negative discrete random variables is at least k , the expected value of the sum must be at least k . Lastly, from the interpretation of z_0 in (3.38), it is clear that the objective function values of the two linear programs coincide. Hence we have proved that the optimal values of the large-sized and compact primal linear programs are related as $\bar{P}_d(n, k, p) \leq \bar{P}_d^c(n, k, p)$. \square

3.2.2 Closed-form upper bounds

We next show that the compact linear program (3.30) admits a closed-form expression for the optimal solution $\bar{P}_d^c(n, k, p)$ when the discrete random variables are identical or symmetric identical.

Theorem 11. *When the marginals of the discrete random vector \tilde{c} are identical, i.e., $p_{ij} = p_j$, $i \in [n]$, $j \in [0, m-1]$, the optimum solution of the exponential-sized linear program in (3.29) is upper bounded by the following closed-form expression:*

$$\bar{P}_d(n, k, p) \leq \min \left(\frac{n}{k - nt} (\psi_t - t\pi_t), 1 \right), \quad \forall k \in [n(m-1)] \quad (3.39)$$

where

$$\begin{aligned} \psi_r &= \sum_{j=r}^{m-1} jp_j \quad r \in [0, m-1] \\ \pi_r &= \sum_{j=r}^{m-1} p_j \quad r \in [0, m-1] \end{aligned}$$

are the r^{th} discrete partial mean and partial marginal sum respectively of any discrete variable c_i , $i \in [n]$ and $t = \sum_{j=1}^{m-2} \mathbb{1}_{(k-n\psi_j/\pi_j) \geq 0}$ is an integer in $[0, m-2]$.

Proof. When the marginals are identical, we can replace the z_{ij} , $i \in [n]$ decision variables with z_j for all $j \in [0, m-1]$ and the compact linear program (3.30) along with its dual can thus be written as:

$$\begin{array}{l|l}
\max & z_0 \\
\text{s.t.} & 0 \leq z_j \leq p_j, \quad \forall j \in [0, m-1], \\
& \sum_{j=0}^{m-1} z_j = z_0, \\
& n \sum_{j=0}^{m-1} j z_j \geq k z_0 \\
\end{array} \quad (3.40) \qquad \left| \qquad \begin{array}{l}
\min & \sum_{j=1}^n \alpha_j p_j \\
\text{s.t.} & \gamma - \beta - 1 \geq 0 \\
& \beta + \alpha_j - \frac{n j \gamma}{k} \geq 0, \quad \forall j \in [0, m-1], \\
& \alpha_j \geq 0, \quad \forall j \in [0, m-1], \\
& \gamma \geq 0, \\
& \beta \text{ free} \\
\end{array} \quad (3.41)$$

We will show that there exists an optimal solution of the compact primal-dual linear program pair (3.40)-(3.41) that attains the closed-form bound in (3.39). Consider the following optimal solution of the compact primal-dual linear program pair:

Range of k	Primal optimal solution (3.40)	Dual optimal solution (3.41)	Optimum attained (z_0)
$\frac{n\psi_t}{\pi_t} \leq k \leq \frac{n\psi_{t+1}}{\pi_{t+1}}$ $t = \sum_{j=1}^{m-2} \mathbb{1}_{(k \geq n\psi_j/\pi_j)}$	$z_j = \begin{cases} 0, & j \in [0, t-1] \\ z_0 - \pi_{t+1}, & j = t \\ 1/m, & j \in [t+1, m-1] \end{cases}$ $z_0 = \frac{n}{k - nt} (\psi_t - t\pi_t)$	$\alpha_j = \begin{cases} 0, & j \in [0, t] \\ \frac{n(j-t)}{k - nt}, & j \in [t+1, m-1] \end{cases}$ $\beta = nt/(k - nt)$ $\gamma = k/(k - nt)$	$\frac{n}{k - nt} (\psi_t - t\pi_t)$
$k \leq n\psi_0 = S_1$	$z_j = 1/m, \quad j \in [0, m-1],$ $z_0 = 1$	$\alpha_j = 1, \quad j \in [0, m-1],$ $\beta = -1,$ $\gamma = 0$	1

TABLE 3.2: Extremal distribution of the compact linear program pair (3.40)-(3.41) for identical discrete random variables

where S_1 is the first binomial moment $\mathbb{E}[\sum_{i=1}^n \tilde{c}_i]$. It can be easily verified that the above solutions are feasible for both the primal and the dual and attain the closed-form bound in (3.39), which is thus the best upper bound attainable by the compact linear program. The result then follows from $\overline{P}_d(n, k, \mathbf{p}) \leq \overline{P}_d^c(n, k, \mathbf{p})$. \square

We note that (3.39) can be expressed more precisely as:

$$\overline{P}_d(n, k, \mathbf{p}) \leq \begin{cases} 1, & k \leq n\psi_0 \\ \frac{n}{k - nt} (\psi_t - t\pi_t), & \frac{n\psi_t}{\pi_t} \leq k \leq \frac{n\psi_{t+1}}{\pi_{t+1}}, \quad \forall t \in [0, m-2], \forall k \in [n(m-1)] \end{cases} \quad (3.42)$$

When $\frac{n\psi_0}{\pi_0} \leq k \leq \frac{n\psi_1}{\pi_1}$, we have $t = 0$ and the tight bound in (3.42) reduces to the

Markov bound $\frac{n\psi_0}{k} = \frac{S_1}{k}$.

Corollary 6. *When the marginals of the discrete random vector $\tilde{\mathbf{c}}$ are symmetric identical, i.e., $p_{ij} = 1/m$, $i \in [n], j \in [0, m-1]$, the optimum solution of the exponential-sized linear program in (3.29) is upper bounded by the following closed-form expression:*

$$\bar{P}_d(n, k, \mathbf{p}) \leq \min \left(\frac{n(m-t)(m-t-1)}{2m(k-nt)}, 1 \right), \quad \forall k \in [n(m-1)] \quad (3.43)$$

where $t = \left\lceil \frac{2k}{n} - m \right\rceil$ and $\lceil x \rceil$ maps x to the smallest integer greater than or equal to x .

Proof. The proof is straightforward from Theorem 11 by using $p_j = 1/m$, $j \in [0, m-1]$ and noting that

$$\frac{\psi_t}{\pi_t} = \frac{\sum_{j=t}^{m-1} j p_j}{\sum_{j=t}^{m-1} p_j} = \frac{(m+t-1)}{2}$$

and further from (3.42), for any $k \geq n(m-1)/2$, the non-trivial bound is valid when

$$\frac{(m+t-1)}{2} \leq \frac{k}{n} \leq \frac{(m+t)}{2},$$

which is satisfied by

$$t = \left\lceil \frac{2k}{n} - m \right\rceil, \quad t \in [0, m-2]$$

and the result follows. We note that (3.43) can be expressed more precisely as:

$$\bar{P}_d(n, k, \mathbf{p}) \leq \begin{cases} 1, & k < \frac{n(m-1)}{2} \\ \frac{n(m-t)(m-t-1)}{2m(k-nt)}, & k \geq \frac{n(m-1)}{2} \end{cases}$$

□

3.2.3 Numerical results

We next demonstrate the usefulness of the compact linear program derived in Theorem 10 in computing upper bounds on $\bar{P}_d(n, k, \mathbf{p})$. We compare the tight bound $\bar{P}_d(n, k, \mathbf{p})$ derived in Corollary 2.2 of Padmanabhan et al. (2021) (from a more involved compact linear program as noted earlier) with our upper bound $\bar{P}_d^c(n, k, \mathbf{p})$ derived as the optimal value of the compact linear program in (3.30) (alternatively the closed-form solutions in Theorem 11 and Corollary 6 for identical marginals) and the Markov bound $\frac{\sum_{i=1}^n \sum_{j=0}^{m-1} j p_{ij}}{k}$.

Example 8 (Non-identical marginals). *We first consider $n = 4$ discrete random variables with $m = 5$ support points each, i.e., each variable can assume values from $\{0, 1, 2, 3, 4\}$. In this example, we plot the three bounds by generating 300 instances of random probabilities p_{ij} , $i \in [4]$, $j \in [0, 4]$ where the probabilities are uniformly and independently generated in $(0, 1)$ such that $\sum_{j=0}^{m-1} p_{ij} = 1$, $\forall i \in [n]$.*

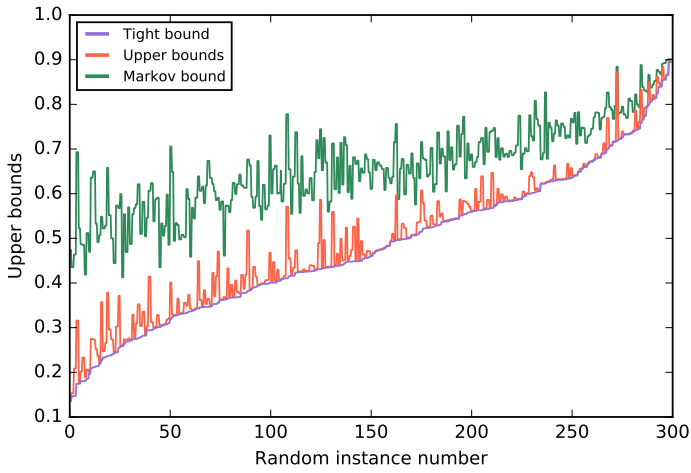
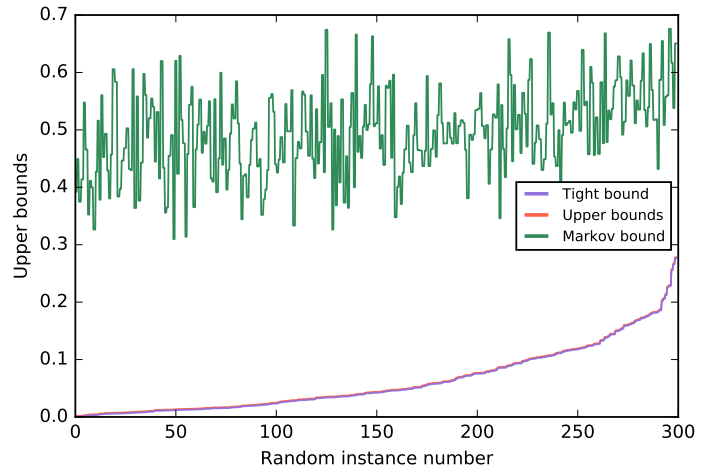
(a) $k=12$ (b) $k=16$ FIGURE 3.3: Comparison with tight bound for $n = 4$, $m = 5$ and 300 random instances

Figure 3.3a plots the three bounds for $k = 12$ while Figure 3.3b plots them for $k = 16$. Our upper bounds (in red) exactly coincide with the tight bound (in purple) when $k = n(m - 1) = 16$, which is the largest possible value of k , while it is marginally weaker than the tight bound when $k = 12$. The Markov bound performs better for smaller k .

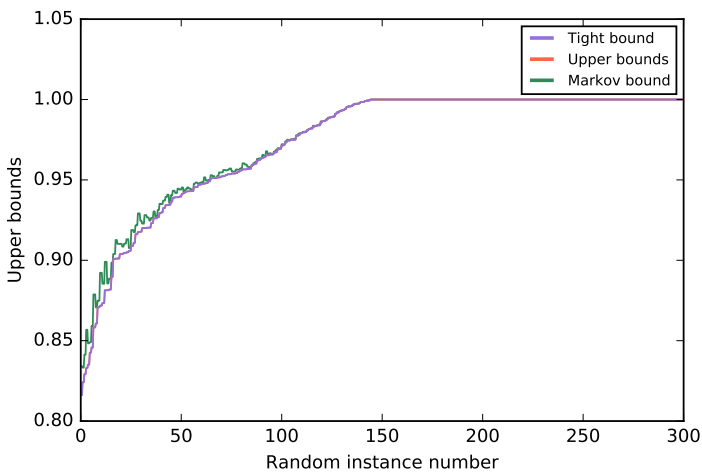
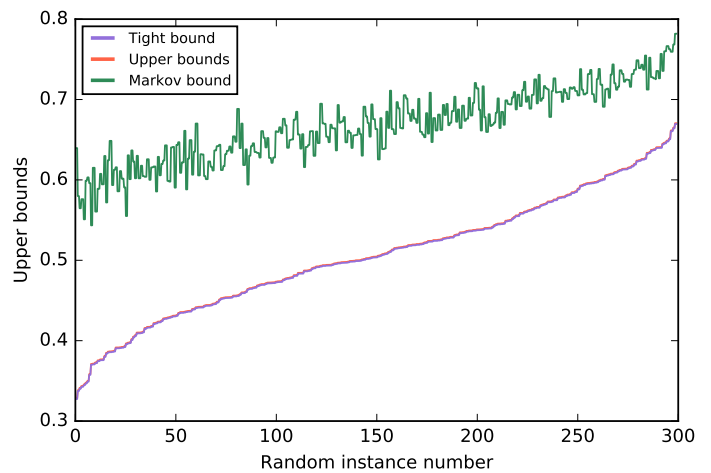
(a) $k=40$ (b) $k=60$ FIGURE 3.4: Comparison with tight bound for $n = 20$, $m = 5$ and 300 random instances

Figure 3.4 shows similar plots for $n = 20$ variables with $k = 40$ and 60 for 300 randomly generated instances. In this case, our upper bound exactly coincides with the tight bound in both the plots while the Markov bound becomes weaker with increasing k . Numerical illustrations show that as n increases, the upper bounds are increasingly stronger for all $k \in [0, n(m - 1)]$. Note that the plots in figures 3.3 and 3.4 are shown with the bounds sorted according to the increasing value of the tight bound.

In the next example, we demonstrate the usefulness of the closed-form bound in Theorem 11 and Corollary 6 in providing upper bounds on $\bar{P}_d(n, k, \mathbf{p})$ when the marginals are identical.

Example 9 (Identical marginals). Consider $n = 10$ discrete random variables with $m = 10$ support points each. We generate 200 instances of identical random probabilities p_j , $j \in [0, 9]$ where $p_{ij} = p_j$, $\forall i \in [10]$, $\forall j \in [0, 9]$ and the probabilities are uniformly and independently generated in $(0, 1)$ such that $\sum_{j=0}^{m-1} p_j = 1$. Figure 3.5a plots the closed-form bound in (3.39) and the tight bound $\bar{P}_d(n, k, \mathbf{p})$ derived in Padmanabhan et al. (2021) for a selected k values where the bounds are non-trivial. As seen in Figure 3.5a, the upper bounds are almost always tight for all chosen k values.

Figure 3.5b plots the closed-form bound in (3.43) with the tight bound when the marginals are symmetric identical, i.e., when $p_{ij} = 1/m$, $\forall i \in [10]$, $\forall j \in [0, m-1]$ for $m = 6, 8, 10, 12, 14$. Note that we do not generate random instances here since the marginals are fixed and thus the bounds are plotted against their respective valid ranges of k , i.e., $k \in [0, 10(m-1)]$. It is observed that the upper bound in Corollary 6 is always tight for all the selected values of m and $k \in [0, 10(m-1)]$. We deliberately exclude the Markov bound in Figure 3.5 to avoid clutter, but our results show similar behaviour of weaker performance with increasing k as observed in Example 8.

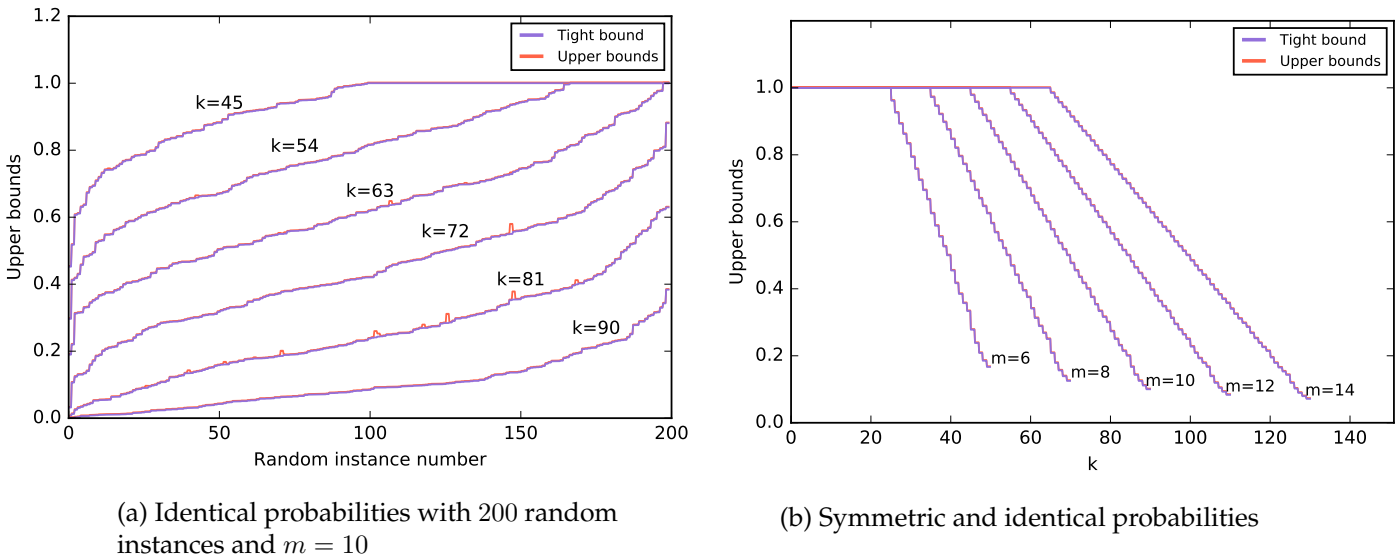


FIGURE 3.5: Comparison of bounds for identical probabilities with $n = 10$

In conclusion, the closed-form bounds in (3.39) and (3.43) appear to be tight in many instances such as when the marginals are identical or symmetric identical. Even with random marginals, the upper bounds derived as the optimal value of the compact linear program (3.30) appear to be tight in many cases such as when $k = n(m-1)$ or large n values.

3.2.4 Extension to real-valued discrete support

We next show that the results of Theorem 10 can be generalized to the case when the discrete variables assume *rational* values. Suppose, each discrete random variable \tilde{c}_i

assumes a value from the set $A_i = \{a_{i0}, a_{i1}, \dots, a_{i(m-1)}\}$ where $a_{ij} \in \mathbb{Q}$ (the set of rational numbers), for all $j \in [0, m-1], i \in [n]$ and $\mathbb{P}(\tilde{c}_i = a_{ij}) = p_{ij}$, for $i \in [n], j \in [0, m-1]$. In this case, the set of realizations of \tilde{c} can be written as the cross product of the sets A_i , i.e., $\mathcal{C}_d = \prod_{i \in [n]} A_i$ and

$$\bar{P}_d(n, k, \mathbf{p}) = \max_{\theta \in \Theta_d} \mathbb{P}_\theta \left(\sum_{i=1}^n \tilde{c}_i \geq k \right), \quad \forall k \in [a_{\min}, a_{\max}] \quad (3.44)$$

where

$$a_{\min} = \sum_{i=1}^n \min_{j \in [0, m-1]} a_{ij}, \quad a_{\max} = \sum_{i=1}^n \max_{j \in [0, m-1]} a_{ij}$$

and

$$\Theta_d = \left\{ \theta \in \Theta \left(\prod_{i \in [n]} A_i \right) : \mathbb{P}_\theta (\tilde{c}_i = a_{ij}) = p_{ij}, \forall i \in [n], \forall j \in [0, m-1] \right\}$$

Corollary 7. *The tight bound $\bar{P}_d(n, k, \mathbf{p})$ in (3.44) on the probability that n real-valued discrete random variables add up to at least k where $k \in [a_{\min}, a_{\max}]$, is upper bounded by the optimal solution of the following compact linear program:*

$$\begin{aligned} \bar{P}_d(n, k, \mathbf{p}) &\leq \max z_0 \\ \text{s.t.} \quad &0 \leq z_{ij} \leq p_{ij}, \quad \forall i \in [n], \forall j \in [0, m-1], \\ &\sum_{j=0}^{m-1} z_{ij} = z_0, \quad \forall i \in [n], \\ &\sum_{i=1}^n \sum_{j=0}^{m-1} a_{ij} z_{ij} \geq k z_0 \end{aligned} \quad (3.45)$$

Proof. The proof follows from the proof of Theorem 10 by redefining $y_{ij} = \mathbb{1}_{c_i = a_{ij}}$, $i \in [n], j \in [0, m-1]$ which thus satisfies the constraints

$$\sum_{j=0}^{m-1} y_{ij} = 1, \quad \forall i \in [n], \quad \sum_{j=0}^{m-1} a_{ij} y_{ij} = c_i, \quad \forall i \in [n]$$

for any realization \mathbf{c} of the random vector \tilde{c} . □

If the support points *and* marginal probabilities are identical, i.e.,

$$a_{ij} = a_j, \quad \forall i \in [n], \forall j \in [0, m-1], \quad p_{ij} = p_j, \quad \forall i \in [n], \forall j \in [0, m-1],$$

we can replace the z_{ij} , $i \in [n]$ decision variables with z_j for all $j \in [0, m-1]$ and the optimal solution to (3.45) can be derived as a closed form expression similar that in Theorem 11. The results in this section can be extended to derive lower bounds on the tail probability of the sum of real-valued discrete random variables using similar ideas.

3.3 Generalization to weighted tail probability bounds

In this section, we generalize the results of Section 3.1 to weighted tail probability bounds of sums of Bernoulli random variables. Denote by $\mathbf{w} = (w_1, w_2, \dots, w_n)$, $w_i \in \mathbb{R}$, $\forall i \in [n]$ a vector of pre-specified weights. We are interested in computing the following tight upper bound on the weighted sum of the tail probabilities

$$\max_{\theta \in \Theta_u} \sum_{l=0}^n w_l \mathbb{P}_\theta \left(\sum_{i=1}^n \tilde{c}_i \geq l \right).$$

We recall that the ambiguity set Θ_u ensures consistency of the considered distributions with the given univariate marginals for each c_i , $i \in [n]$. Note that without loss of generality, we can ignore $l = 0$ and consider $\mathbb{P}_\theta(\sum_{i=1}^n \tilde{c}_i = l)$ for $l \in [n]$ instead of tail probabilities by a suitable transformation of weights. Denote by $\bar{P}_{uw}(n, \mathbf{w}, \mathbf{p})$ the tight bound

$$\bar{P}_{uw}(n, \mathbf{w}, \mathbf{p}) = \max_{\theta \in \Theta_u} \sum_{l=1}^n w_l \mathbb{P}_\theta \left(\sum_{i=1}^n \tilde{c}_i = l \right)$$

which can be computed as the optimal value of the following exponential-sized linear program:

$$\begin{aligned} \bar{P}_{uw}(n, \mathbf{w}, \mathbf{p}) = \max \quad & \sum_{l=1}^n w_l \sum_{\mathbf{c} \in \mathcal{C}: \sum_{t=1}^n \tilde{c}_t = l} \mathbb{P}(\mathbf{c}) \\ \text{s.t.} \quad & \sum_{\mathbf{c} \in \mathcal{C}: c_i = 1} \mathbb{P}(\mathbf{c}) = p_i, \quad \forall i \in [n], \\ & \sum_{\mathbf{c} \in \mathcal{C}} \mathbb{P}(\mathbf{c}) = 1, \\ & \mathbb{P}(\mathbf{c}) \geq 0 \quad \forall \mathbf{c} \in \mathcal{C} \end{aligned} \quad (3.46)$$

We note that the feasible region of the above linear program is non-empty and since the weights w_i , $\forall i \in [n]$ are real-valued, the linear program cannot be unbounded and an optimal solution exists. Also note that when $\mathbf{w} = [\mathbf{0}_{k-1}, \mathbf{1}_{n-k+1}]$ (zeros up to index $k - 1$ and ones thereafter), the objective function in (3.46) reduces to the tail probability bounds considered in (3.1). We next derive a compact reformulation of (3.46) by considering the linear relaxation of its dual separation problems, similar to the proof of Theorem 8.

3.3.1 Compact linear program and primal proof of correctness

Theorem 12. *The exponential-sized linear program in (3.46) is equivalent to the following compact linear program:*

$$\begin{aligned}
\bar{P}_{uw}(n, \mathbf{w}, \mathbf{p}) = \max \quad & \sum_{l=0}^n x_l w_l \\
\text{s.t.} \quad & \sum_{l=0}^n x_l = 1, \\
& \sum_{l=0}^n y_{li} = p_i, \quad \forall i \in [n], \\
& x_l \geq y_{li}, \quad \forall i \in [n], \forall l \in [n], \\
& \sum_{i=1}^n y_{li} = l x_l, \quad \forall l \in [n], \\
& x_l \geq 0, \quad \forall l \in [n], \\
& y_{li} \geq 0, \quad \forall i \in [n], \forall l \in [n],
\end{aligned} \tag{3.47}$$

The corresponding lower bound $\underline{P}_{uw}(n, \mathbf{w}, \mathbf{p})$ can be computed as the optimal value of (3.47), with a minimization objective instead of maximization.

Proof. Consider the dual of the large-sized linear program (3.46)

$$\begin{aligned}
\bar{P}_{uw}(n, \mathbf{w}, \mathbf{p}) = \min \quad & \sum_{i=1}^n \lambda_i p_i + \lambda_0 \\
\text{s.t.} \quad & \sum_{i=1}^n \lambda_i c_i + \lambda_0 \geq w_l, \quad \forall \mathbf{c} \in \mathcal{C} : \sum c_i = l, \forall l \in [n], \\
& \lambda_i \text{ free}, \quad \forall i \in [n], \\
& \lambda_0 \text{ free}
\end{aligned} \tag{3.48}$$

The dual has 2^n constraints, which can be divided into n sets of $\binom{n}{l}$ constraints for $l \in [n]$. Similar to the steps followed in (3.6)-(3.11), for each $l \in [n]$, the set of $\binom{n}{l}$ constraints corresponding to the scenarios $\mathbf{c} \in \mathcal{C} : \sum c_i = l$ can be replaced with equivalent polynomial-sized constraint sets by converting them into optimization problems with $\{c_i, i \in [n]\}$ as decision variables for fixed $\{\lambda_0, \lambda_i, i \in [n]\}$ as follows:

$$\begin{aligned}
& \lambda_0 + \left\{ \min \sum_{i=1}^n \lambda_i c_i : \mathbf{c} \in \mathcal{C}, \sum_{i=1}^n c_i = l \right\} \geq w_l \quad \forall l \in [n] \\
\equiv & \lambda_0 + \left\{ \min \sum_{i=1}^n \lambda_i c_i : 0 \leq c_i \leq 1, \forall i \in [n], \sum_{i=1}^n c_i = l \right\} \geq w_l, \quad \forall l \in [n]
\end{aligned} \tag{3.49}$$

where the equivalence of the linear program relaxation follows from the totally unimodular structure of the constraint matrix in (3.49). We now dualize this resulting

linear program as follows:

$$\lambda_0 + \left\{ \begin{array}{l} \max \sum_{i=1}^n u_{li} + lv_l \\ \text{s.t. } u_{li} + v_l \leq \lambda_i, \quad \forall i \in [n], \\ u_{li} \leq 0, \quad \forall i \in [n], \\ v_l \text{ free} \end{array} \right\} \geq w_l, \quad \forall l \in [n] \quad (3.50)$$

Since an optimal solution to the primal (3.46) exists, by strong duality, the dual (3.48) must also have an optimal solution. Consequently there must exist a feasible solution to the linear program (3.50) and the constraint sets corresponding to each $l \in [n]$ in (3.48) can be replaced by the following polynomial-sized set of constraints:

$$\left\{ \begin{array}{l} \lambda_0 + \sum_{i=1}^n u_{li} + lv_l \geq w_l, \\ u_{li} + v_l \leq \lambda_i, \quad \forall i \in [n], \\ u_{li} \leq 0, \quad \forall i \in [n], \\ v_l \text{ free} \end{array} \right\}, \quad \forall l \in [n] \quad (3.51)$$

and thus the compact version of the dual (3.48) can be written as:

$$\begin{aligned} \bar{P}_{uw}(n, \mathbf{w}, \mathbf{p}) = & \min \sum_{i=1}^n \lambda_i p_i + \lambda_0 \\ \text{s.t. } & \lambda_0 - \sum_{i=1}^n u_{li} + lv_l \geq w_l, \quad \forall l \in [n], \\ & v_l - u_{li} \leq \lambda_i, \quad \forall i \in [n], \forall l \in [n], \\ & u_{li} \geq 0, \quad \forall i \in [n], \forall l \in [n], \\ & v_l \text{ free}, \quad \forall l \in [n], \\ & \lambda_i \text{ free} \quad \forall i \in [n], \\ & \lambda_0 \text{ free} \end{aligned} \quad (3.52)$$

Finally, dualizing (3.52) leads to the compact linear program (3.47) with $\mathcal{O}(n^2)$ variables and constraints. Their feasible regions remaining the same, it is straightforward to see that the corresponding lower bound $\underline{P}_{uw}(n, \mathbf{w}, \mathbf{p})$ can be computed as the optimal value of the compact linear program (3.47) with a minimization objective instead of maximization. \square

Connection to existing work: Weighted objective functions as in (3.46) have been considered in Kwerel (1975b) albeit with aggregated information in the form of the first two binomial moments. Assuming more information in the form of m -variate joint probabilities

$$\mathbb{P}(\tilde{c}_{i_1} = 1, \tilde{c}_{i_2} = 1, \dots, \tilde{c}_{i_r} = 1), \quad 1 \leq i_1 < i_2 \cdots < i_r \leq n, \quad r \leq m \leq n$$

Prékopa, Vizvári, and Regös (1997) formulate partially aggregated-disaggregated linear programs (see Section 3) with multivariate binomial moments to provide bounds on the linear functionals of the probabilities $\mathbb{P}(\sum_{i=1}^n \tilde{c}_i = l)$, $l \in [0, n]$. However, these works only restrict attention to the case when $\mathbf{w} = [\mathbf{0}_{k-1}, \mathbf{1}_{n-k+1}]$ to derive bounds on the probability that at least k out of n events occur or $w_i = \mathbb{1}_{i=k}$, $i \in [n]$ to derive bounds on the probability that exactly k out of n events occur. Thus the compact linear program (3.47) and its minimization version, which compute the tightest upper and lower bounds on the weighted tail probability function in (3.46), appear to be unknown in the literature to the best of our knowledge.

Primal proof of correctness

We next provide a direct proof of equivalence of the primal formulations of the large-sized compact linear programs with the weighted tail probability objective (without going through the dual formulations) and also interpret the decision variables of the compact primal formulation in terms of the probabilities from a feasible joint distribution of the large-sized primal formulation.

Proposition 9. *The large-sized primal linear program (3.46) is equivalent to the compact primal linear program (3.47), where for any extremal distribution $\theta^* \in \Theta_u$ of the large-sized linear program and any $l \in [n]$, the corresponding optimal solution of the compact linear program satisfies:*

$$\begin{aligned} x_l &= \mathbb{P}_\theta\left(\sum_{t=1}^n \tilde{c}_t = l\right) & \forall l \in [n] \\ y_{li} &= \mathbb{P}_\theta\left(\sum_{t=1}^n \tilde{c}_t = l, \tilde{c}_i = 1\right) & \forall l \in [n], \forall i \in [n] \end{aligned} \quad (3.53)$$

Proof. Denote the optimal value of the compact linear program in (3.47) by $\bar{P}_{uw}^c(n, \mathbf{w}, \mathbf{p})$.

Step (1): $\bar{P}_{uw}(n, k, \mathbf{p}) \leq \bar{P}_{uw}^c(n, k, \mathbf{p})$

Given a feasible solution $\mathbb{P}_\theta(\mathbf{c})$, $\forall \mathbf{c} \in \mathcal{C}$ of the large-sized primal linear program (3.46) for some distribution $\theta \in \Theta_u$, construct an optimal solution of the compact linear program in (3.47) as follows:

$$x_l = \sum_{\mathbf{c} \in \mathcal{C}: \sum_{t=1}^n c_t = l} \mathbb{P}_\theta(\mathbf{c}) \quad \forall l \in [n], \quad y_{li} = \sum_{\mathbf{c} \in \mathcal{C}: \sum_{t=1}^n c_t = l, c_i = 1} \mathbb{P}_\theta(\mathbf{c}) \quad \forall l \in [n], \forall i \in [n] \quad (3.54)$$

Using the fact that $\mathbb{P}_\theta(\tilde{c}_i = 1) = p_i$, $\forall i \in [n]$, it is straightforward to see that the interpretation satisfies the first constraint and next two constraint sets in (3.47), while the third constraint set is satisfied as follows:

$$\sum_{i=0}^n y_{li} = \sum_{i=0}^n \mathbb{P}_\theta\left(\sum_{t=1}^n \tilde{c}_t = l, \tilde{c}_i = 1\right) = l \mathbb{P}_\theta\left(\sum_{t=1}^n \tilde{c}_t = l\right) = l x_l, \quad \forall l \in [n],$$

Step (2): $\bar{P}_{uw}(n, k, \mathbf{p}) \geq \bar{P}_{uw}^c(n, k, \mathbf{p})$

Given a feasible solution x_l, y_{li} , $\forall l \in [n], \forall i \in [n]$ of the compact linear program (3.47), we can show that there exists a feasible solution of the large-sized linear program (3.46) that attains the same objective function value while satisfying the interpretation in (3.54). The proof is similar to that of Lemma 7 and we omit further details for the sake of brevity. \square

One of the criticism of considering tail probability functions of sums of extremally dependent random variables, is that the computed tight bounds $\bar{P}_u(n, \mathbf{w}, \mathbf{p})$ are often too conservative given that only the univariate marginal information of each random variable c_i is known. At the other end of the spectrum, mutually independent variables provide better bounds but are often impractical in many real-world situations. To offset the conservatism in our approach, we next consider introducing a limited degree of independence into our model by splitting the set of random variables into two sets, one of which contains extremally dependent variables while the other contains mutually independent variables. The two sets of variables are assumed independent of each other. We then show that under the given assumptions, the tail probability of the total sum of variables in both sets can be reformulated as a weighted tail probability function and thus the tightest bound on this tail probability can be computed by direct application of Theorem 12.

3.3.2 Applications to limited dependency

Consider two sets of Bernoulli random variables M_1 and M_2 of cardinality n_1 and n_2 as follows:

$$M_1 = \{\alpha_i : P(\tilde{\alpha}_i = 1) = p_i, i \in [n_1]\} \quad M_2 = \{\beta_j : P(\tilde{\beta}_j = 1) = p_{n_1+j}, j \in [n_2]\}$$

We assume that the variables in set M_1 are extremally dependent (there is no defined correlation between them), while the variables in M_2 are mutually independent. Further, we assume that the two sets of variables are independent of each other. We are interested in computing tail probability bounds on the total sum of variables of both sets. Denote the tightest upper bound on this tail probability as:

$$\bar{P}_\ell(n_1, n_2, k, \mathbf{p}) = \max_{\theta \in \Theta_\ell} \mathbb{P}_\theta \left(\sum_{i=1}^{n_1} \tilde{\alpha}_i + \sum_{j=1}^{n_2} \tilde{\beta}_j \geq k \right), \quad \forall k \in [n_1 + n_2] \quad (3.55)$$

where $\mathbf{p} = (p_1, p_2, \dots, p_{n_1+n_2})$ is the vector of concatenated probabilities and Θ_ℓ is the set of distributions consistent with the given assumptions:

$$\Theta_\ell = \left\{ \theta \in \Theta(\{0, 1\}^{n_1+n_2}) : \mathbb{P}_\theta((\boldsymbol{\alpha}, \boldsymbol{\beta})) = \mathbb{P}_\theta(\boldsymbol{\alpha}) \mathbb{P}_{\theta_{ind}}(\boldsymbol{\beta}), \quad \forall (\boldsymbol{\alpha}, \boldsymbol{\beta}) \in \{0, 1\}^{n_1+n_2} \right. \\ \left. \mathbb{P}_\theta(\tilde{\alpha}_i = 1) = p_i, \quad \forall i \in [n_1] \right\}.$$

where $(\boldsymbol{\alpha}, \boldsymbol{\beta})$ is the concatenated random vector of dimension $n_1 + n_2$ and θ_{ind} is the product distribution of the independent variables in M_2 supported on $\{0, 1\}^{n_2}$. We term this arrangement as *limited dependency* to indicate that the extremally dependent variables are restricted to the set M_1 . Note that for any feasible distribution $\theta \in \Theta_\ell$, since the variables in the sets M_1 and M_2 are independent of each other, we can write:

$$\mathbb{P}_\theta \left(\sum_{i=1}^{n_1} \tilde{\alpha}_i + \sum_{j=1}^{n_2} \tilde{\beta}_j \geq k \right) = \sum_{\ell=0}^{n_2} \left[\mathbb{P}_{\theta_\alpha} \left(\sum_{i=1}^{n_1} \tilde{\alpha}_i \geq k - \ell \right) \mathbb{P}_{\theta_{ind}} \left(\sum_{j=1}^{n_2} \tilde{\beta}_j = \ell \right) \right], \quad (3.56)$$

where θ_α is a feasible distribution in the set Θ_α of joint distributions of the variables in M_1 supported on $\{0, 1\}^{n_1}$ and consistent with the given univariate information, *i.e.*,

$$\Theta_\alpha = \{\theta_\alpha \in \Theta(\{0, 1\}^{n_1}) : \mathbb{P}_{\theta_\alpha}(\tilde{\alpha}_i = 1) = p_i, \forall i \in [n_1]\}.$$

Since the random variables in M_2 are Bernoulli and mutually independent, it is possible to compute $\mathbb{P}_{\theta_{ind}}(\sum_{j=1}^{n_2} \tilde{\beta}_j = \ell)$, $\ell \in [0, n_2]$ in polynomial time using a dynamic programming recursion as follows:

$$\mathbb{P}_{\theta_{ind}}\left(\sum_{j=1}^{n_2} \tilde{\beta}_j = \ell\right) = \mathbb{P}_{\theta_{ind}}\left(\sum_{j=1}^{n_2-1} \tilde{\beta}_j = \ell\right)\mathbb{P}(\tilde{\beta}_{n_2} = 0) + \mathbb{P}_{\theta_{ind}}\left(\sum_{j=1}^{n_2-1} \tilde{\beta}_j = \ell - 1\right)\mathbb{P}(\tilde{\beta}_{n_2} = 1), \quad \ell \in [n_2],$$

$$\text{where } n_2 \geq 2, \quad \mathbb{P}(\tilde{\beta}_j = 0) = 1 - p_{n_1+j}, \quad \mathbb{P}(\tilde{\beta}_j = 1) = p_{n_1+j}, \quad \forall j \in [n_2] \quad (3.57)$$

We also note that there is a one-one mapping between the set of feasible distributions in Θ_ℓ and Θ_α as follows:

$$\begin{aligned} \forall \theta_\alpha \in \Theta_\alpha, \exists \theta \in \Theta_\ell \mid \mathbb{P}_\theta((\alpha, \beta)) &= \mathbb{P}_{\theta_\alpha}(\alpha) \times \mathbb{P}_{\theta_{ind}}(\beta), \quad \forall (\alpha, \beta) \in \{0, 1\}^{n_1+n_2} \\ \forall \theta \in \Theta_\ell, \exists \theta_\alpha \in \Theta_\alpha \mid \mathbb{P}_{\theta_\alpha}(\alpha) &= \sum_{\beta \in \{0, 1\}^{n_2}} \mathbb{P}_\theta((\alpha, \beta)), \quad \forall \alpha \in \{0, 1\}^{n_1} \end{aligned}$$

where \times indicates the cross product of the probability masses in the two joint distributions considered. Thus, the extremal distribution $\theta^* \in \Theta_\ell$ that maximizes the right hand side of (3.56) will correspond to the extremal distribution $\theta_\alpha^* \in \Theta_\alpha$ that maximizes the right hand side, through the relation $\theta^* = \theta_\alpha^* \times \theta_{ind}$. Hence we can reformulate (3.55) as follows:

$$\begin{aligned} \bar{P}_\ell(n_1, n_2, k, \mathbf{p}) &= \max_{\theta \in \Theta_\ell} \mathbb{P}_\theta\left(\sum_{i=1}^{n_1} \tilde{\alpha}_i + \sum_{j=1}^{n_2} \tilde{\beta}_j \geq k\right) \\ &= \max_{\theta_\alpha \in \Theta_\alpha} \sum_{\ell=0}^{n_2} \left[\mathbb{P}_{\theta_\alpha}\left(\sum_{i=1}^{n_1} \tilde{\alpha}_i \geq k - \ell\right) \mathbb{P}_{\theta_{ind}}\left(\sum_{j=1}^{n_2} \tilde{\beta}_j = \ell\right) \right], \end{aligned} \quad (3.58)$$

By re-writing the tail probabilities as $\mathbb{P}_{\theta_\alpha}(\sum_{i=1}^{n_1} \tilde{\alpha}_i \geq k - \ell) = \sum_{r=k-\ell}^{n_1} \mathbb{P}_{\theta_\alpha}(\sum_{i=1}^{n_1} \tilde{\alpha}_i = r)$ we can cast (3.58) in the form of a weighted tail probability function (similar to that in (3.46)) with n_1 decision variables. It can be shown that the corresponding weights w_ℓ , $\forall \ell \in [0, n_1]$ are:

$$w_\ell = \begin{cases} \begin{cases} \Phi(n_2 - k + \ell), & 0 \leq \ell \leq k - 1, \\ 1, & k \leq \ell \leq n_1 \end{cases}, & k < \min(n_1, n_2) \\ \Phi(n_2 - k + \ell), & 0 \leq \ell \leq n_1, & n_1 \leq k \leq n_2 \\ \begin{cases} \Phi(n_2 - k + \ell), & k - n_2 \leq \ell \leq k - 1, \\ 1, & k \leq \ell \leq n_1 \end{cases}, & n_2 \leq k \leq n_1 \\ \Phi(n_2 - k + \ell), & k - n_2 \leq \ell \leq n_1, & k > \max(n_1, n_2) \end{cases}$$

where

$$\Phi(r) = \sum_{i=0}^r \mathbb{P}\left(\sum_{j=1}^{n_2} \tilde{\beta}_j = n_2 - i\right), \quad 0 \leq r \leq n_2$$

is the reverse cumulative sum (up to index r) of the independent tail probabilities computed using (3.57) and $\Phi(n_2) = 1$. The compact linear program (3.47) can now be directly used with $n = n_1$, $\mathbf{p} = (p_1, p_2, \dots, p_{n_1})$ and the weights defined above to compute $\bar{P}_\ell(n_1, n_2, k, \mathbf{p})$ even for relatively large values of n as demonstrated in the numerical results below.

Other related bounds:

Denote the total number of variables in (α, β) by $n = n_1 + n_2$. We first consider the two extremes of the *limited dependency*, i.e., extremal dependence and complete independence. When $n_1 = n$, all the random variables are extremally dependent ($\Theta_\ell = \Theta_u$) and the tight bound $\bar{P}_u(n, k, \mathbf{p})$ is retrieved. Similarly, when $n_2 = n$, all the variables are mutually independent and the tail probability bound $P_{ind}(n, k, \mathbf{p})$, computed using the dynamic program recursion in (3.57) is retrieved. These bounds must satisfy the relation:

$$P_{ind}(n, k, \mathbf{p}) \leq \bar{P}_\ell(n_1, n_2, k, \mathbf{p}) \leq \bar{P}_u(n, k, \mathbf{p}), \quad \forall n_1, n_2 : 1 \leq n_1 \leq n, n_2 = n - n_1$$

We additionally compare these bounds with the following three valid upper bounds on the tail probability $\mathbb{P}(\sum_{i=1}^n \tilde{c}_i \geq k)$ for $k \in [n]$:

$$\begin{aligned} \text{Poisson approximation: } & \sum_{r=k}^n e^{-\lambda} \frac{\lambda^r}{r!} \\ \text{Comonotonic bound: } & \sum_{r=k}^n p_{(n-r+1)} - p_{(n-r)} = p_{(n-k+1)} \\ \text{Markov bound: } & \frac{\sum_{i=1}^n p_i}{k} \end{aligned} \tag{3.59}$$

where $\lambda = \mathbb{E}[\sum_{i=1}^n \tilde{c}_i] = \sum_{i=1}^n p_i$ and $p_{(i)}$ is the i^{th} order statistic of the marginal probability vector \mathbf{p} when its components are arranged in ascending order. Le Cam (1960) showed that the Poisson distribution can be used to approximate the probability distribution of sums of *non-identical* independent Bernoulli random variables (Poisson binomial distribution), where the error is minimal when the probabilities are small. The Chen-Stein (see Stein, 1972; Chen, 1975) approximation method extends this idea to compute error bounds for the Poisson approximation of the distribution of sums of dependent Bernoulli variables. This method provides the best approximation when the probabilities are small and the variables are close to being independent. The utility and far-reaching impact of the Chen-Stein method has been illustrated through several applications in graph theory, combinatorics, molecular biology (see Arratia, Goldstein, and Gordon, 1990, for a non-exhaustive list of examples). The comonotonic distribution is known to be extremal for supermodular functions (Tchen, 1980; Müller, 1997). However in our context, for the tail probability function, it provides a valid lower bound on $\bar{P}_u(n, k, \mathbf{p})$. Similarly the Markov bound is known to be tight for identical extremally

dependent Bernoulli variables (Rüger, 1978), but in our context provides a valid upper bound on $\bar{P}_u(n, k, \mathbf{p})$.

Numerical results with limited dependency

In this section, we compare our *limited dependency* bounds computed from the compact linear program (3.47) with the two extremes of extremal dependency and complete independence and the three bounds in (3.59). Figure 3.6 shows the six bounds for $n = 30$ variables where the *limited dependency* bounds (in purple) have been selectively shown for $n_1 = 6, 10, 14, 18, 22, 26$ (left to right). In Figure 3.6a, we consider non-identical small marginal probabilities by uniformly and independently generating the entries of \mathbf{p} between 0.1 and 0.15 while in Figure 3.6b, we uniformly generate the probabilities in $[0, 1]$.

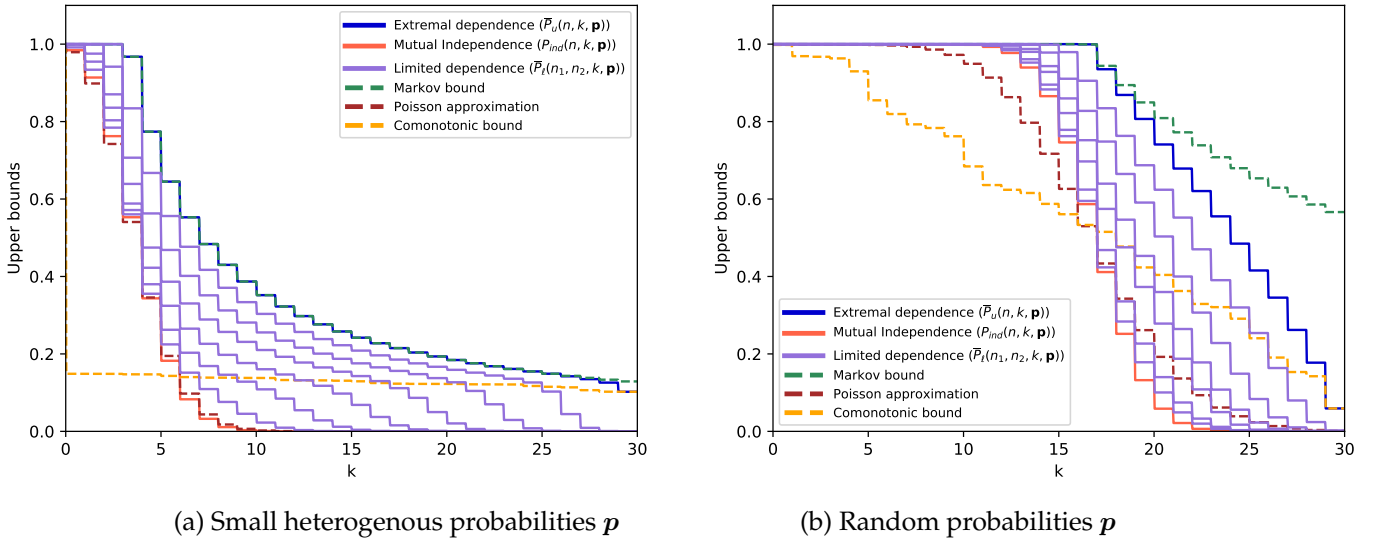


FIGURE 3.6: Limited dependency: Step plots of upper bounds with $n = 30$

It can be observed from both figures that with change in n_1, n_2 , the limited dependency bounds $\bar{P}_\ell(n_1, n_2, k, \mathbf{p})$ move away faster from the extremally dependent bound $\bar{P}_u(n, k, \mathbf{p})$ than from the independent tail probability $P_{ind}(n, k, \mathbf{p})$. More specifically, when n_1 changes from n to $n - 1$, there is a larger deviation of $\bar{P}_\ell(n_1, n_2, k, \mathbf{p})$ from $\bar{P}_u(n, k, \mathbf{p})$ (in blue) than from $P_{ind}(n, k, \mathbf{p})$ (in red), when n_2 changes from n to $n - 1$. In other words, introducing a small degree of independence into the extremal dependence model has a larger impact on the extremal tail probability than by introducing a small degree of dependence into the mutual independence model. As a sanity check, it was observed that when $n_2 = n - 1$, there is exactly one variable $\alpha_1 \in M_1$ and since it is independent of all variables in M_2 , the entire set of variables M is independent and thus we retrieve the bound $P_{ind}(n, k, \mathbf{p})$.

The Poisson approximation closely follows the independent tail probability $P_{ind}(n, k, \mathbf{p})$ in Figure 3.6a due to the assumption of small probabilities while in Figure 3.6b, it initially underestimates the independent tail probability (for $k \leq 15$) and then overestimates it while remaining close to the limited dependency bounds with high degree of independence (n_2 close to n). This observation is consistent with the results in the

literature which state that the Poisson approximation provides better approximations of tail probabilities when the variables are close to being independent (see Section 4 in Chen, 1975). Due to the almost identical nature of the small probabilities in Figure 3.6a, the comonotonic bound plot remains almost flat for $k \geq 1$ and the Markov bound is very close to the extremally dependent bound $P_u(n, k, \mathbf{p})$ while this is not true in Figure 3.6b due to the non-identical probabilities.

We next provide a more comprehensive view of Figure 3.6 with 3D plots of the absolute deviation of the *limited dependency* bounds from $\bar{P}_u(n, k, \mathbf{p})$ and $\bar{P}_{ind}(n, k, \mathbf{p})$ (over an added dimension n_1).

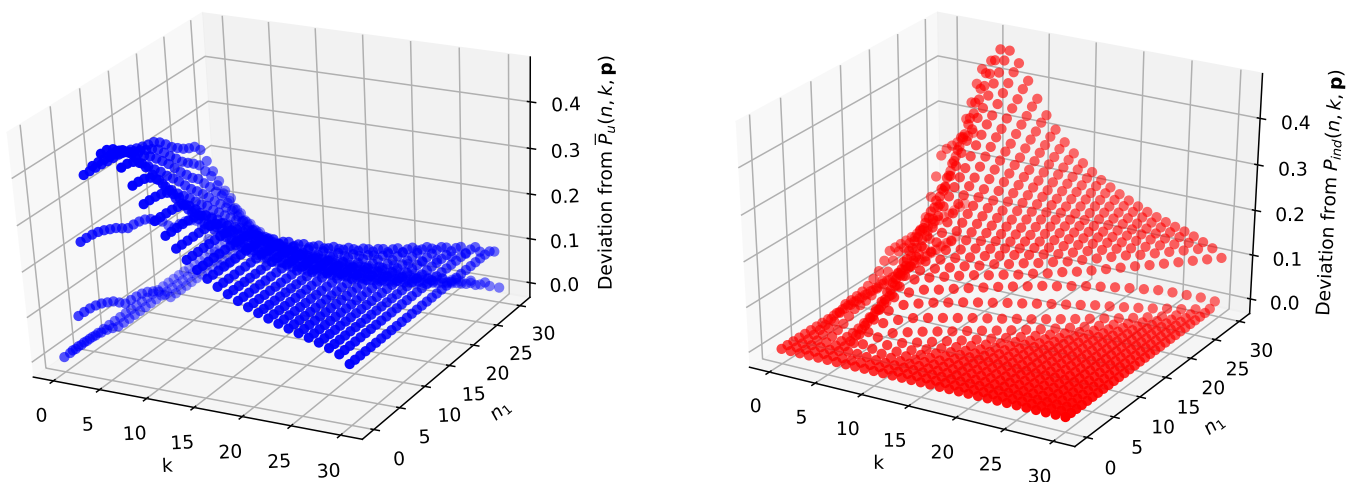


FIGURE 3.7: 3D plots of absolute deviation from extremal dependency bounds (left) and independent tail probability (right) with $n = 30$, small heterogeneous probabilities \mathbf{p}

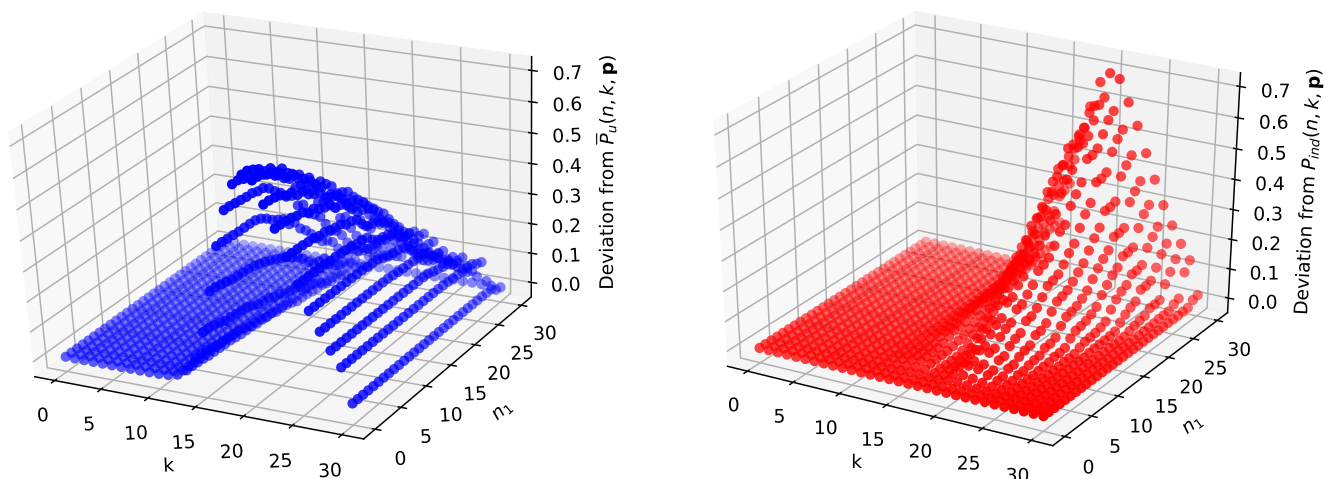


FIGURE 3.8: 3D plots of absolute deviation from extremal dependency bounds (left) and independent tail probability (right) with $n = 30$, random probabilities \mathbf{p}

Figures 3.7 and 3.8 show the plots with randomly generated non-identical small marginals \mathbf{p} and general probabilities $\mathbf{p} \in [0, 1]^n$ respectively. The deviation in both

figures is significant when the bounds being compared are *non-trivial*, i.e., when at least one of them is not zero or trivially one. The deviation starts increasing from a certain k and reaches a peak before decreasing as both bounds tend to zero. This peak is reached much earlier (for $k \leq n/2$) in Figure 3.7 than in Figure 3.8 (for $k \geq n/2$) due to the small probabilities. The observation made in Figure 3.6 that introducing a small degree of independence into the extremal dependence model has a larger impact on the extremal tail probability than by introducing a small degree of dependence into the mutual independence model is corroborated in both the 3D plots, where with $n_1 = 29$ the deviation from $\bar{P}_u(n, k, \mathbf{p})$ (left plots in blue) is already significant while with $n_1 = 1$, the deviation from $\bar{P}_{ind}(n, k, \mathbf{p})$ (right plots in red) is still close to zero.

3.4 Bounds on expected stop-loss functions

In this section, we revisit the objective with expected stop-loss functions considered in Section 2.7.3, but in the context of extremally dependent random variables. We denote the tight upper bound on the expected stop-loss function over the set of distributions θ in the univariate ambiguity set Θ_u as:

$$\bar{E}_u(n, k, \mathbf{p}) = \max_{\theta \in \Theta_u} \mathbb{E}_\theta \left[\left(\sum_{j=1}^n \tilde{c}_j - k \right)^+ \right], \quad \forall k \in [n]$$

which can be computed as the optimal value of the following exponential-sized linear program:

$$\begin{aligned} \bar{E}_u(n, k, \mathbf{p}) = \max \quad & \mathbb{E} \left[\left(\sum_{j=1}^n \tilde{c}_j - k \right)^+ \right] \\ \text{s.t.} \quad & \sum_{\mathbf{c} \in \mathcal{C}: c_i=1} \mathbb{P}(\mathbf{c}) = p_i, \quad \forall i \in [n], \\ & \sum_{\mathbf{c} \in \mathcal{C}} \mathbb{P}(\mathbf{c}) = 1, \\ & \mathbb{P}(\mathbf{c}) \geq 0 \quad \forall \mathbf{c} \in \mathcal{C} \end{aligned} \quad (3.60)$$

Expected value functions like that in (3.60) involving sums of extremally dependent Bernoulli random variables find application in many problems. For example, c_i could represent the uncertain scenario where the loss accrued from the i^{th} financial instrument exceeds a given limit with a probability p_i , where the correlation between the instruments is assumed to be unknown. Then, $\bar{E}_u(n, k, \mathbf{p})$ represents the maximum possible average number of non-viable extremally dependent instruments exceeding a threshold k . For further details, we refer the interested reader to Dhaene et al. (2002b), who provide a comprehensive overview of the actuarial theory on this topic while Dhaene et al. (2002a) demonstrate their usefulness in several financial and actuarial applications.

This next theorem derives $\bar{E}_u(n, k, \mathbf{p})$ as the optimal value of a compact linear program, using familiar techniques of considering the linear relaxation of the dual separation problem, as used throughout this chapter. We further use this compact linear program to retrieve a familiar closed-form expression for $\bar{E}_u(n, k, \mathbf{p})$ in Theorem 14.

3.4.1 Compact linear program and primal proof of correctness

Theorem 13. *The exponential-sized linear program in (3.60) is equivalent to the following compact linear program:*

$$\begin{aligned} \bar{E}_u(n, k, \mathbf{p}) = \max \quad & \sum_{i=1}^n y_i - ky_0 \\ \text{s.t.} \quad & 0 \leq y_0 - y_i \leq 1 - p_i, \quad \forall i \in [n], \\ & 0 \leq y_i \leq p_i, \quad \forall i \in [n], \\ & \sum_{i=1}^n y_i \geq ky_0 \end{aligned} \quad (3.61)$$

Proof. Since it is only the objective function which has changed from probability in (3.1) to expectation in (3.60), the proof broadly parallels that of Theorem 8 and thus we only preserve the most important steps and highlight differences for the purpose of exposition. Consider the dual of the large-sized linear program (3.60):

$$\begin{aligned} \bar{P}_u(n, k, \mathbf{p}) = \min \quad & \sum_{i=1}^n \lambda_i p_i + \lambda_0 \\ \text{s.t.} \quad & \sum_{i=1}^n \lambda_i c_i + \lambda_0 \geq \left(\sum_{j=1}^n c_j - k \right)^+, \quad \forall \mathbf{c} \in \mathcal{C}, \\ & \lambda_i \text{ free}, \quad \forall i \in [n], \\ & \lambda_0 \text{ free} \end{aligned} \quad (3.62)$$

Splitting the dual (3.62) constraints into two parts we have:

$$\sum_{i=1}^n \lambda_i c_i + \lambda_0 \geq 0 \quad \forall \mathbf{c} \in \mathcal{C} \quad (3.63a)$$

$$\sum_{i=1}^n \lambda_i c_i + \lambda_0 \geq \left(\sum_{j=1}^n c_j - k \right) \quad \forall \mathbf{c} \in \mathcal{C} : \sum_{i=1}^n c_i \geq k \quad (3.63b)$$

As usual, we next convert both the above constraint sets into optimization problems with $\{c_i, i \in [n]\}$ as decision variables for fixed $\{\lambda_0, \lambda_i, i \in [n]\}$. The first constraint set is exactly the same as in (3.5a) and thus handled identically.

The second constraint set (3.63b) can be similarly transformed as:

$$\lambda_0 + k + \left\{ \min \sum_{i=1}^n (\lambda_i - 1) c_i : \sum_{i=1}^n c_i \geq k, 0 \leq c_i \leq 1, \forall i \in [n] \right\} \geq 0 \quad (3.64)$$

where once again, the linear program relaxation yields integer extreme points due to the totally unimodular structure of the constraint set.

Dualizing the linear program relaxations and forcing a single instance to satisfy the resulting dual as in (3.8) and (3.10), and replacing both constraint sets (3.63a) and (3.63b) by the resultant compact set of equations, the transformed version of the dual (3.62) is:

$$\begin{aligned}
\min \quad & \sum_{i=1}^n \lambda_i p_i + \lambda_0 \\
\text{s.t.} \quad & \lambda_0 - \sum_{i=1}^n w_i \geq 0, \\
& \lambda_0 + k v_0 - \sum_{i=1}^n v_i + k \geq 0, \\
& \lambda_i + w_i \geq 0, & \forall i \in [n], \\
& \lambda_i + v_i - v_0 - 1 \geq 0, & \forall i \in [n], \\
& w_i \geq 0, & \forall i \in [n], \\
& v_i \geq 0, & \forall i \in [n], \\
& v_0 \geq 0
\end{aligned} \tag{3.65}$$

Finally, we dualize (3.65) to get exactly the same linear program as (3.12) except that the objective function is $\sum_{i=1}^n y_i - k y_0$ instead of y_0 . Eliminating redundant variables $x_0, x_i, \forall i \in [n]$, we obtain the compact primal linear program (3.61). \square

Primal proof of correctness

Similar to earlier sections, we can prove the direct equivalence of the large-size and compact primal linear program formulations with the expected stop-loss objective without going through the dual formulations, where the interpretation of the decision variables of the compact primal formulation is exactly similar to that of the tail probability objective function in Lemma 7.

Proposition 10. *The large-sized primal linear program (3.60) is equivalent to the compact primal linear program (3.61), where for any extremal distribution $\theta^* \in \Theta_u$ of the large-sized linear program and any $k \in [n]$, the corresponding optimal solution (y_0, y_1, \dots, y_n) of the compact linear program satisfies*

$$\begin{aligned}
y_0 &= \mathbb{P}_{\theta^*} \left(\sum_{t=1}^n \tilde{c}_t \geq k \right) \\
y_i &= \mathbb{P}_{\theta^*} \left(\sum_{t=1}^n \tilde{c}_t \geq k, \tilde{c}_i = 1 \right), \quad \forall i \in [n]
\end{aligned} \tag{3.66}$$

Proof. Given a feasible solution $\mathbb{P}_\theta(\mathbf{c})$, $\forall \mathbf{c} \in \mathcal{C}$ to the exponential-sized linear program (3.60) for some $\theta \in \Theta_u$, construct a feasible solution of the compact linear program by aggregating the probabilities exactly similar to that of the tail probability objective in (3.15). The objective function of the compact linear program (3.61) can be written as

$$\begin{aligned}
\sum_{i=1}^n y_i - k y_0 &= \sum_{i=1}^n \mathbb{P}_\theta \left(\sum_{t=1}^n \tilde{c}_t \geq k, \tilde{c}_i = 1 \right) - k \mathbb{P}_\theta \left(\sum_{t=1}^n \tilde{c}_t \geq k \right) \\
&= \sum_{\ell=k}^n \sum_{i=1}^n \mathbb{P}_\theta \left(\sum_{t=1}^n \tilde{c}_t = \ell, \tilde{c}_i = 1 \right) - k \sum_{\ell=k}^n \mathbb{P}_\theta \left(\sum_{t=1}^n \tilde{c}_t = \ell \right) \\
&= \sum_{\ell=k}^n \ell \mathbb{P}_\theta \left(\sum_{t=1}^n \tilde{c}_t = \ell \right) - k \sum_{\ell=k}^n \mathbb{P}_\theta \left(\sum_{t=1}^n \tilde{c}_t = \ell \right) \\
&= \mathbb{E}_\theta \left[\left(\sum_{j=1}^n \tilde{c}_j - k \right)^+ \right]
\end{aligned}$$

which coincides with that of the exponential-sized linear program (3.60). The rest of the proof follows that of Lemma 7 and we omit further details here for the sake of brevity. \square

The next theorem uses the compact linear program formulation derived in Theorem 13 to retrieve a well-known closed-form expression for $\bar{E}_u(n, k, \mathbf{p})$.

Theorem 14. (Dhaene et al., 2000) Sort the probabilities in increasing value as $0 \leq p_1 \leq p_2 \leq \dots \leq p_n \leq 1$. Then, the tight upper bound $\bar{E}_u(n, k, \mathbf{p})$ admits a closed-form expression in the form of the comonotonic bound, i.e.,

$$\bar{E}_u(n, k, \mathbf{p}) = \sum_{i=1}^{n-k} p_i, \quad k \in [n] \quad (3.67)$$

Proof. We consider the dual of the compact linear program (3.61) as follows:

$$\begin{aligned} \bar{E}_u(n, k, \mathbf{p}) = \min \quad & \sum_{i=1}^n w_i p_i + \sum_{i=1}^n v_i (1 - p_i) \\ \text{s.t.} \quad & \sum_{i=1}^n v_i - \sum_{i=1}^n u_i + k\lambda + k \geq 0 \\ & u_i - v_i + w_i - \lambda - 1 \geq 0, \quad \forall i \in [n], \\ & u_i \geq 0, \quad \forall i \in [n], \\ & v_i \geq 0, \quad \forall i \in [n], \\ & w_i \geq 0, \quad \forall i \in [n], \\ & \lambda \geq 0 \end{aligned} \quad (3.68)$$

Table 3.3 provides an optimal solution of the compact primal-dual linear program pair (3.61)-(3.68) that attains the comonotonic closed-form bound in Theorem 14.

Range of k	Primal optimal solution (3.61)	Dual optimal solution (3.68)	Optimum attained ($\bar{E}_u(n, k, \mathbf{p})$)
$k \in [n]$	$y_i = \begin{cases} p_i, & i \leq n - k \\ p_{n-k+1}, & i \geq n - k + 1 \end{cases}$ $y_0 = p_{n-k+1}$	$w_i = \begin{cases} 1, & i \leq n - k \\ 0, & i \geq n - k + 1 \end{cases}$ $\begin{aligned} u_i &= 1 - w_i, \quad \forall i \in [n], \\ v_i &= 0, \quad \forall i \in [n], \\ \lambda &= 0 \end{aligned}$	$\sum_{i=1}^{n-k} p_i$
$k = 0$	$\begin{aligned} y_i &= p_i, \quad \forall i \in [n], \\ y_0 &= 1 \end{aligned}$	$\begin{aligned} u_i &= 0, \quad \forall i \in [n], \\ v_i &= 0, \quad \forall i \in [n], \\ w_i &= 1, \quad \forall i \in [n], \\ \lambda &= 0 \end{aligned}$	$\sum_{i=1}^n p_i$

TABLE 3.3: Optimal solution that attains the comonotonic bound (3.67)

It can be easily verified that the above solutions are both primal and dual feasible and attain the desired bound.

Connection to earlier work: Expected value functions like that in (3.60) involve sums of random variables which are commonly encountered in many applied problems. With continuous random variables whose marginal distributions are known, Dhaene et al. (2002b) and Dhaene et al. (2002a) provide interesting results with applications in actuarial science and mathematical finance. The fact that the comonotonic copula forms the extremal distribution for the expected stop-loss objective function in (3.60) over the set of distributions $\theta \in \Theta_u$ is well known in the literature. While Tchen (1980) and Müller (1997) provide proofs using properties of supermodular functions, Dhaene et al. (2000) and Dhaene et al. (2002b) provide alternative proofs (see Section 5 of Dhaene et al., 2002b, and references therein for other proofs). However, the use of the compact linear programming formulation in (3.61) to derive this bound does not appear in the literature to the best of our knowledge. \square

3.4.2 Lower bounds

We now extend the results of the previous section to show that the corresponding lower bounds on the expected stop-loss functions can be similarly computed. Denote by $\underline{E}_u(n, k, \mathbf{p})$ the tight lower bound on this function over the set of distributions θ in the univariate ambiguity set Θ_u , i.e.,

$$\underline{E}_u(n, k, \mathbf{p}) = \min_{\theta \in \Theta_u} \mathbb{E}_\theta \left[\left(\sum_{j=1}^n \tilde{c}_j - k \right)^+ \right], \quad \forall k \in [n]$$

Corollary 8. *The tight lower bound $\underline{E}_u(n, k, \mathbf{p})$ can be computed as the optimal value of the following compact linear program:*

$$\begin{aligned} \underline{E}_u(n, k, \mathbf{p}) = \min \quad & \sum_{i=1}^n y_i - ky_0 \\ \text{s.t.} \quad & 0 \leq y_0 - y_i \leq 1 - p_i, \quad \forall i \in [n], \\ & 0 \leq y_i \leq p_i, \quad \forall i \in [n], \\ & \sum_{i=1}^n y_i \geq ky_0 + (S_1 - k)^+ \end{aligned} \quad (3.69)$$

where $S_1 = \mathbb{E}(\sum_{i=1}^n \tilde{c}_i) = \sum_{i=1}^n p_i$ is the first binomial moment.

Proof. We first write down the dual of the minimization version of (3.60) which computes the tight lower bound as its optimum value:

$$\begin{aligned} \underline{E}_u(n, k, \mathbf{p}) = \max \quad & \sum_{i=1}^n \lambda_i p_i + \lambda_0 \\ \text{s.t.} \quad & \sum_{i=1}^n \lambda_i c_i + \lambda_0 \leq \left(\sum_{j=1}^n c_j - k \right)^+, \quad \forall \mathbf{c} \in \mathcal{C}, \\ & \lambda_i \text{ free} \quad \forall i \in [n], \\ & \lambda_0 \text{ free} \end{aligned} \quad (3.70)$$

The constraints in the dual (3.70) can be split up as follows:

$$\sum_{i=1}^n \lambda_i c_i + \lambda_0 \leq 0, \quad \forall c \in \mathcal{C} : \sum_{i=1}^n c_i \leq k \quad (3.71a)$$

$$\sum_{i=1}^n \lambda_i c_i + \lambda_0 \leq \left(\sum_{j=1}^n c_j - k \right), \quad \forall c \in \mathcal{C} : \sum_{i=1}^n c_i \geq k \quad (3.71b)$$

Note that we are forced to retain the k in both the above two sets of constraints unlike in (3.24a)-(3.24b) where we could absorb k into (3.24a) only. This is because the inequalities here do not have a constant term like 1 (which appears due to the probability objective in (3.24b)) on the right hand side, but rather a function of the random vector \tilde{c} in the form of $\sum_{j=1}^n c_j - k$. Thus, there is no constant value which can upper bound the left hand side of (3.71b) for all $c \in \mathcal{C}$. We now proceed in similar steps as earlier for the upper bound but reformulate the above constraint sets as maximization problems instead of minimization:

$$\lambda_0 + \left\{ \max \sum_{i=1}^n \lambda_i c_i : \sum_{i=1}^n c_i \leq k, 0 \leq c_i \leq 1, \forall i \in [n] \right\} \leq 0$$

$$\lambda_0 + k + \left\{ \max \sum_{i=1}^n (\lambda_i - 1) c_i : \sum_{i=1}^n c_i \geq k, 0 \leq c_i \leq 1, \forall i \in [n] \right\} \leq 0$$

where once again, the linear program relaxation yields integer extreme points due to the totally unimodular structure of the constraint set. Similar techniques of dualizing and forcing a single instance to satisfy the resulting dual leads us to the following primal:

$$\begin{aligned} \min \quad & \sum_{i=1}^n y_i - k y_0 \\ \text{s.t.} \quad & x_0 + y_0 = 1, \\ & x_i + y_i = p_i, \quad \forall i \in [n], \\ & x_0 - x_i \geq 0, \quad \forall i \in [n], \\ & y_0 - y_i \geq 0, \quad \forall i \in [n], \\ & \sum_{i=1}^n y_i \geq k y_0 \\ & \sum_{i=1}^n x_i \leq k x_0 \\ & x_i \geq 0, \quad \forall i \in [n], \\ & y_i \geq 0, \quad \forall i \in [n], \\ & x_0 \geq 0, \\ & y_0 \geq 0 \end{aligned} \quad (3.72)$$

Note the similarities and differences in structure of (3.72) to (3.13) with an additional constraint $\sum_{i=1}^n x_i \leq k x_0$ and the different objective along with being a minimization problem instead of maximization. The compact linear program (3.69) whose feasible

region is very similar to that of (3.61) except the extra $(S_1 - k)^+$ term in the last constraint, then follows by eliminating the $x_0, x_i, i \in [n]$ variables. \square

Theorem 15. *The tight lower bound $\underline{E}_u(n, k, \mathbf{p})$ admits a closed-form expression in the form of the Jensen (1906) bound, i.e.,*

$$\underline{E}_u(n, k, \mathbf{p}) = (S_1 - k)^+, \quad k \in [n] \quad (3.73)$$

Proof. We consider the dual of the compact linear program (3.69) as follows:

$$\begin{aligned} \bar{E}_u(n, k, \mathbf{p}) = \min \quad & \lambda(S_1 - k)^+ - \sum_{i=1}^n w_i p_i - \sum_{i=1}^n v_i(1 - p_i) \\ \text{s.t.} \quad & \sum_{i=1}^n v_i - \sum_{i=1}^n u_i + k\lambda - k \geq 0 \\ & u_i - v_i + w_i - \lambda + 1 \geq 0, \quad \forall i \in [n], \quad (3.74) \\ & u_i \geq 0, \quad \forall i \in [n], \\ & v_i \geq 0, \quad \forall i \in [n], \\ & w_i \geq 0, \quad \forall i \in [n], \\ & \lambda \geq 0 \end{aligned}$$

Table 3.4 shows that there exists an optimal solution of the compact primal-dual linear program pair (3.69)-(3.74) that attains the Jensen (1906) bound.

Range of k	Primal optimal solution (3.69)	Dual optimal solution (3.74)	Optimum attained ($\underline{E}_u(n, k, \mathbf{p})$)
$k \leq S_1$	$y_i = p_i, \quad \forall i \in [n],$ $y_0 = 1$	$\lambda = 1,$ $u_i = 0, \quad \forall i \in [n],$ $v_i = 0, \quad \forall i \in [n],$ $w_i = 0, \quad \forall i \in [n]$	$S_1 - k$
$k > S_1$	$y_i = 0, \quad \forall i \in [n],$ $y_0 = 0$	$\lambda = 1$ $u_i = 0, \quad \forall i \in [n],$ $v_i = 0, \quad \forall i \in [n],$ $w_i = 0, \quad \forall i \in [n]$	0

TABLE 3.4: Optimal solution that attains Jensen (1906) bound (3.73)

It can be easily verified that the above solutions are both primal and dual feasible and attain the desired bound. \square

Connection to earlier work: It can be verified that the following aggregated linear program proposed by Boros and Prékopa (1989):

$$\begin{aligned}
 BP_u(n, k, \mathbf{p}) = \min & \sum_{\ell=k+1}^n (\ell - k)v_\ell \\
 \text{s.t.} & \sum_{\ell=1}^n \ell v_\ell = S_1 \\
 & \sum_{\ell=0}^n v_\ell = 1 \\
 & v_\ell \geq 0, \quad \forall \ell \in [0, n],
 \end{aligned} \tag{3.75}$$

also attains the Jensen (1906) bound with the primal and dual feasible basis indices

$$\{i, j\} : i = \lfloor S_1 \rfloor, j = \lceil S_1 \rceil.$$

However, the tightness of the bound with general disaggregated univariate probabilities as shown in Theorem 15 does not seem to be explicitly known to the best of our knowledge. We also note that the corresponding maximization version of the aggregated linear program in (3.75) does not attain the upper bound in Theorem 14 unless the marginals are identical, since the comonotonic bound needs more information (than that provided by the first binomial moment S_1) for general non-identical marginals.

3.5 Summary of Part I and future directions

This section summarizes the results in Part I of this dissertation and provides some useful directions for future research. Table 3.5 provides a high-level view of the most important results.

Tail Probability / Expected stop-loss functions	Extremal dependence	Pairwise independence		t -wise independence ($t \geq 3$)
	General probabilities $p \in [0, 1]^n$	Identical probabilities $p \in [0, 1]$	General probabilities $p \in [0, 1]^n$	Identical probabilities $p \in [0, 1]$
\max $\mathbb{P}(\sum_{t=1}^n c_t \geq k)$	Bernoulli variables	Boros and Prékopa (1989) \checkmark^*	$k = 1$	Boros and Prékopa (1989) \checkmark^*
	Rüger (1978) \checkmark		Hunter (1976)-Worsley (1982) \checkmark^*	
	Discrete variables		$k \geq 2$ (Improved bounds)	
	Ramachandra and Natarajan (2021) \checkmark^{**}		Ramachandra and Natarajan (2021) \checkmark^{**}	
\min $\mathbb{P}(\sum_{t=1}^n c_t \geq k)$	Rüger (1981) \checkmark	Boros and Prékopa (1989) \checkmark^*	$k = 1$ Bonferroni (1936) (Tight for small probabilities only) \checkmark^*	Boros and Prékopa (1989) \checkmark^*
\max / \min $\sum_{l=0}^n w_l \mathbb{P}_\theta(\sum_{i=1}^n \tilde{c}_i \geq l)$	Ramachandra and Natarajan (2021) \checkmark^{**}			
\max $\mathbb{E}\left[\left(\sum_{t=1}^n c_t - k\right)^+\right]$	Dhaene et al. (2000) (comonotonic bound) \checkmark	Ninh, Hu, and Allen (2019) \checkmark^*		Boros and Prékopa (1989) \checkmark^*
\min $\mathbb{E}\left[\left(\sum_{t=1}^n c_t - k\right)^+\right]$	Jensen (1906) \checkmark^*	Ninh, Hu, and Allen (2019) \checkmark^*		Boros and Prékopa (1989) \checkmark^*

\checkmark : Earlier known tight closed-form bound with alternative proof \checkmark^* : Closed-form bound known but tightness unknown
 \checkmark^{**} : Unknown closed-form bound \checkmark^{**} : Known linear program bound but tightness unknown, \checkmark^{**} : Unknown linear program bound

TABLE 3.5: Summary of tight bounds in Part I

Summary:

The results in Table 3.5 can be categorized as follows:

i) *Closed-form bounds that are known in the literature and whose tightness is also established under the given input assumptions (indicated with \checkmark):*

Bounds such as Rüger (1978), Rüger (1981), and Dhaene et al. (2000) are known to be tight when only the univariate marginal probabilities are known. In this case, we provided alternative proofs in Sections 3.1.1 and 3.4, that involved deriving a compact linear programming formulation, whose optimal solution could be captured as a closed-form expression.

ii) *Closed-form bounds that are known in the literature but whose tightness under assumptions of extremal dependence or pairwise independence has not been established (indicated with \checkmark^*):*

Closed-form bounds such as Jensen (1906), Bonferroni (1936), Boros and Prékopa (1989), and Ninh, Hu, and Allen (2019) can be expressed in terms of the binomial moments alone. While they are known to be tight with such aggregated information, we additionally proved their tightness in some special instances of disaggregated information such as when the variables are identical, extremally dependent or pairwise independent in Sections 3.4.2, 2.6, 2.4.1 and 2.7.3 respectively. The Hunter (1976)-Worsley (1982) bound in (2.15) requires more information than these aggregated bounds (such as the sum of bivariate probabilities in each spanning tree on the complete graph), and it was shown to be tight with pairwise independent variables for any marginal vector $\mathbf{p} \in [0, 1]^n$. To the best of our knowledge, this result is not known thus far in the literature dedicated to this topic. In fact, paraphrasing from Boros et al. (2014) (section 1.2), “As far as we know, in spite of the several studies dedicated to this problem, the complexity status of this problem, for feasible input, seems to be still open even for bivariate probabilities”. With pairwise independent random variables, feasibility is guaranteed and Theorem 2 shows that the tightest upper bound is computable in polynomial time (in fact in a simple closed form), thus providing a partial positive answer towards this question.

iii) *Closed-form bounds derived in our work that do not appear to be known in the literature and which are not necessarily tight (indicated with \checkmark^{**}):*

In Theorem 11 and Corollary 6 of Section 3.2, we derived closed-form upper bounds on the tail probability of the sum of identical discrete integer-valued random variables which do not appear to be known in the literature. Numerical illustrations in Example 9 demonstrated that these upper bounds are tight in many instances for identical and symmetric identical marginals. In Section 2.3, for $k \geq 2$, we proposed new bounds exploiting ordering of the probabilities, which are at least as good as the unordered bounds. To the best of our knowledge the idea of ordering has not been exploited thus far to tighten probability bounds for pairwise independent random variables. Section 2.3.1 demonstrated through numerical examples that while the Boros and Prékopa bound is uniformly the best performing of the three ordered bounds, the Schmidt, Siegel and Srinivasan bound shows the best improvement with ordering, in the examples considered.

iv) *Bounds computable in polynomial time as the optimal solution of a known aggregated linear program but whose tightness under assumptions of identical t -wise independent variables has not been established (indicated with \checkmark^*):*

The aggregated linear program proposed in Boros and Prékopa (1989) was shown to provide the tightest bound on the tail probability of sums of identical t -wise ($t \geq 2$) independent variables in Section 2.7.1. While closed-form bounds can be derived for $t = 2, 3$, the optimal value of the linear program provides the tight bounds for $t \geq 4$. The result in Proposition 5 can be easily extended to expected stop-loss functions such as those in the last two rows of Table 3.5.

v) *Bounds computable as the optimal solution of a compact linear program derived in our work that do not appear to be known in the literature (indicated with \checkmark^{**}):*

In Section 3.3, we derived a compact linear program that computes the tightest upper and lower bounds on the weighted tail probability function which does appear to be known in the literature. Similarly, in Section 3.2, we derived a compact linear program that computes valid upper bounds on the tail probability of the sum of discrete real-valued random variables which also does not seem to be known in the literature.

Numerical results in Example 8 showed that the upper bounds derived were tight in many instances of randomly generated non-identical marginal probabilities and with increasing number of random variables n . The results with discrete variables with integer support were generalized to variables with real support in Section 3.2.4.

vi) *Results of independent interest*

In Section 2.2.1, we established with Lemma 1 that given an arbitrary univariate probability vector $\mathbf{p} \in [0, 1]^n$ and transformed bivariate probabilities $p_i p_j / p$ where $p \in [\max_i p_i, 1]$, a Bernoulli random vector \tilde{c} consistent with the given information always exists. This feasibility result is significant, since with general bivariate probabilities p_{ij} , even verifying if there exists a feasible joint distribution is already known to be a NP-complete problem (Pitowsky, 1991).

vii) *Applications of derived bounds:*

a) *Star-shaped system and limited dependency:*

The usefulness of the Rüger (1978) bound in Theorem 9 was demonstrated with an application to a *star-shaped* marginal structure system in Section 3.1.4, while the usefulness of the weighted tail probability bounds in Section 3.3 was demonstrated with an application to the *limited-dependency* system in Section 3.3.2, where the conservativeness of extremal dependency was alleviated by considering varying degrees of dependence and independence among the variables.

b) *Correlation gap analysis:*

A $4/3$ attainable upper bound on the ratio of the Boole's union bound and the pairwise independent bound was shown in Proposition 1, by using the result derived in Theorem 2. Instances when the correlation gap analysis can be improved with pairwise independence instead of extremal dependence, for a specific non-decreasing, non-negative, submodular set function were presented in Example 2. Section 2.5 generalizes these results to show that, with $n = 2$ random variables, for any non-decreasing, non-negative, submodular set function, the upper bound on the correlation gap can be improved from $e/(e - 1)$ to $4/3$ while it can be arbitrarily large with supermodular set functions under similar assumptions. Even for the simple case of $n = 2$ variables, this result does not appear to be known in the literature.

c) *Tightness of existing bounds:*

Section 2.4 provided instances when the unordered and ordered bounds are tight. The tightness of the Boros and Prekopa bound for identical pairwise independent variables established in Theorem 4 was used in Section 2.4.1 to identify instances when other existing unordered bounds are tight. Section 2.4.2 demonstrated the usefulness of the ordered bounds by identifying an instance with $n - 1$ identical probabilities (along with additional conditions on the identical probability and k), when the ordered bounds are tight.

d) *Small deviation bounds:*

In Section 2.7.2, for the case of identical marginals, we identified instances when non-trivial and tight small deviation bounds are provided by the Boros and Prekopa bound while the Chebyshev and Schmidt, Siegel, Srinivasan bounds are trivial.

Future research questions:

We believe several interesting research questions arise from the results in Part I that need to be answered, a few of which we list below:

(a) To the best of our knowledge, the computational complexity of evaluating (or approximating) the bound $\bar{P}(n, k, \mathbf{p})$ for general n, k and $\mathbf{p} \in [0, 1]^n$ is still unresolved. While we provide the answer in closed form for $k = 1$ in Section 2.2, a natural question that arises is whether the tight bounds for general $k \geq 2$ with pairwise independent random variables are efficiently computable (or efficient to approximate) using linear program formulations? We leave this for future research.

(b) The upper bound of $4/3$ in Section 2.2.3 is derived for the ratio between the maximum probability for the union of extremally dependent events and the probability of the union of pairwise independent events. Similarly, the $4/3$ bound in Section 2.5 is derived for $n = 2$ random variables when pairwise independence is identical to mutual independence. We conjecture that this upper bound is valid for the expected value of all non-decreasing, non-negative, submodular functions (of which the probability of the union is a special case) for any $n \geq 2$ and leave it as an open question.

(c) While we proved that the tightest upper bound on the union of pairwise independent events is computable in a closed-form expression in Theorem 2, the complexity status of the Boolean probability bounding problem (Boros et al. (2014)) for general bivariate appears to be unresolved even if feasibility is guaranteed.

(d) Tree bounds for sums of extremally dependent Bernoulli random variables have been studied in Padmanabhan and Natarajan (2021) under the assumption that the bivariate probabilities are specified on a tree structure. If we additionally enforce pairwise independence, these results will provide valid upper bounds on $\bar{P}(n, k, \mathbf{p})$, which can then be compared with our improved bounds in Section 2.3.

(e) It would be of interest to perform a sensitivity analysis of the factors contributing to the performance gap of the improved bounds in Section 2.3 and further attempt to quantify the improvement beyond the numerical results in Section 2.3.1.

(f) The weighted tail probability bounds in Section 3.3 can be extended to pairwise independent Bernoulli variables by using the improved bounds from Section 2.3.1 as follows:

$$\max_{\theta \in \Theta_{pw}} \sum_{l=0}^n w_l \mathbb{P}_{\theta}(\sum_{i=1}^n \tilde{c}_i \geq l) \leq \sum_{l=0}^n w_l \bar{P}(n, l, \mathbf{p})$$

where $\bar{P}(n, l, \mathbf{p}) = \max_{\theta \in \Theta_{pw}} \mathbb{P}_{\theta}(\sum_{i=1}^n \tilde{c}_i \geq l)$ and the bounds from Theorem 3 can be directly applied to provide valid upper bounds on the required weighted tail probability, although the tightest bound may not be efficiently computable.

(g) While we proved in Section 2.6 that the tight lower bound $\underline{P}(n, 1, \mathbf{p})$ reduces to the Bonferroni (1936) bound for small probabilities, it remains an open question if the tight lower union bound and more generally $\underline{P}(n, k, \mathbf{p})$ (for any $k \geq 2$) are efficiently computable for any $\mathbf{p} \in [0, 1]^n$?

(h) In Section 2.7.1, we proved that the tight upper and lower bounds for tail probabilities of sums of identical t -wise independent variables is computable as the optimal

value of an aggregated linear program. For non-identical marginal probabilities, it remains an open question if the pairwise independence results from Sections 2.2 and 2.3 for the union bound and improved bounds respectively can be extended to t -wise independent variables.

(i) Can the results in Part I for sums of finite set of Bernoulli random variables be extended to sums of countably infinite set of Bernoulli variables?

(j) For expected stop-loss functions, while we provided in Section 2.7.3 that tight upper and lower bounds are captured in a closed-form expression for identical pairwise independent variables, it is not clear if $\bar{E}(n, k, \mathbf{p})$, and $\underline{E}(n, k, \mathbf{p})$ are efficiently computable for any $k \in [n]$ and $\mathbf{p} \in [0, 1]^n$.

(k) Extending the work of Padmanabhan et al., 2021, it would be of interest to investigate if the efficient computability of the bounds

$$\max_{\theta \in \Theta_u} \mathbb{P}_\theta(Z(\tilde{\mathbf{c}}) \geq k), \quad \forall k \in [n]$$

(where $Z(\tilde{\mathbf{c}})$ is the optimal value of a combinatorial optimization problem as considered in 3.2), flows over to pairwise independent Bernoulli random variables and compact 0/1 V-polytopes.

Part II

Satisficing with Uncertainty Sets

Chapter 4

Robust Conic Satisficing

In Part I, we considered bounds on tail probability and expected stop-loss functions of sums of random variables when the joint distribution satisfies conditions on the univariate probabilities (Chapter 3) and pairwise independence (Chapter 2). In this part of the dissertation, uncertainty is viewed from the lens of sets instead of distributions. More specifically, in the context of a recently proposed framework known as *robust satisficing*, we consider finding tractable solutions or approximations to uncertain conic optimization problems, when the uncertainty is adversarially chosen from an ellipsoidal or polyhedral support set. The suggested formulation employs a constraint function that evaluates to the optimal objective value of a standard conic optimization problem and generalizes several existing models considered in the recent literature. Numerical examples clearly illustrate the benefits of this new framework over classical robust optimization models. The technical content of this chapter is primarily derived from our paper Ramachandra, Rujeerapaiboon, and Sim (2021).

4.1 Introduction

“Of the impermanent there is no certainty” - Gita (2.16)

Uncertainty is an integral part of optimization problems without accounting for which, the deterministic optimal solution is fragile and does not provide meaningful insights (Ben-Tal, El Ghaoui, and Nemirovski, 2009). While the need to introduce uncertainty is well documented, the form in which it appears varies. In stochastic optimization problems, the uncertainty appears as random variables that are governed by an explicit probability distribution, which is assumed to be either available or else has to be estimated from historical data (Shapiro, Dentcheva, and Ruszczyński, 2014; Birge and Louveaux, 2011). On the other hand, robust optimization only assumes that the uncertainty dwells in a restricted set, also known as *uncertainty set*, without any further statistical information (Soyster, 1973; Ben-Tal and Nemirovski, 1998; El Ghaoui, Oustry, and Lebret, 1998). Robust optimization minimizes the worst-case cost while enforcing that the constraints are satisfied for every realization of the uncertainty within this set.

The selling point of robust optimization models is that their computational tractability is typically on par with their deterministic counterparts for many classes of constraints and characterizations of the uncertainty set (Bertsimas and Sim, 2003; Bertsimas and Sim, 2004; Bertsimas and Sim, 2006). Ben-Tal et al. (2004) extend robust optimization to an adaptive optimization framework, where recourse decisions can adapt to the uncertain parameters that are realized. Not all recourse adaptations would lead to computationally tractable optimization problems, and Ben-Tal et al. (2004) propose a tractable safe approximation by restricting the recourse to an affine function

of the uncertain parameters (see also Delage and Iancu, 2015; Kuhn, Wiesemann, and Georghiou, 2011; Bertsimas, Iancu, and Parrilo, 2010; Iancu, Sharma, and Sviridenko, 2013). Distributionally robust optimization, which generalizes robust optimization, assumes that the probability distribution governing the uncertain parameters lies in an ambiguity set of distributions characterized by known properties of the unknown data-generating distribution (Delage and Ye, 2010; Wiesemann, Kuhn, and Sim, 2014; Bertsimas, Sim, and Zhang, 2019). In the data-driven framework, distributionally robust optimization models with Wasserstein ambiguity sets (Mohajerin Esfahani and Kuhn, 2018), or Φ -divergence based ambiguity sets (Ben-Tal et al., 2013) could effectively overcome poor out-of-sample performance. Chen, Sim, and Xiong (2020) provide a unified framework for modeling distributionally robust optimization problems including data-driven models, and develop an algebraic modeling toolbox “RSOME” for this purpose.

Long, Sim, and Zhou (2021) recently proposed a new paradigm to model uncertainty called *robustness optimization*, which, in the stochastic-free version, corresponds to a case of the GRC (globalized robust counterpart)-sum model of Ben-Tal et al. (2017). Unlike robust optimization methods, which only hedge against pre-defined uncertainty, robustness optimization offers full protection by giving nature a free-hand to vary over the entire uncertainty support. The robustness optimization model compensates for this increased protection by allowing the constraints to be violated while simultaneously controlling the degree of infeasibility. The decision maker has the flexibility to choose the degree of sub-optimality relative to the nominal objective value, by specifying a target, unlike the robust optimization model, where the size of the uncertainty set needs to be known a priori. Simon (1955), who proposes the term *satisficing*, argues that target plays an important role in decision making, especially in complex situations involving uncertainty. To emphasize the role of the target, we prefer to use the term *robust satisficing* in place of *robustness optimization* proposed in Long, Sim, and Zhou (2021). The same term has also been used in Schwartz, Ben-Haim, and Dacso (2011) to describe a decision model that maximizes the robustness to uncertainty of achieving a satisfactory target. The decision criterion in our robust satisficing framework belongs to the family of satisficing decision criteria axiomatized by Brown and Sim (2009), which has an embedded preference for diversification that, serendipitously, also leads to computational tractability when used in convex optimization problems.

Since the inception of robust optimization, we now have an arsenal of tools to address and solve either exactly, or providing tractable safe approximations for various kinds of robust optimization models. We wish to highlight Bertsimas and Ruiters (2016) for proposing the dualizing technique and applying affine dual recourse adaptation to address an adaptive robust linear optimization problem. When the uncertainty set is polyhedral, this approach can also be used to provide safe approximations for robust optimization models with biconvex constraint functions including those with recourse adaptation (Ruiters, Zhen, and Hertog, 2018; Roos et al., 2020). We use this approach to obtain solutions to our proposed robust conic satisficing models. We summarize the contributions of this chapter below:

i) We provide a unifying framework for conic optimization under uncertainty that is based on minimizing a linear objective function and a constraint function that evaluates to the optimal objective value of a standard conic optimization problem. We demonstrate that it can be used to model a wide range of robust optimization problems studied in the literature including biconvex linear or quadratic constraint functions (Ben-Tal and Nemirovski, 1998), saddle constraint functions (Ben-Tal et al., 2017),

non-linear biconvex constraint functions (Roos et al., 2020; Zhen, Ruiter, and Hertog, 2017), adaptive linear optimization model (Ben-Tal et al., 2004; Bertsimas and Ruiter, 2016) and adaptive convex optimization model (Ruiter, Zhen, and Hertog, 2018).

ii) Based on the conic optimization framework, we demonstrate how we could solve the robust satisficing model, which has potentially infinite number of conic constraints, either exactly when possible, or safely approximated to a practicably solvable optimization problem. For a biconvex quadratic constraint with a quadratic penalty and quadratic uncertainty support, we derive the exact reformulation in the form of a tractable semidefinite optimization problem. Then, for a more general constraint with polyhedral support and penalty, we derive a tractable safe approximation using the *affine dual recourse adaptation* technique first proposed by Bertsimas and Ruiter (2016). The key challenge is to show that under a condition of complete recourse, and reasonably chosen polyhedral support set and penalty function, the exact reformulation and safe approximations do not lead to infeasible problems as long as the chosen targets are above the optimum objective obtained when the nominal optimization problem is minimized.

iii) We explore how the affine dual recourse adaptation can be used to provide safe approximations to two-stage adaptive conic optimization problems, including those in the data-driven settings explored in Long, Sim, and Zhou (2021). For the important case of adaptive linear optimization, we show that the affine dual recourse adaptation provides a better approximation than the non-affine recourse adaptation proposed in Long, Sim, and Zhou (2021).

iv) We showcase the modeling and the computational benefits of the robust satisficing framework over the robust optimization counterpart with three numerical examples: portfolio selection, log-sum-exp optimization and adaptive lot-sizing problem. Using *Monte-Carlo* simulations, we show that the robust satisficing model obtains a family of solutions that have better statistical performance compared to the solutions generated by an equivalent robust optimization model. Additionally, we present computational results to show that the robust satisficing model has a remarkable improvement in computational time over the robust optimization model.

Notation: We use \mathbb{R} to denote the space of reals while \mathbb{R}_+ and \mathbb{R}_{++} denote the sets of non-negative and strictly positive real numbers respectively. We use boldface small-case letters (e.g. \mathbf{x}) to denote vectors, capitals (e.g. \mathbf{A}) to denote matrices and capital calligraphic letters to denote sets (e.g. \mathcal{Z}) including cones (e.g. \mathcal{K}). $\mathcal{R}^{m,n}$ and $\mathcal{L}^{m,n}$ are used to denote the set of all functions and its sub-class of affine functions, respectively, from \mathbb{R}^m to \mathbb{R}^n . The transpose of a vector (matrix) is denoted by \mathbf{x}^\top (\mathbf{A}^\top). A random vector is denoted with a tilde sign (e.g. $\tilde{\mathbf{z}}$), and $[n]$ is used to denote the running index set $\{1, 2, \dots, n\}$. We use superscript indexing (e.g. \mathbf{w}^i) to denote the i^{th} vector (matrix) among a countable set of vectors $\{\mathbf{w}^i\}$ (matrices) and subscript indexing (e.g. \mathbf{A}_i) to denote the i^{th} row of a matrix \mathbf{A} . Finally, $\mathbf{0}$ ($\mathbf{1}$) denotes the vector of all zeros (ones) and its dimension should be clear from the context, while the identity matrix of order n is denoted by \mathbf{I}_n .

4.2 Unifying framework for conic optimization under uncertainty

In this section, we propose a unifying conic optimization framework where the exact values of the model's parameters are unknown, or unobservable, but proximal to some given nominal values. We first consider a deterministic *nominal conic optimization problem* as follows:

$$\begin{aligned} Z_0 = \min \quad & \mathbf{c}^\top \mathbf{x} \\ \text{s.t.} \quad & g(\mathbf{x}, \hat{\mathbf{z}}) \leq 0 \\ & \mathbf{x} \in \mathcal{X}, \end{aligned} \quad (4.1)$$

for a given function $g : \mathcal{X} \times \mathcal{Z} \mapsto \mathbb{R}$ where the input to the second argument may be subjected to uncertainty and $\hat{\mathbf{z}} \in \mathcal{Z}$ is the nominal value. The model's decision variable is denoted by the vector $\mathbf{x} \in \mathcal{X} \subseteq \mathbb{R}^{n_x}$ and the uncertain parameters are represented by the vector $\mathbf{z} \in \mathcal{Z} \subseteq \mathbb{R}^{n_z}$, where \mathcal{X} and \mathcal{Z} are respectively the feasible set and uncertainty support set. Central to our conic optimization model is how we define the function g , which is designed to be as expressive as possible, yet allowing the conic optimization problem under uncertainty to be amendable to tractable reformulations or approximations. Specifically, the function g is a conic representable function of the form

$$\begin{aligned} g(\mathbf{x}, \mathbf{z}) = \min \quad & \mathbf{d}^\top \mathbf{y} \\ \text{s.t.} \quad & \mathbf{B}\mathbf{y} \succeq_{\mathcal{K}} \mathbf{f}(\mathbf{x}) + \mathbf{F}(\mathbf{x})\mathbf{z} \\ & \mathbf{y} \in \mathbb{R}^{n_y}, \end{aligned} \quad (4.2)$$

where $\mathbf{f} : \mathbb{R}^{n_x} \mapsto \mathbb{R}^{n_f}$, $\mathbf{F} : \mathbb{R}^{n_x} \mapsto \mathbb{R}^{n_f \times n_z}$ are affine mappings in \mathbf{x} , and \mathcal{K} is a proper cone. Since the decision variable \mathbf{y} in Problem (4.2) is made after observing \mathbf{x} and \mathbf{z} , we will call \mathbf{y} the *recourse* variable. Indeed, if the cone \mathcal{K} is the non-negative orthant, then the g function would represent the second stage optimization problem of a standard two-stage stochastic optimization model. However, as we will show, the function g is sufficiently generic to represent many types of functions considered in the robust optimization literature, for instance a biconvex quadratic function (Ben-Tal and Nemirovski, 1998), which are not necessarily associated with a two-stage optimization problem.

Assumption 1 (Convexity and practicable solvability). *We assume that \mathcal{X} and \mathcal{Z} are compact and convex sets. Moreover, we assume that any convex optimization problem over $\mathbf{x} \in \mathcal{X}$, involving a modest number of additional decision variables, linear and \mathcal{K} -conic inequalities are practicably solvable, i.e., it can be solved to optimality within reasonable time using current available solvers such as CPLEX, Gurobi, Mosek, SDPT3, among others.*

The nominal problem is practicably solvable under Assumption 1. However, most optimization problems become much harder to solve when they are subject to uncertainty. Note that as \mathbf{x} and \mathbf{z} appear on the right-hand side of the conic constraint, g is a biconvex function, and we would expect the problem to be much harder to solve exactly if the second argument is subject to uncertainty. In the simplest case, where g is a biaffine function given by

$$g(\mathbf{x}, \mathbf{z}) = \mathbf{x}^\top \mathbf{A}\mathbf{z} + \mathbf{b}^\top \mathbf{x} + \mathbf{c}^\top \mathbf{z} + d,$$

we can express

$$g(\mathbf{x}, \mathbf{z}) = \min_{y \in \mathbb{R}} \left\{ y \mid y \geq \left(\mathbf{b}^\top \mathbf{x} + d \right) + \left(\mathbf{x}^\top \mathbf{A} + \mathbf{c}^\top \right) \mathbf{z} \right\}.$$

In addition, the following example demonstrates how we can convert commonly used biconvex functions to the form of Problem (4.2).

Example 10 (Common bi-convex function). *Consider a biconvex function of the following form*

$$g(\mathbf{x}, \mathbf{z}) = h(\mathbf{b}(\mathbf{x}) + \mathbf{A}(\mathbf{x})\mathbf{z})$$

where $h : \mathbb{R}^{n_\alpha} \mapsto \mathbb{R} \cup \{\infty\}$ is a convex map, $\mathbf{b} : \mathbb{R}^{n_x} \rightarrow \mathbb{R}^{n_\alpha}$, $\mathbf{A} : \mathbb{R}^{n_x} \rightarrow \mathbb{R}^{n_\alpha \times n_z}$ are affine mappings in \mathbf{x} . This is a bi-convex function, which is common in classical robust convex optimization models (see for e.g. Roos et al., 2020). Observe that

$$g(\mathbf{x}, \mathbf{z}) = \inf_y \quad y \\ \text{s.t.} \quad \underbrace{\begin{pmatrix} \mathbf{0} \\ 1 \\ 0 \end{pmatrix}}_B y \succeq_{\mathcal{K}} \underbrace{\begin{pmatrix} -\mathbf{b}(\mathbf{x}) \\ 0 \\ -1 \end{pmatrix}}_{f(\mathbf{x})} + \underbrace{\begin{pmatrix} -\mathbf{A}(\mathbf{x}) \\ \mathbf{0}^\top \\ \mathbf{0}^\top \end{pmatrix}}_{F(\mathbf{x})} \mathbf{z},$$

where the conic inequality involves a cone

$$\mathcal{K} = \text{cl} \{ (\boldsymbol{\alpha}, \beta, \gamma) \in \mathbb{R}^{n_\alpha} \times \mathbb{R} \times \mathbb{R}_+ \mid \gamma h(\boldsymbol{\alpha}/\gamma) \leq \beta, \gamma > 0 \},$$

which is proper and convex because a perspective function preserves convexity. For instance, a quadratic constraint

$$\|\mathbf{A}(\mathbf{x})\mathbf{z} + \mathbf{a}(\mathbf{x})\|_2^2 + \mathbf{b}(\mathbf{x})^\top \mathbf{z} + c(\mathbf{x}) \leq 0$$

can be expressed as

$$g(\mathbf{x}, \mathbf{z}) = \min_{y \in \mathbb{R}} \left\{ y \mid (\mathbf{A}(\mathbf{x})\mathbf{z} + \mathbf{a}(\mathbf{x}), y - \mathbf{b}(\mathbf{x})^\top \mathbf{z} - c(\mathbf{x}), 1) \in \mathcal{K} \right\},$$

where here \mathcal{K} denotes the rotated second-order cone given by

$$\mathcal{K} = \left\{ (\boldsymbol{\alpha}, \beta, \gamma) \in \mathbb{R}^{n_\alpha} \times \mathbb{R}_+ \times \mathbb{R}_+ \mid \boldsymbol{\alpha}^\top \boldsymbol{\alpha} \leq \beta\gamma \right\}.$$

In this regard, the two-stage adaptive convex optimization framework proposed in Ruitter, Zhen, and Hertog (2018) can also be represented in our unified conic optimization framework.

4.2.1 Robust optimization

To better protect the constraints against infeasibility, robust optimization fashions an uncertainty set of a given size r around the nominal parameter $\hat{\mathbf{z}}$ as follows:

$$\begin{aligned} Z_r = \min \quad & \mathbf{c}^\top \mathbf{x} \\ \text{s.t.} \quad & g(\mathbf{x}, \mathbf{z}) \leq 0 \quad \forall \mathbf{z} \in \mathcal{U}_r, \\ & \mathbf{x} \in \mathcal{X}, \end{aligned} \tag{4.3}$$

where \mathcal{U}_r is typically a distance-calibrated uncertainty set that contains \hat{z} and is given by

$$\mathcal{U}_r = \{z \in \mathcal{Z} \mid p(z - \hat{z}) \leq r\},$$

and $p(\zeta) : \mathbb{R}^{n_z} \mapsto \mathbb{R}_+$ is a convex penalty function that penalizes deviations of ζ from the origin such that $p(\zeta) = 0$ if and only if $\zeta = \mathbf{0}$. Hence, $\mathcal{U}_0 = \{\hat{z}\}$ and $\mathcal{U}_r \subseteq \mathcal{U}_{r'}$ for all $0 \leq r \leq r'$.

It has well been known that the tractability of the robust optimization depends on the constraint function g along with the characterization of the uncertainty set, and there are few examples beyond linear constraints that would yield tractable reformulations. Notably, if \mathcal{U}_r is a compact convex set, and the function associated with the robust constraint $h(\mathbf{x}, z) \leq 0$, $\forall z \in \mathcal{U}_r$ is a saddle function, *i.e.*, $h(\mathbf{x}, z)$ is convex in \mathbf{x} for a given z and concave in z for a given \mathbf{x} , then in many interesting examples, we would be able to use standard robust optimization techniques (see, *e.g.*, Ben-Tal et al., 2017) to tractably address the robust constraint through a reformulation. As we will show, although such a saddle function may not necessarily be represented as a g function of Problem (4.2), we can always transform the constraint to an equivalent one where the constraint function can be expressed as the g function.

Example 11 (Saddle function). Consider a saddle function $h(\mathbf{x}, z) : \mathcal{X} \times \mathbb{R}^{n_z} \mapsto \mathbb{R} \cup \{-\infty\}$ on an extended real number line. Specifically, for a given $\mathbf{x} \in \mathcal{X}$, $h(\mathbf{x}, z)$ is upper-semicontinuous and concave in $z \in \mathbb{R}^{n_z}$, and for a given $z \in \mathbb{R}^{n_z}$, the function is convex in $\mathbf{x} \in \mathcal{X}$. Hence, due the biconjugate property, for a given $(\mathbf{x}, z) \in \mathcal{X} \times \mathbb{R}^{n_z}$, the function can be rewritten as

$$h(\mathbf{x}, z) = \inf_{\mathbf{v} \in \mathbb{R}^{n_z}} \left\{ f(\mathbf{x}, \mathbf{v}) - \mathbf{v}^\top z \right\}$$

where f is the convex conjugate of $-h$ with respect to the second argument as follows

$$f(\mathbf{x}, \mathbf{v}) = \sup_{\mathbf{y} \in \mathbb{R}^{n_z}} \left\{ \mathbf{v}^\top \mathbf{y} + h(\mathbf{x}, \mathbf{y}) \right\},$$

which is a jointly convex function, since it can be expressed as a maximum of functions that are convex in (\mathbf{x}, \mathbf{v}) . Therefore, we can express

$$h(\mathbf{x}, z) = \inf_{(u, \mathbf{v}) : (u, \mathbf{v}, \mathbf{x}) \in \mathcal{Y}} \left\{ u - \mathbf{v}^\top z \right\} \quad (4.4)$$

where

$$\mathcal{Y} = \{(u, \mathbf{v}, \mathbf{x}) \in \mathbb{R} \times \mathbb{R}^{n_z} \times \mathcal{X} \mid u \geq f(\mathbf{x}, \mathbf{v})\}$$

is an epigraph of a jointly convex function and thus a convex set. However, it should be noted that Problem (4.4) is not in the same form expressed in Problem (4.2) because the recourse matrix \mathbf{B} in the latter does not depend on z . Note that the robust optimization constraint

$$h(\mathbf{x}, z) \leq 0 \quad \forall z \in \mathcal{U}_r$$

is equivalent to

$$\max_{z \in \mathcal{U}_r} \inf_{(u, \mathbf{v}) : (u, \mathbf{v}, \mathbf{x}) \in \mathcal{Y}} \left\{ u - \mathbf{v}^\top z \right\} \leq 0.$$

Since \mathcal{U}_r is a convex compact set, we can use Sion (1958) minimax result to obtain an equivalent representation,

$$\max_{z \in \mathcal{U}_r} \inf_{(u, \mathbf{v}): (u, \mathbf{v}, \mathbf{x}) \in \mathcal{Y}} \{u - \mathbf{v}^\top \mathbf{z}\} \leq 0 \iff \inf_{(u, \mathbf{v}): (u, \mathbf{v}, \mathbf{x}) \in \mathcal{Y}} \max_{z \in \mathcal{U}_r} \{u - \mathbf{v}^\top \mathbf{z}\} \leq 0.$$

Hence, we can express the robust optimization constraint as

$$g(u, \mathbf{v}, \mathbf{z}) \leq 0 \quad \forall \mathbf{z} \in \mathcal{U}_r,$$

where $g(u, \mathbf{v}, \mathbf{z}) = \min_y \{y \mid y \geq u - \mathbf{v}^\top \mathbf{z}\}$ for some first-stage variables $(u, \mathbf{v}, \mathbf{x}) \in \mathcal{Y}$. Therefore, we can always transform a robust optimization problem with saddle constraint function to an equivalent robust optimization problem with a biaffine constraint function.

4.2.2 Robust satisficing

Long, Sim, and Zhou (2021) have recently proposed a target-oriented *robustness optimization* framework for data-driven optimization, which we term as *robust satisficing* to emphasize the role of the target in the model specification. We focus on the stochastic-free model, where the robust satisficing model also corresponds to the GRC (globalized robust counterpart)-sum model of Ben-Tal et al. (2017) as follows:

$$\begin{aligned} \min \quad & k \\ \text{s.t.} \quad & g(\mathbf{x}, \mathbf{z}) \leq kp(\mathbf{z} - \hat{\mathbf{z}}), \quad \forall \mathbf{z} \in \mathcal{Z} \\ & \mathbf{c}^\top \mathbf{x} \leq \tau \\ & \mathbf{x} \in \mathcal{X}, k \in \mathbb{R}_+. \end{aligned} \tag{4.5}$$

In contrast to the robust formulation in Problem (4.3), where the protection offered is only against the subset $\mathcal{U}_r \subseteq \mathcal{Z}$ of all possible realizations of \mathbf{z} , the robust satisficing model allows the uncertainty to range over the entire support \mathcal{Z} , but controls the level of constraint violations as much as possible whenever \mathbf{z} deviates from its nominal value, $\hat{\mathbf{z}}$. Additionally, as a trade-off for the model's greater ability to withstand uncertainty, an acceptable loss in optimality is specified by a target that satisfies $\tau \geq Z_0$. As also observed in Long, Sim, and Zhou (2021), the robust satisficing model is almost in the same complexity class as its robust optimization counterpart. We also note that if the constraint function $h(\mathbf{x}, \mathbf{z})$ is a saddle function, then the function $h(\mathbf{x}, \mathbf{z}) - kp(\mathbf{z} - \hat{\mathbf{z}})$ is also a saddle function on domains $\{(\mathbf{x}, k) \in \mathcal{X} \times \mathbb{R}_+\}$ and $\{\mathbf{z} \in \mathcal{Z}\}$, which, as illustrated in Example 11, can be transformed to a robust constraint in which the constraint function can be represented as a g function of Problem (4.2).

Depending on the nominal problem, there are different variants of the robust optimization and satisficing models. If the nominal problem has g appearing in the objective function, then we can introduce artificial variables so that it can be framed as Problem (4.1). For instance

$$Z_0 = \min_{\mathbf{x} \in \mathcal{X}} \mathbf{c}^\top \mathbf{x} + g(\mathbf{x}, \mathbf{z}) \iff Z_0 = \min_{\mathbf{x} \in \mathcal{X}, x_0 \in \mathbb{R}} x_0 \quad \text{s.t.} \quad \bar{g}((x_0, \mathbf{x}), \mathbf{z}) \leq 0 \tag{4.6}$$

where $\bar{g}((x_0, \mathbf{x}), \mathbf{z}) = \min_{y \in \mathbb{R}} \{g(\mathbf{x}, \mathbf{z}) + y \mid y \geq \mathbf{c}^\top \mathbf{x} - x_0\}$. Hence, the corresponding robust optimization problem becomes

$$Z_r = \min_{\mathbf{x} \in \mathcal{X}, x_0 \in \mathbb{R}} x_0 \quad \text{s.t.} \quad \bar{g}((x_0, \mathbf{x}), \mathbf{z}) \leq 0 \quad \forall \mathbf{z} \in \mathcal{U}_r \quad \iff \quad Z_r = \min_{\mathbf{x} \in \mathcal{X}} \mathbf{c}^\top \mathbf{x} + \max_{\mathbf{z} \in \mathcal{U}_r} g(\mathbf{x}, \mathbf{z})$$

and the robust satisficing problem would be

$$\begin{aligned} \min \quad & k \\ \text{s.t.} \quad & \bar{g}((x_0, \mathbf{x}), \mathbf{z}) \leq kp(\mathbf{z} - \hat{\mathbf{z}}) \quad \forall \mathbf{z} \in \mathcal{Z} \\ & x_0 \leq \tau \\ & \mathbf{x} \in \mathcal{X}, x_0 \in \mathbb{R} \end{aligned} \quad \iff \quad \begin{aligned} \min \quad & k \\ \text{s.t.} \quad & \mathbf{c}^\top \mathbf{x} + g(\mathbf{x}, \mathbf{z}) \leq \tau + kp(\mathbf{z} - \hat{\mathbf{z}}) \quad \forall \mathbf{z} \in \mathcal{Z} \\ & \mathbf{x} \in \mathcal{X}. \end{aligned} \quad (4.7)$$

We can also extend these frameworks to consider an arbitrary number of constraints, say $m \in \mathbb{N}$ as follows,

Nominal problem	Robust optimization	Robust satisficing ($\tau \geq Z_0$)
$Z_0 = \min_{\mathbf{x} \in \mathcal{X}} \mathbf{c}^\top \mathbf{x}$ $\text{s.t.} \quad g_i(\mathbf{x}, \hat{\mathbf{z}}) \leq 0 \quad \forall i \in [m]$	$\min_{\mathbf{x} \in \mathcal{X}} \mathbf{c}^\top \mathbf{x}$ $\text{s.t.} \quad g_i(\mathbf{x}, \mathbf{z}) \leq 0 \quad \forall \mathbf{z} \in \mathcal{U}(r_i), i \in [m]$	$\min_{\mathbf{x} \in \mathcal{X}, \mathbf{k} \in \mathbb{R}_+^m} \mathbf{w}^\top \mathbf{k}$ $\text{s.t.} \quad g_i(\mathbf{x}, \mathbf{z}) \leq k_i p(\mathbf{z} - \hat{\mathbf{z}}) \quad \forall \mathbf{z} \in \mathcal{Z}, i \in [m]$ $\mathbf{c}^\top \mathbf{x} \leq \tau$

where $\{r_i\}_{i \in [m]}$ is a collection of the non-negative radii of the uncertainty set, and $\{w_i\}_{i \in [m]}$ is a collection of non-negative weights.

4.3 Tractable reformulations and safe approximations

In this section, we demonstrate how we could solve the robust satisficing of Problem (4.5) that has infinite number of conic constraints, either exactly when possible, or safely approximated to a practicably solvable optimization problem under Assumption 1. For a biconvex quadratic function with a quadratic penalty and quadratic uncertainty support, we derive the exact reformulation in the form of a tractable semidefinite optimization problem. Then, for a more general function with polyhedral support and penalty, we focus on obtaining a tractable safe approximation using *affine dual recourse adaptation* technique. The key challenge is to provide the conditions under which the exact reformulation and safe approximations would not lead to infeasible problems for any reasonably chosen target above the optimum objective obtained when the nominal optimization problem is minimized, *i.e.*, $\tau > Z_0$.

4.3.1 Biconvex quadratic constraint with quadratic penalty

This problem is motivated from the classical robust optimization proposed in Ben-Tal and Nemirovski (1998) involving a quadratic constraint and an ellipsoidal uncertainty

set

$$\begin{aligned} Z_r = \min \quad & \mathbf{c}^\top \mathbf{x} \\ \text{s.t.} \quad & \|\mathbf{A}(\mathbf{x})\mathbf{z} + \mathbf{a}(\mathbf{x})\|_2^2 + \mathbf{b}(\mathbf{x})^\top \mathbf{z} + c(\mathbf{x}) \leq 0 \quad \forall \mathbf{z} \in \mathcal{E}_r \\ & \mathbf{x} \in \mathcal{X}, \end{aligned} \quad (4.8)$$

where $\mathcal{E}_r = \{\mathbf{z} \in \mathbb{R}^{n_z} \mid \mathbf{z}^\top \mathbf{z} \leq r\}$, $r \geq 0$, is a non-empty ellipsoidal uncertainty set and $\mathbf{a} : \mathbb{R}^{n_x} \mapsto \mathbb{R}^{n_a}$, $\mathbf{A} : \mathbb{R}^{n_x} \mapsto \mathbb{R}^{n_a \times n_z}$, $\mathbf{b} : \mathbb{R}^{n_x} \mapsto \mathbb{R}^{n_z}$, $c : \mathbb{R}^{n_x} \mapsto \mathbb{R}$ are affine mappings of the decision variables \mathbf{x} . Note that here the nominal value is $\hat{\mathbf{z}} = \mathbf{0}$, which can be assumed without any loss of generality. Biconvex robust optimization problems are typically difficult to deal with; however, as shown below, Problem (4.8) is a notable exception. Besides, we assume that the nominal problem is strictly feasible.

Theorem 16. (Ben-Tal and Nemirovski, 1998, Theorem 3.2). *For any $r > 0$, the constraints*

$$\|\mathbf{A}(\mathbf{x})\mathbf{z} + \mathbf{a}(\mathbf{x})\|_2^2 + \mathbf{b}(\mathbf{x})^\top \mathbf{z} + c(\mathbf{x}) \leq 0, \quad \forall \mathbf{z} \in \mathcal{E}_r$$

are equivalent to the following positive semidefinite constraint:

$$\exists \lambda \geq 0 : \begin{bmatrix} \mathbf{I}_{n_a} & \mathbf{a}(\mathbf{x}) & \mathbf{A}(\mathbf{x}) \\ \mathbf{a}(\mathbf{x})^\top & -c(\mathbf{x}) - \lambda r & -\frac{1}{2}\mathbf{b}(\mathbf{x})^\top \\ \mathbf{A}(\mathbf{x})^\top & -\frac{1}{2}\mathbf{b}(\mathbf{x}) & \lambda \mathbf{I}_{n_z} \end{bmatrix} \succeq \mathbf{0}.$$

Proof. To avoid clutter, we first drop the dependency of $\mathbf{A}, \mathbf{b}, c$ on \mathbf{x} , and then we expand the squared Euclidean norm in the robust constraint $\|\mathbf{A}(\mathbf{x})\mathbf{z} + \mathbf{a}(\mathbf{x})\|_2^2 + \mathbf{b}(\mathbf{x})^\top \mathbf{z} + c(\mathbf{x}) \leq 0, \forall \mathbf{z} \in \mathcal{E}_r$ to equivalently express it as

$$\begin{bmatrix} 1 \\ \mathbf{z} \end{bmatrix}^\top \begin{bmatrix} -c - \mathbf{a}^\top \mathbf{a} & -(\mathbf{A}^\top \mathbf{a} + \frac{1}{2}\mathbf{b})^\top \\ -(\mathbf{A}^\top \mathbf{a} + \frac{1}{2}\mathbf{b}) & -\mathbf{A}^\top \mathbf{A} \end{bmatrix} \begin{bmatrix} 1 \\ \mathbf{z} \end{bmatrix} \geq 0 \quad \forall \mathbf{z} : \begin{bmatrix} 1 \\ \mathbf{z} \end{bmatrix}^\top \begin{bmatrix} r & \mathbf{0}^\top \\ \mathbf{0} & -\mathbf{I}_{n_z} \end{bmatrix} \begin{bmatrix} 1 \\ \mathbf{z} \end{bmatrix} \geq 0.$$

Applying \mathcal{S} -lemma leads to another equivalent representation of our quadratic constraint which is

$$\begin{aligned} \exists \lambda \geq 0 : \quad & \begin{bmatrix} -c - \mathbf{a}^\top \mathbf{a} & -(\mathbf{A}^\top \mathbf{a} + \frac{1}{2}\mathbf{b})^\top \\ -(\mathbf{A}^\top \mathbf{a} + \frac{1}{2}\mathbf{b}) & -\mathbf{A}^\top \mathbf{A} \end{bmatrix} - \lambda \begin{bmatrix} r & \mathbf{0}^\top \\ \mathbf{0} & -\mathbf{I}_{n_z} \end{bmatrix} \succeq \mathbf{0} \\ \iff \quad & \exists \lambda \geq 0 : \begin{bmatrix} -c - \lambda r & -\frac{1}{2}\mathbf{b}^\top \\ -\frac{1}{2}\mathbf{b} & \lambda \mathbf{I}_{n_z} \end{bmatrix} - \begin{bmatrix} \mathbf{a}^\top \\ \mathbf{A}^\top \end{bmatrix} \mathbf{I}_{n_a} \begin{bmatrix} \mathbf{a}^\top \\ \mathbf{A}^\top \end{bmatrix}^\top \succeq \mathbf{0}. \end{aligned}$$

Finally, using Schur's complement and recovering the dependency of $\mathbf{A}, \mathbf{b}, c$ on \mathbf{x} yields the desired result. \square

Analogously, we now consider a robust quadratic satisficing model by choosing the penalty function to be the squared Euclidean norm $p(\mathbf{z}) = \|\mathbf{z}\|_2^2 = \mathbf{z}^\top \mathbf{z}$. Suppose we

consider the ellipsoidal support set $\mathcal{Z} = \mathcal{E}_{\bar{r}}$, $\bar{r} \geq r$, which contains the earlier uncertainty set \mathcal{E}_r . The arising robust satisficing problem can then be written down as

$$\begin{aligned} \min \quad & k \\ \text{s.t.} \quad & \|\mathbf{A}(\mathbf{x})\mathbf{z} + \mathbf{a}(\mathbf{x})\|_2^2 + \mathbf{b}(\mathbf{x})^\top \mathbf{z} + c(\mathbf{x}) \leq k\mathbf{z}^\top \mathbf{z} \quad \forall \mathbf{z} \in \mathcal{Z}, \\ & \mathbf{c}^\top \mathbf{x} \leq \tau \\ & \mathbf{x} \in \mathcal{X}, k \in \mathbb{R}_+, \end{aligned} \tag{4.9}$$

where $\tau > Z_0$ is the prescribed target.

Theorem 17. For any $\bar{r} > 0$, the constraints

$$\|\mathbf{A}(\mathbf{x})\mathbf{z} + \mathbf{a}(\mathbf{x})\|_2^2 + \mathbf{b}(\mathbf{x})^\top \mathbf{z} + c(\mathbf{x}) \leq k\mathbf{z}^\top \mathbf{z}, \quad \forall \mathbf{z} \in \mathcal{Z}$$

are equivalent to the following positive semidefinite constraint:

$$\exists \lambda \geq 0 : \begin{bmatrix} \mathbf{I}_{n_a} & \mathbf{a}(\mathbf{x}) & \mathbf{A}(\mathbf{x}) \\ \mathbf{a}(\mathbf{x})^\top & -c(\mathbf{x}) - \lambda\bar{r} & -\frac{1}{2}\mathbf{b}(\mathbf{x})^\top \\ \mathbf{A}(\mathbf{x})^\top & -\frac{1}{2}\mathbf{b}(\mathbf{x}) & (k + \lambda)\mathbf{I}_{n_z} \end{bmatrix} \succeq \mathbf{0}.$$

Under Assumption 1 and that the nominal problem is strictly feasible, Problem (4.9) is feasible for any chosen target, $\tau > Z_0$.

Proof. By relocating $k\mathbf{z}^\top \mathbf{z}$ to the left-hand side, the constraint function is still quadratic in \mathbf{x} and in \mathbf{z} . Using similar arguments of the \mathcal{S} -lemma and Schur's complement from the proof of Theorem 16 thus completes the first half of the theorem.

For the second half of the proof, we denote by $\mathbf{x}^s \in \mathcal{X}$ any Slater's point of the nominal problem. Let $\hat{\mathbf{x}}$ be the optimum solution to the nominal problem so that $Z_0 = \mathbf{c}^\top \hat{\mathbf{x}}$. Since \mathcal{X} is a convex set, it follows that there is a point $\hat{\mathbf{x}}^s \in \mathcal{X}$ on the line segment connecting $\hat{\mathbf{x}}$ and \mathbf{x}^s such that

$$\mathbf{c}^\top \hat{\mathbf{x}}^s \leq \tau \quad \text{and} \quad \|\mathbf{a}(\hat{\mathbf{x}}^s)\|_2^2 + c(\hat{\mathbf{x}}^s) < 0.$$

It thus suffices to show that there exists a sufficiently large positive \hat{k} such that $(\mathbf{x}, k, \lambda) = (\hat{\mathbf{x}}^s, \hat{k}, 0)$ is feasible in Problem (4.9). To this end, we first note from the above quadratic inequality that

$$\begin{bmatrix} \mathbf{I}_{n_a} & \mathbf{a}(\hat{\mathbf{x}}^s) \\ \mathbf{a}(\hat{\mathbf{x}}^s)^\top & -c(\hat{\mathbf{x}}^s) \end{bmatrix} \succ \mathbf{0}.$$

Thus, there exists $\hat{k} > 0$ such that

$$\hat{k} \begin{bmatrix} \mathbf{I}_{n_a} & \mathbf{a}(\hat{\mathbf{x}}^s) \\ \mathbf{a}(\hat{\mathbf{x}}^s)^\top & -c(\hat{\mathbf{x}}^s) \end{bmatrix} \succeq \begin{bmatrix} \mathbf{A}(\hat{\mathbf{x}}^s) \\ -\frac{1}{2}\mathbf{b}(\hat{\mathbf{x}}^s)^\top \end{bmatrix} \begin{bmatrix} \mathbf{A}(\hat{\mathbf{x}}^s) \\ -\frac{1}{2}\mathbf{b}(\hat{\mathbf{x}}^s)^\top \end{bmatrix}^\top.$$

Therefore, by the virtue of Schur's complement, $(\mathbf{x}, k, \lambda) = (\hat{\mathbf{x}}^s, \hat{k}, 0)$ satisfies the semidefinite constraint presented in the theorem. The proof is now complete. \square

Theorems 16 and 17 show that both the robust quadratic optimization and satisficing problems can be reformulated as tractable semidefinite optimization problems that can be solved exactly in polynomial time by, for instance, the interior point algorithm. These results heavily rely on the nature of the problem: g is a biconvex quadratic

function, the uncertainty set and the support are ellipsoidal, and the penalty function is quadratic in the form of squared Euclidean norm. For a more general robust conic satisficing problem of the form of Problem (4.5), exact tractable reformulations may not exist, and thus approximations would be needed. We consider next the case of polyhedral support sets, and we use polyhedral penalty function to penalize the deviation of the uncertain parameter z from its nominal value \hat{z} .

4.3.2 Tractable safe approximation with affine dual recourse adaptation

Assuming again without loss of generality that $\hat{z} = \mathbf{0}$, we denote the optimal solution of the nominal optimization problem (4.1) by \hat{x} and by \hat{y} the corresponding optimal recourse, that is,

$$\hat{y} \in \operatorname{argmin}_{\mathbf{y}} \left\{ \mathbf{d}^\top \mathbf{y} : \mathbf{B}\mathbf{y} \succeq_{\mathcal{K}} \mathbf{f}(\hat{x}) \right\}. \quad (4.10)$$

As a consequence of our notation, we have $Z_0 = \mathbf{c}^\top \hat{x}$. Problem (4.5) can be expressed in the following explicit formulation,

$$\begin{aligned} \min \quad & k \\ \text{s.t.} \quad & \mathbf{d}^\top \mathbf{y}(z) \leq kp(z) & \forall z \in \mathcal{Z} \\ & \mathbf{B}\mathbf{y}(z) \succeq_{\mathcal{K}} \mathbf{f}(x) + \mathbf{F}(x)z & \forall z \in \mathcal{Z} \\ & \mathbf{c}^\top x \leq \tau \\ & x \in \mathcal{X}, \mathbf{y} \in \mathcal{R}^{n_z, n_y}, k \in \mathbb{R}_+, \end{aligned} \quad (4.11)$$

where $\mathcal{R}^{m,n}$ denotes the family of all functions from \mathbb{R}^m to \mathbb{R}^n , *i.e.*,

$$\mathcal{R}^{m,n} = \{ \mathbf{y} \mid \mathbf{y} : \mathbb{R}^m \mapsto \mathbb{R}^n \}.$$

The problem remains intractable even if we restrict the recourse \mathbf{y} to a static function that does not depend on z . As we will reveal, we overcome this challenge by using a technique of dualizing twice similar to that in Roos et al. (2020), first over the recourse variables \mathbf{y} and then over the uncertain parameters z to absorb the conic nature of the original problem into a new uncertainty set while the polyhedral support and penalty show up as linear constraints of the resultant formulation. We can thus use familiar approximation methods such as affine recourse adaptation for this resulting problem. Although feasibility is not guaranteed with such approximations even under assumptions of complete recourse (see for *e.g.*, Bertsimas, Sim, and Zhang, 2019), our results however show that whenever the target satisfies $\tau \geq Z_0$, the *affine dual recourse adaptation* would always yield a feasible solution under the stated assumptions as follows.

Assumption 2. *We assume the following:*

- (i) **Solvable:** *The optimal nominal solutions \hat{x} and \hat{y} exist.*
- (ii) **Complete and bounded recourse:** *For any $\mathbf{v} \in \mathbb{R}^{n_f}$, there exists a $\mathbf{y} \in \mathbb{R}^{n_y}$ such that $\mathbf{B}\mathbf{y} \succeq_{\mathcal{K}} \mathbf{v}$. Moreover, there does not exist $\mathbf{y} \in \mathbb{R}^{n_y}$ such that $\mathbf{B}\mathbf{y} \succeq \mathbf{0}$ and $\mathbf{d}^\top \mathbf{y} < 0$. These conditions ensure that Problem (4.2) is always finite and strictly feasible.*
- (iii) **Polyhedral support:** *The uncertainty set \mathcal{Z} is a polytope*

$$\mathcal{Z} = \{ z \in \mathbb{R}^{n_z} \mid \mathbf{H}z \leq \mathbf{h} \},$$

for some $\mathbf{H} \in \mathbb{R}^{n_h \times n_z}$ and $\mathbf{h} \in \mathbb{R}_+^{n_h}$.

(iv) **Polyhedral penalty:** The polyhedral penalty function $p(\zeta) : \mathbb{R}^{n_z} \mapsto \mathbb{R}_+$ can be expressed as

$$p(\zeta) = \max_{(\lambda, \eta) \in \mathcal{V}} \{\lambda^\top \zeta - \eta\},$$

where \mathcal{V} is a polyhedral

$$\mathcal{V} = \{(\lambda, \eta) \in \mathbb{R}^{n_z} \times \mathbb{R}_+ \mid \exists \mu \in \mathbb{R}^{n_\mu} : \mathbf{M}\lambda + \mathbf{N}\mu + s\eta \leq \mathbf{t}\},$$

for some $\mathbf{M} \in \mathbb{R}^{n_m \times n_z}$, $\mathbf{N} \in \mathbb{R}^{n_m \times n_\mu}$, and $\mathbf{s}, \mathbf{t} \in \mathbb{R}^{n_m}$. In addition, (i) \mathcal{V} contains the origin so that $p(\zeta) \geq 0$ and $p(\mathbf{0}) = 0$, (ii) there exists $\hat{\mu} \in \mathbb{R}^{n_\mu}$ such that $\mathbf{N}\hat{\mu} < \mathbf{t}$, which ensures $p(\zeta) > 0$ if $\zeta \neq \mathbf{0}$, and (iii) \mathcal{V} is bounded, which ensures $p(\zeta) < \infty$.

We remark that the term *complete recourse* is an extension of the same term used in stochastic linear optimization (see for e.g., Birge and Louveaux, 2011) to our model where the second stage problem is a conic optimization problem. It ensures that Problem (4.2) is strictly feasible. To see the strict feasibility, let $\mathbf{v} \in \mathbb{R}^{n_f}$ such that $\mathbf{v} \succ_{\mathcal{K}} \mathbf{0}$, and under complete recourse, there exists a $\mathbf{y} \in \mathbb{R}^{n_y}$ such that $\mathbf{B}\mathbf{y} \succeq_{\mathcal{K}} \mathbf{f}(\mathbf{x}) + \mathbf{F}(\mathbf{x})\mathbf{z} + \mathbf{v} \succ_{\mathcal{K}} \mathbf{f}(\mathbf{x}) + \mathbf{F}(\mathbf{x})\mathbf{z}$. The bounded recourse condition ensures that the g function of Problem (4.2) is always finite.

It is common to choose a polyhedral norm as the penalty function, which has a similar representation.

Proposition 11 (Polyhedral norm). *Under Assumption 2, if the penalty function p is a norm, then it has the representation*

$$p(\zeta) = \max_{\lambda \in \mathbb{R}^{n_z}, \mu \in \mathbb{R}^{n_\mu}} \left\{ \lambda^\top \zeta \mid \mathbf{M}\lambda + \mathbf{N}\mu \leq \mathbf{t} \right\},$$

for which

$$\{\lambda \mid \mathbf{M}\lambda + \mathbf{N}\mu \leq \mathbf{t}\} = \{\lambda \mid -\mathbf{M}\lambda + \mathbf{N}\mu \leq \mathbf{t}\}.$$

Its dual norm is given by

$$p^*(\zeta) = \min_{\mu \in \mathbb{R}^{n_\mu}, \delta \in \mathbb{R}_+} \{\delta \mid \mathbf{M}\zeta + \mathbf{N}\mu \leq \delta\mathbf{t}\}.$$

Proof. Suppose that p is a norm function and define

$$\mathcal{J} = \bigcup_{\zeta \in \mathbb{R}^{n_z}} \operatorname{argmax}_{(\lambda, \eta) \in \mathcal{V}} \{\lambda^\top \zeta - \eta\}.$$

We will first show that $(\lambda^*, \eta^*) \in \mathcal{J}$ implies $\eta^* = 0$, that is, η is superfluous in the optimization problem underlying the definition of p . Suppose otherwise for the sake of a contradiction that there exists $(\zeta^*, \lambda^*, \eta^*) \in \mathbb{R}^{n_z} \times \mathbb{R}^{n_z} \times \mathbb{R}_{++}$ such that $(\lambda^*, \eta^*) \in \operatorname{argmax}_{(\lambda, \eta) \in \mathcal{V}} \{\lambda^\top \zeta^* - \eta\}$. It follows that $p(\zeta^*) = (\lambda^*)^\top \zeta^* - \eta^*$ and, as p is a norm, $p(2\zeta^*) = 2(\lambda^*)^\top \zeta^* - 2\eta^*$. Note also that

$$p(2\zeta^*) = \max_{(\lambda, \eta) \in \mathcal{V}} \{\lambda^\top (2\zeta^*) - \eta\} \geq (\lambda^*)^\top (2\zeta^*) - \eta^*.$$

By comparing $p(2\zeta^*)$ with its lower bound, we find $\eta^* \leq 0$, reaching hence a contradiction. In conclusion, η always vanishes at optimality, and we can assume that $\mathbf{s} = \mathbf{0}$

without any loss of generality:

$$p(\zeta) = \max_{\lambda \in \mathbb{R}^{n_z}, \mu \in \mathbb{R}^{n_\mu}} \left\{ \lambda^\top \zeta \mid M\lambda + N\mu \leq t \right\}.$$

Since $p(\zeta) = p(-\zeta)$ for all $\zeta \in \mathbb{R}^{n_z}$, the polytope $\mathcal{Q}_1 = \{\lambda \mid M\lambda + N\mu \leq t\}$ must be identical to the polytope $\mathcal{Q}_2 = \{\lambda \mid -M\lambda + N\mu \leq t\}$. Otherwise, suppose $\lambda^* \in \mathcal{Q}_1$ but $\lambda^* \notin \mathcal{Q}_2$, then by a separating hyperplane argument there would exist a vector $\zeta^* \in \mathbb{R}^{n_z}$ such that

$$p(\zeta^*) = \max_{\lambda \in \mathcal{Q}_1} \{\lambda^\top \zeta^*\} \geq \lambda^{*\top} \zeta^* > \max_{\lambda \in \mathcal{Q}_2} \{\lambda^\top \zeta^*\} = p(-\zeta^*),$$

which is a contradiction. Likewise, similar contradiction can be established if $\lambda^* \in \mathcal{Q}_2$ but $\lambda^* \notin \mathcal{Q}_1$. Hence, $\mathcal{Q}_1 = \mathcal{Q}_2$. Next, we derive the dual norm p^* :

$$\begin{aligned} p^*(\zeta) &= \max_{\omega \in \mathbb{R}^{n_z}} \left\{ \omega^\top \zeta \mid p(\omega) \leq 1 \right\} \\ &= \max_{\omega \in \mathbb{R}^{n_z}} \left\{ \omega^\top \zeta \mid \lambda^\top \omega \leq 1, \forall (\lambda, \mu) : M\lambda + N\mu \leq t \right\} \\ &= \max_{\omega \in \mathbb{R}^{n_z}, \alpha \in \mathbb{R}_+^{n_m}} \left\{ \omega^\top \zeta \mid \alpha^\top t \leq 1, M^\top \alpha = \omega, N^\top \alpha = 0 \right\} \\ &= \max_{\alpha \in \mathbb{R}_+^{n_m}} \left\{ \alpha^\top M\zeta \mid \alpha^\top t \leq 1, N^\top \alpha = 0 \right\} \\ &= \min_{\mu \in \mathbb{R}^{n_\mu}, \delta \in \mathbb{R}_+} \left\{ \delta \mid M\zeta + N\mu \leq \delta t \right\}, \end{aligned}$$

where the third maximization problem constitutes a robust counterpart of the second and the fifth equation holds due to the standard linear optimization duality argument. \square

Example 12 (Budgeted norm). We illustrate the modeling potential of the norm-based penalty defined in Proposition 11 with a budgeted norm which computes the sum of the $\Gamma \in \{1, \dots, n_z\}$ largest absolute components of an n_z -dimensional vector, i.e.,

$$p_\Gamma(\zeta) = \max_{\mathcal{S} \subseteq [n_z], |\mathcal{S}| = \Gamma} \sum_{i \in \mathcal{S}} |\zeta_i|$$

so that $p_1(\zeta) = \|\zeta\|_\infty$ and $p_{n_z}(\zeta) = \|\zeta\|_1$. This can be represented as the following linear optimization problem

$$\begin{aligned} p_\Gamma(\zeta) &= \max_{\lambda \in \mathbb{R}^{n_z}} \left\{ \lambda^\top \zeta \mid \sum_{i \in [n_z]} |\lambda_i| \leq \Gamma, |\lambda_i| \leq 1, \forall i \in [n_z] \right\} \\ &= \max_{\lambda, \mu \in \mathbb{R}^{n_z}} \left\{ \lambda^\top \zeta \mid \begin{array}{l} \sum_{i \in [n_z]} \mu_i \leq \Gamma \\ \lambda_i - \mu_i \leq 0 \\ -\lambda_i - \mu_i \leq 0 \\ \mu_i \leq 1 \end{array} \quad \forall i \in [n_z] \right\}, \end{aligned}$$

which satisfies the properties of the polyhedral penalty in Assumption 2.

We also remark that since second-order conic constraints can be approximated accurately via a modest sized polyhedron (Ben-Tal and Nemirovski, 2001), the representation of polyhedral penalty is quite broad and can be used to approximate many different types of convex nonlinear penalty functions such as, *inter alia*, convex polynomials and ℓ_p -norms, for $p \geq 1$.

Under Assumption 2, we will show that the robust satisficing problem (4.5) with a conic constraint and a polyhedral uncertainty set admits an equivalent reformulation as a problem of a similar nature but with linear constraints and a conic uncertainty set. The following result is a precursor for obtaining the alternate formulation of the robust satisficing problem, which would enable us to obtain a safe approximation via affine dual recourse adaptation.

Proposition 12. *Under Assumption 2, for any $\mathbf{a} \in \mathbb{R}^{n_z}$ and $k \geq 0$, we have*

$$\max_{\mathbf{z} \in \mathcal{Z}} \left\{ \mathbf{a}^\top \mathbf{z} - kp(\mathbf{z}) \right\} = \min_{\eta \in \mathbb{R}_+, \boldsymbol{\beta} \in \mathbb{R}_+^{n_h}} \left\{ \boldsymbol{\beta}^\top \mathbf{h} + \eta \mid (\mathbf{a} - \mathbf{H}^\top \boldsymbol{\beta}, \eta, k) \in \bar{\mathcal{V}} \right\}$$

where $\bar{\mathcal{V}}$ is the perspective cone of \mathcal{V} given by

$$\bar{\mathcal{V}} = \{(\boldsymbol{\lambda}, \eta, k) \in \mathbb{R}^{n_z} \times \mathbb{R}_+^2 \mid \exists \boldsymbol{\mu} \in \mathbb{R}^{n_\mu} : \mathbf{M}\boldsymbol{\lambda} + \mathbf{N}\boldsymbol{\mu} + \mathbf{s}\eta \leq \mathbf{t}k\}.$$

If the penalty function p is a norm, then we have

$$\max_{\mathbf{z} \in \mathcal{Z}} \left\{ \mathbf{a}^\top \mathbf{z} - kp(\mathbf{z}) \right\} = \min_{\boldsymbol{\beta} \in \mathbb{R}_+^{n_h}} \left\{ \boldsymbol{\beta}^\top \mathbf{h} \mid p^*(\mathbf{a} - \mathbf{H}^\top \boldsymbol{\beta}) \leq k \right\}.$$

Proof. We first consider $k > 0$. From the definition of p in Assumption 2, we find

$$\max_{\mathbf{z} \in \mathcal{Z}} \left\{ \mathbf{a}^\top \mathbf{z} - kp(\mathbf{z}) \right\} = \max_{\mathbf{z} \in \mathcal{Z}} \min_{(\boldsymbol{\lambda}, \eta) \in \mathcal{V}} \left\{ (\mathbf{a} - k\boldsymbol{\lambda})^\top \mathbf{z} + k\eta \right\}. \quad (4.12)$$

Since this is linear optimization problem, by the standard linear optimization duality argument, this latter maximization problem can be expressed as

$$\begin{aligned} & \max_{\mathbf{z} \in \mathcal{Z}} \min_{(\boldsymbol{\lambda}, \eta) \in \mathcal{V}} \left\{ (\mathbf{a} - k\boldsymbol{\lambda})^\top \mathbf{z} + k\eta \right\} \\ &= \min_{(\boldsymbol{\lambda}, \eta) \in \mathcal{V}} \max_{\mathbf{z} \in \mathcal{Z}} \left\{ (\mathbf{a} - k\boldsymbol{\lambda})^\top \mathbf{z} + k\eta \right\} \\ &= \min_{(\boldsymbol{\lambda}, \eta) \in \mathcal{V}, \boldsymbol{\beta}} \left\{ \boldsymbol{\beta}^\top \mathbf{h} + k\eta \mid \boldsymbol{\beta} \geq \mathbf{0}, \mathbf{H}^\top \boldsymbol{\beta} = \mathbf{a} - k\boldsymbol{\lambda} \right\} \\ &= \min_{\boldsymbol{\beta} \geq \mathbf{0}, \eta \geq 0} \left\{ \boldsymbol{\beta}^\top \mathbf{h} + k\eta \mid (\mathbf{a} - \mathbf{H}^\top \boldsymbol{\beta}, k\eta, k) \in \bar{\mathcal{V}} \right\} \\ &= \min_{\boldsymbol{\beta} \geq \mathbf{0}, \eta \geq 0} \left\{ \boldsymbol{\beta}^\top \mathbf{h} + \eta \mid (\mathbf{a} - \mathbf{H}^\top \boldsymbol{\beta}, \eta, k) \in \bar{\mathcal{V}} \right\}, \end{aligned}$$

where the first interchange between minimization and maximization is justified because \mathcal{Z} is compact, and this concludes the desired equivalence. Next, we consider the case when $k = 0$. Since \mathcal{V} is bounded, we must have $\{(\boldsymbol{\lambda}, \eta) \mid (\boldsymbol{\lambda}, \eta, 0) \in \bar{\mathcal{V}}\} = \{(\mathbf{0}, 0)\}$. Hence, $(\mathbf{a} - \mathbf{H}^\top \boldsymbol{\beta}, \eta, 0) \in \bar{\mathcal{V}}$ is equivalent to $\eta = 0$ and $\mathbf{H}^\top \boldsymbol{\beta} = \mathbf{a}$. By noting that $\max_{\mathbf{z} \in \mathcal{Z}} \mathbf{a}^\top \mathbf{z} = \min_{\boldsymbol{\beta} \in \mathbb{R}_+^{n_h}} \{\boldsymbol{\beta}^\top \mathbf{h} \mid \mathbf{H}^\top \boldsymbol{\beta} = \mathbf{a}\}$, the first half of the proposition follows.

If the penalty function p is a norm, from the derivation of the dual norm in Proposition 11, we have

$$\begin{aligned} & \min_{\beta \in \mathbb{R}_+^{n_h}} \left\{ \beta^\top \mathbf{h} \mid p^*(\mathbf{a} - \mathbf{H}^\top \beta) \leq k \right\} \\ &= \min_{\beta \in \mathbb{R}_+^{n_h}, \mu \in \mathbb{R}^{n_\mu}, \delta \in \mathbb{R}_+} \left\{ \beta^\top \mathbf{h} \mid \delta \leq k, M(\mathbf{a} - \mathbf{H}^\top \beta) + \mathbf{N}\mu \leq \delta \mathbf{t} \right\} \\ &= \min_{\beta \in \mathbb{R}_+^{n_h}, \mu \in \mathbb{R}^{n_\mu}} \left\{ \beta^\top \mathbf{h} \mid M(\mathbf{a} - \mathbf{H}^\top \beta) + \mathbf{N}\mu \leq k \mathbf{t} \right\}, \end{aligned}$$

where the second equality follows because, to ensure that $(\mathbf{0}, 0) \in \mathcal{V}$, \mathbf{t} must be non-negative making the constraint $\delta \leq k$ binding at optimality. Noting from the previous half of this proposition and the proof of Proposition 11 that, as s vanishes when the penalty function is a norm, the latter minimization problem is equivalent to $\max_{z \in \mathcal{Z}} \{ \mathbf{a}^\top z - kp(z) \}$ completes the proof. \square

Theorem 18. Under Assumption 2, for any $\mathbf{x} \in \mathbb{R}^{n_x}$ and $k \geq 0$, the robust satisficing constraint

$$g(\mathbf{x}, z) \leq kp(z), \quad \forall z \in \mathcal{Z}$$

is equivalent to

$$\forall \rho \in \mathcal{P}, \exists \beta \in \mathbb{R}^{n_h}, \mu \in \mathbb{R}^{n_\mu}, \eta \in \mathbb{R} : \begin{cases} \rho^\top \mathbf{f}(\mathbf{x}) + \beta^\top \mathbf{h} + \eta \leq 0 \\ M(\mathbf{F}(\mathbf{x})^\top \rho - \mathbf{H}^\top \beta) + \mathbf{N}\mu + s\eta \leq tk \\ \beta \geq \mathbf{0}, \eta \geq 0, \end{cases}$$

where $\mathcal{P} = \{ \rho \in \mathcal{K}^* \mid \mathbf{B}^\top \rho = \mathbf{d} \}$.

Proof. First, it follows from the specificity of g in (4.2) that

$$g(\mathbf{x}, z) \leq kp(z), \quad \forall z \in \mathcal{Z} \iff \max_{z \in \mathcal{Z}} \min_{\mathbf{y}} \left\{ \mathbf{d}^\top \mathbf{y} - kp(z) \mid \mathbf{B}\mathbf{y} \succeq_{\mathcal{K}} \mathbf{f}(\mathbf{x}) + \mathbf{F}(\mathbf{x})z \right\} \leq 0.$$

Under complete and bounded recourse, observe that the inner minimization (over \mathbf{y}) is strictly feasible and its objective is finite. Thus, we can transform it into a maximization problem via conic duality, that is,

$$\begin{aligned} g(\mathbf{x}, z) \leq kp(z), \quad \forall z \in \mathcal{Z} &\iff \max_{z \in \mathcal{Z}} \max_{\rho \in \mathcal{P}} \left\{ \rho^\top (\mathbf{f}(\mathbf{x}) + \mathbf{F}(\mathbf{x})z) - kp(z) \right\} \leq 0 \\ &\iff \max_{\rho \in \mathcal{P}} \left\{ \rho^\top \mathbf{f}(\mathbf{x}) + \max_{z \in \mathcal{Z}} \left\{ \rho^\top \mathbf{F}(\mathbf{x})z - kp(z) \right\} \right\} \leq 0. \end{aligned}$$

Invoking Proposition 12 to transform the inner maximization (over z) to a minimization problem (over β, μ and η) completes the proof. \square

Theorem 18 allows us to reformulate Problem (4.5), which is the same as Problem (4.11), as a classical adaptive robust linear optimization model with a conic uncertainty set as follows,

$$\begin{aligned}
& \min && k \\
& \text{s.t.} && \boldsymbol{\rho}^\top \mathbf{f}(\mathbf{x}) + \boldsymbol{\beta}(\boldsymbol{\rho})^\top \mathbf{h} + \eta(\boldsymbol{\rho}) \leq 0 && \forall \boldsymbol{\rho} \in \mathcal{P} \\
& && \mathbf{M}(\mathbf{F}(\mathbf{x})^\top \boldsymbol{\rho} - \mathbf{H}^\top \boldsymbol{\beta}(\boldsymbol{\rho})) + \mathbf{N}\boldsymbol{\mu}(\boldsymbol{\rho}) + s\eta(\boldsymbol{\rho}) \leq tk && \forall \boldsymbol{\rho} \in \mathcal{P} \\
& && \boldsymbol{\beta}(\boldsymbol{\rho}) \geq \mathbf{0}, \eta(\boldsymbol{\rho}) \geq 0 && \forall \boldsymbol{\rho} \in \mathcal{P} \\
& && \mathbf{c}^\top \mathbf{x} \leq \tau \\
& && \mathbf{x} \in \mathcal{X}, k \in \mathbb{R}_+, \boldsymbol{\beta} \in \mathcal{R}^{n_f, n_h}, \boldsymbol{\mu} \in \mathcal{R}^{n_f, n_\mu}, \eta \in \mathcal{R}^{n_f, 1},
\end{aligned} \tag{4.13}$$

where $(\boldsymbol{\beta}, \boldsymbol{\mu}, \eta)$ replaces \mathbf{y} as the recourse variables and \mathcal{P} represents the (dual) uncertainty set defined in Theorem 18. To distinguish the two different recourse variables, we may refer \mathbf{y} as the *primal recourse* and $(\boldsymbol{\beta}, \boldsymbol{\mu}, \eta)$ as the *dual recourse*. Comparing Problems (4.11) and (4.13), we find that, even though Problem (4.11) is always feasible (thanks to Assumption 2), it is not necessarily easy to construct a feasible solution, let alone computing the optimal solution. In contrast, we will argue below that Problem (4.13) admits an almost trivial feasible dual recourse solution. The existence of this feasible solution will then be used to support the appropriateness of approximately solving Problem (4.13) using *affine dual recourse adaption* as follows:

$$\begin{aligned}
& \min && k \\
& \text{s.t.} && \boldsymbol{\rho}^\top \mathbf{f}(\mathbf{x}) + \boldsymbol{\beta}(\boldsymbol{\rho})^\top \mathbf{h} + \eta(\boldsymbol{\rho}) \leq 0 && \forall \boldsymbol{\rho} \in \mathcal{P} \\
& && \mathbf{M}(\mathbf{F}(\mathbf{x})^\top \boldsymbol{\rho} - \mathbf{H}^\top \boldsymbol{\beta}(\boldsymbol{\rho})) + \mathbf{N}\boldsymbol{\mu}(\boldsymbol{\rho}) + s\eta(\boldsymbol{\rho}) \leq tk && \forall \boldsymbol{\rho} \in \mathcal{P} \\
& && \boldsymbol{\beta}(\boldsymbol{\rho}) \geq \mathbf{0}, \eta(\boldsymbol{\rho}) \geq 0 && \forall \boldsymbol{\rho} \in \mathcal{P} \\
& && \mathbf{c}^\top \mathbf{x} \leq \tau \\
& && \mathbf{x} \in \mathcal{X}, k \in \mathbb{R}_+, \boldsymbol{\beta} \in \mathcal{L}^{n_f, n_h}, \boldsymbol{\mu} \in \mathcal{L}^{n_f, n_\mu}, \eta \in \mathcal{L}^{n_f, 1},
\end{aligned} \tag{4.14}$$

where $\mathcal{L}^{m,n}$ denotes the sub-class of functions in $\mathcal{R}^{m,n}$ that are affinely dependent on the inputs as follows:

$$\mathcal{L}^{m,n} = \{ \mathbf{y} \in \mathcal{R}^{m,n} \mid \exists \boldsymbol{\pi} \in \mathbb{R}^n, \boldsymbol{\Pi} \in \mathbb{R}^{n \times m} : \mathbf{y}(\mathbf{z}) = \boldsymbol{\pi} + \boldsymbol{\Pi}\mathbf{z} \}.$$

Theorem 19. *Under Assumption 2, there exists a feasible solution for Problem (4.14) whenever the target satisfies $\tau \geq Z_0$. Moreover, Problem (4.14) is practicably solvable under Assumption 1.*

Proof. We first show that the solution $\mathbf{x} = \hat{\mathbf{x}}$, $\boldsymbol{\beta}(\boldsymbol{\rho}) = \mathbf{0}$, and $\eta(\boldsymbol{\rho}) = 0$ robustly satisfies the first and third constraints of Problem (4.14). To achieve this, it suffices to derive the maximum value that the left-hand side of the first constraint could take, *i.e.*,

$$\max_{\boldsymbol{\rho} \in \mathcal{P}} \boldsymbol{\rho}^\top \mathbf{f}(\hat{\mathbf{x}}) = \min_{\mathbf{y}} \left\{ \mathbf{d}^\top \mathbf{y} \mid \mathbf{B}\mathbf{y} \succeq_{\mathcal{K}} \mathbf{f}(\hat{\mathbf{x}}) \right\} = \mathbf{d}^\top \hat{\mathbf{y}} = g(\hat{\mathbf{x}}, \mathbf{0}) \leq 0,$$

where the first equality is due to the strong duality (as the minimization problem is strictly feasible) and the second equality holds because of the optimality of the recourse variable $\hat{\mathbf{y}}$ given the decision $\hat{\mathbf{x}}$ in (4.10).

We next show that the remaining constraints can be satisfied because there exists $\hat{k} > 0$ such that

$$MF(\hat{x})^\top \rho + N\hat{\mu}\hat{k} \leq t\hat{k} \quad \forall \rho \in \mathcal{P}. \quad (4.15)$$

Indeed, since $N\hat{\mu} < t$, it implies that the set $\{\lambda \mid M\lambda + N\hat{\mu} \leq t\}$ must contain the origin in its interior. Hence, there exists a norm $\|\cdot\|$ such that

$$\{\lambda \mid \|\lambda\| \leq 1\} \subseteq \{\lambda \mid M\lambda + N\hat{\mu} \leq t\}.$$

Therefore, it suffices to show that there exists a finite $\hat{k} > 0$ such that

$$\max_{\rho \in \mathcal{P}} \|F(\hat{x})^\top \rho\| \leq \hat{k}.$$

Suppose that the dual uncertainty set \mathcal{P} is unbounded for the sake of a contradiction. Then, there exists a vector $v \in \mathbb{R}^{n_f}$ such that $\max_{\rho \in \mathcal{P}} \rho^\top v$ is unbounded, and therefore its corresponding dual $\min_y \{d^\top y \mid By \succeq_{\mathcal{K}} v\}$ must be infeasible, which contradicts Assumption 2. Hence, \mathcal{P} is a bounded set, and a finite and positive \hat{k} exists. Hence, the solution $x = \hat{x}$, $\beta(\rho) = \mathbf{0}$, $\mu(\rho) = \hat{\mu}\hat{k}$, $k = \hat{k}$ and $\eta(\rho) = 0$ robustly satisfies the second constraint of Problem (4.14).

To show that Problem (4.14) can be expressed as a modest sized conic optimization problem, observe that since the recourse variables are restricted to affine functions, we can express Problem (4.14) more compactly as

$$\begin{aligned} \min \quad & k \\ \text{s.t.} \quad & \gamma(x, k, L) + \Gamma(x, k, L)\rho \leq \mathbf{0} \quad \forall \rho \in \mathcal{P} \\ & x \in \mathcal{X}, k \in \mathbb{R}_+, L \in \mathbb{R}^{(n_h+n_\mu+1) \times (n_f+1)}, \end{aligned}$$

where L gathers the affine dual recourse adaption coefficients of (β, μ, η) and γ, Γ are appropriate affine mappings. We next show that under Assumption 2, for any $\gamma \in \mathbb{R}^{n_\gamma}$ and $\Gamma \in \mathbb{R}^{n_\gamma \times n_f}$, the robust counterpart of $\gamma + \Gamma\rho \leq \mathbf{0}$, $\forall \rho \in \mathcal{P}$ is given by the following linear conic constraint

$$\exists V \in \mathbb{R}^{n_\gamma \times n_y} : \begin{cases} \gamma + Vd \leq \mathbf{0} \\ B(V_i)^\top \succeq_{\mathcal{K}} \Gamma_i^\top \quad \forall i \in [n_\gamma]. \end{cases}$$

Indeed, observe that the given robust constraint can be written down as

$$\max_{\rho \in \mathcal{P}} \gamma_i + \Gamma_i \rho \leq 0 \quad \forall i \in [n_\gamma] \iff \min_{v^i \in \mathbb{R}^{n_y}} \left\{ \gamma_i + d^\top v^i \mid Bv^i \succeq_{\mathcal{K}} \Gamma_i^\top \right\} \leq 0 \quad \forall i \in [n_\gamma],$$

where the equivalence holds because the minimization problem is convex and strictly feasible. We then denote $[v^1, \dots, v^{n_\gamma}]^\top$ by V . Hence, the problem is practicably solvable under Assumption 1, which completes the proof. \square

This result is computationally significant since, despite the difficulty to solve it exactly, if $\tau \geq Z_0$, we can still obtain a feasible solution of Problem (4.14) by solving a modest sized conic optimization problem.

4.4 Two-stage adaptive optimization

In this section, we explore how the affine dual recourse adaptation can be used to provide safe approximations to two-stage adaptive optimization problems. We investigate a two-stage adaptive linear optimization problem under complete recourse focusing on the ℓ_1 -norm penalty function, $p(\zeta) = \|\zeta\|_1$, which has been previously tackled by Long, Sim, and Zhou (2021) in the data-driven setting. For simplicity, we first focus on the stochastic-free setting with the nominal value being $\hat{z} = \mathbf{0}$. With $\mathcal{K} = \mathbb{R}_+^{n_f}$, the two-stage nominal problem can be written as:

$$\begin{aligned} Z_0 = \min \quad & \mathbf{c}^\top \mathbf{x} + \mathbf{d}^\top \mathbf{y} \\ \text{s.t.} \quad & \mathbf{B}\mathbf{y} \geq \mathbf{f}(\mathbf{x}) \\ & \mathbf{x} \in \mathcal{X}, \mathbf{y} \in \mathbb{R}^{n_y}, \end{aligned} \quad (4.16)$$

which has the same format as Problem (4.6). We analogously denote by $(\hat{\mathbf{x}}, \hat{\mathbf{y}})$ an optimal nominal solution. Assuming further that $\hat{z} = \mathbf{0}$, the robust satisficing model, which is based on Problem (4.7), becomes the following standard two-stage robust linear program with (\mathbf{x}, k) being the first-stage decisions and \mathbf{y} being the recourse or second-stage decisions:

$$\begin{aligned} \min \quad & k \\ \text{s.t.} \quad & \mathbf{c}^\top \mathbf{x} + \mathbf{d}^\top \mathbf{y}(z) \leq \tau + k\|z\|_1 \quad \forall z \in \mathcal{Z} \\ & \mathbf{B}\mathbf{y}(z) \geq \mathbf{f}(\mathbf{x}) + \mathbf{F}(\mathbf{x})z \quad \forall z \in \mathcal{Z} \\ & \mathbf{x} \in \mathcal{X}, \mathbf{y} \in \mathcal{R}^{n_z, n_y}, k \in \mathbb{R}_+. \end{aligned} \quad (4.17)$$

Generally, two-stage robust linear programs are not tractable and are typically solved approximately via affine primal recourse adaptation, that is,

$$\begin{aligned} \min \quad & k \\ \text{s.t.} \quad & \mathbf{c}^\top \mathbf{x} + \mathbf{d}^\top \mathbf{y}(z) \leq \tau + k\|z\|_1 \quad \forall z \in \mathcal{Z} \\ & \mathbf{B}\mathbf{y}(z) \geq \mathbf{f}(\mathbf{x}) + \mathbf{F}(\mathbf{x})z \quad \forall z \in \mathcal{Z} \\ & \mathbf{x} \in \mathcal{X}, \mathbf{y} \in \mathcal{L}^{n_z, n_y}, k \in \mathbb{R}_+. \end{aligned} \quad (4.18)$$

Note that, while Problem (4.17) is always feasible under Assumption 2, it is not necessarily the case for the restricted problem (4.18) (Long, Sim, and Zhou, 2021). As a result, we consider a more flexible, non-affine primal recourse adaptation extension with extra coefficients $\mathbf{q}^\dagger \in \mathbb{R}^{n_y}$:

$$\mathbf{y}(z) = \mathbf{q} + \mathbf{Q}z + \mathbf{q}^\dagger\|z\|_1. \quad (4.19)$$

Observe that when such a non-linear primal recourse adaptation is substituted for $\mathbf{y}(z)$ in Problem (4.17), the resultant optimization problem can be written down as

$$\begin{aligned} \min \quad & k \\ \text{s.t.} \quad & \mathbf{c}^\top \mathbf{x} + \mathbf{d}^\top (\mathbf{q} + \mathbf{Q}z + \mathbf{q}^\dagger\|z\|_1) \leq \tau + k\|z\|_1 \quad \forall z \in \mathcal{Z} \\ & \mathbf{B}(\mathbf{q} + \mathbf{Q}z + \mathbf{q}^\dagger\|z\|_1) \geq \mathbf{f}(\mathbf{x}) + \mathbf{F}(\mathbf{x})z \quad \forall z \in \mathcal{Z} \\ & k - \mathbf{d}^\top \mathbf{q}^\dagger \geq 0, \mathbf{B}\mathbf{q}^\dagger \geq \mathbf{0} \\ & \mathbf{x} \in \mathcal{X}, \mathbf{q} \in \mathbb{R}^{n_y}, \mathbf{Q} \in \mathbb{R}^{n_y \times n_z}, \mathbf{q}^\dagger \in \mathbb{R}^{n_y}, k \in \mathbb{R}_+, \end{aligned} \quad (4.20)$$

where the two linear constraints $k - \mathbf{d}^\top \mathbf{q}^\dagger \geq 0$ and $\mathbf{B}\mathbf{q}^\dagger \geq \mathbf{0}$ are added to ensure that the two robust constraints are concave in the uncertain \mathbf{z} and consequently tractability of Problem (4.20). Observe that with $\mathbf{q}^\dagger = \mathbf{0}$, Problem (4.20) is equivalent to Problem (4.18), implying that the former problem is a less conservative approximation.

Theorem 20. (Long, Sim, and Zhou, 2021). *Under complete recourse, there is always a feasible solution to Problem (4.20) whenever the target satisfies $\tau \geq Z_0$.*

Proof. Consider the following solution to Problem (4.20): $\mathbf{x} = \hat{\mathbf{x}}$, $\mathbf{q} = \hat{\mathbf{y}}$, $\mathbf{Q} = \mathbf{0}$ and $k = \mathbf{d}^\top \hat{\mathbf{q}}^\dagger$ where $\hat{\mathbf{q}}^\dagger \in \mathbb{R}^{n_y}$ satisfies $\mathbf{B}\hat{\mathbf{q}}^\dagger \geq \mathbf{0}$ and $\mathbf{B}\hat{\mathbf{q}}^\dagger \geq \max_{i \in [n_f], j \in [n_z]} |\mathbf{F}_{ij}(\hat{\mathbf{x}})| \cdot \mathbf{1}$. Note that $\hat{\mathbf{q}}^\dagger$ always exists because of complete recourse. The suggested solution robustly satisfies first constraint of Problem (4.20) because

$$\mathbf{c}^\top \hat{\mathbf{x}} + \mathbf{d}^\top (\hat{\mathbf{y}} + \mathbf{q}^\dagger \|\mathbf{z}\|_1) = \mathbf{c}^\top \hat{\mathbf{x}} + \mathbf{d}^\top \hat{\mathbf{y}} + k \|\mathbf{z}\|_1 = Z_0 + k \|\mathbf{z}\|_1 \leq \tau + k \|\mathbf{z}\|_1.$$

Moreover, the second constraint is also robustly satisfied as

$$\begin{aligned} \mathbf{B}(\hat{\mathbf{y}} + \mathbf{q}^\dagger \|\mathbf{z}\|_1) &\geq \mathbf{f}(\hat{\mathbf{x}}) + \mathbf{B}\mathbf{q}^\dagger \|\mathbf{z}\|_1 \\ &\geq \mathbf{f}(\hat{\mathbf{x}}) + \|\mathbf{z}\|_1 \left\{ \max_{i \in [n_f], j \in [n_z]} |\mathbf{F}_{ij}(\hat{\mathbf{x}})| \right\} \cdot \mathbf{1} \geq \mathbf{f}(\hat{\mathbf{x}}) + \mathbf{F}(\hat{\mathbf{x}})\mathbf{z}, \quad \forall \mathbf{z} \in \mathcal{Z} \end{aligned}$$

where the first two inequalities follow from the feasibility of $(\hat{\mathbf{x}}, \hat{\mathbf{y}})$ in the nominal problem (4.16) and the construction of \mathbf{q}^\dagger , respectively. Consequently, it readily follows that the constructed solution is feasible in Problem (4.20). \square

Next, we derive the robust counterpart of Problem (4.20).

Proposition 13. *Problem (4.20) is equivalent to*

$$\begin{aligned} \min \quad & k \\ \text{s.t.} \quad & \mathbf{c}^\top \mathbf{x} + \mathbf{d}^\top \mathbf{q} + \mathbf{h}^\top \mathbf{w}^0 \leq \tau \\ & - (k - \mathbf{d}^\top \mathbf{q}^\dagger) \mathbf{1} \leq \mathbf{H}^\top \mathbf{w}^0 - \mathbf{Q}^\top \mathbf{d} \leq (k - \mathbf{d}^\top \mathbf{q}^\dagger) \mathbf{1} \\ & \mathbf{f}_i(\mathbf{x}) + \mathbf{h}^\top \mathbf{w}^i \leq \mathbf{B}_i \mathbf{q}^\dagger \quad \forall i \in [n_f] \\ & - \mathbf{B}_i \mathbf{q}^\dagger \mathbf{1} \leq \mathbf{H}^\top \mathbf{w}^i - \mathbf{F}_i^\top(\mathbf{x}) + \mathbf{Q}^\top \mathbf{B}_i^\top \leq \mathbf{B}_i \mathbf{q}^\dagger \mathbf{1} \quad \forall i \in [n_f] \\ & \mathbf{x} \in \mathcal{X}, \mathbf{q} \in \mathbb{R}^{n_y}, \mathbf{Q} \in \mathbb{R}^{n_y \times n_z}, \mathbf{q}^\dagger \in \mathbb{R}^{n_y}, \mathbf{w}^0, \dots, \mathbf{w}^{n_f} \in \mathbb{R}_+^{n_h}, k \in \mathbb{R}_+. \end{aligned} \tag{4.21}$$

Proof. The first robust constraint of Problem (4.20) can be expressed as

$$\max_{\mathbf{z}} \left\{ \mathbf{d}^\top \mathbf{Q}\mathbf{z} - (k - \mathbf{d}^\top \mathbf{q}^\dagger) \|\mathbf{z}\|_1 \mid \mathbf{H}\mathbf{z} \leq \mathbf{h} \right\} \leq \tau - \mathbf{d}^\top \mathbf{q} - \mathbf{c}^\top \mathbf{x}.$$

By Proposition 12, we can replace the maximization problem on the left-hand side of by a minimization problem:

$$\min_{\mathbf{w}^0} \left\{ \mathbf{h}^\top \mathbf{w}^0 \mid \|\mathbf{H}^\top \mathbf{w}^0 - \mathbf{Q}^\top \mathbf{d}\|_\infty \leq k - \mathbf{d}^\top \mathbf{q}^\dagger, \mathbf{w}^0 \geq \mathbf{0} \right\}.$$

Similarly, the second robust constraint of problem (4.20) can be written down as

$$\max_{\mathbf{z}} \left\{ (\mathbf{F}_i(\mathbf{x}) - \mathbf{B}_i \mathbf{Q})\mathbf{z} - \mathbf{B}_i \mathbf{q}^\dagger \|\mathbf{z}\|_1 : \mathbf{H}\mathbf{z} \leq \mathbf{h} \right\} \leq \mathbf{B}_i \mathbf{q} - \mathbf{f}_i(\mathbf{x}) \quad \forall i \in [n_f],$$

whose left-hand side maximization problem can be replaced by

$$\min_{\mathbf{w}^i} \left\{ \mathbf{h}^\top \mathbf{w}^i : \|\mathbf{H}^\top \mathbf{w}^i - \mathbf{F}_i^\top(\mathbf{x}) + \mathbf{Q}^\top \mathbf{B}_i^\top\|_\infty \leq \mathbf{B}_i \mathbf{q}^\dagger, \mathbf{w}^i \geq \mathbf{0} \right\} \quad \forall i \in [n_f],$$

Finally, the two deterministic linear constraints (namely, $k - \mathbf{d}^\top \mathbf{q}^\dagger \geq 0$ and $\mathbf{B} \mathbf{q}^\dagger \geq \mathbf{0}$) of (4.20) are redundant in view of problem (4.21) and can therefore be safely omitted. The proof is thus completed. \square

Next, we will similarly analyze the dual robust satisficing problem (4.13) when $p(\zeta) = \|\zeta\|_1$ and $\mathcal{K} = \mathbb{R}_+^{n_f}$. From Proposition 12, with $p^*(\zeta) = \|\zeta\|_\infty$, Problem (4.13) reduces to

$$\begin{aligned} \min \quad & k \\ \text{s.t.} \quad & \mathbf{c}^\top \mathbf{x} + \boldsymbol{\rho}^\top \mathbf{f}(\mathbf{x}) + \boldsymbol{\beta}(\boldsymbol{\rho})^\top \mathbf{h} \leq \tau \quad \forall \boldsymbol{\rho} \in \mathcal{P} \\ & -k\mathbf{1} \leq \mathbf{H}^\top \boldsymbol{\beta}(\boldsymbol{\rho}) - \mathbf{F}(\mathbf{x})^\top \boldsymbol{\rho} \leq k\mathbf{1} \quad \forall \boldsymbol{\rho} \in \mathcal{P} \\ & \boldsymbol{\beta}(\boldsymbol{\rho}) \geq \mathbf{0} \quad \forall \boldsymbol{\rho} \in \mathcal{P} \\ & \mathbf{x} \in \mathcal{X}, k \in \mathbb{R}_+, \boldsymbol{\beta} \in \mathcal{R}^{n_f, n_h}, \end{aligned} \quad (4.22)$$

where the dual uncertainty set \mathcal{P} is $\{\boldsymbol{\rho} \in \mathbb{R}_+^{n_f} \mid \mathbf{B}^\top \boldsymbol{\rho} = \mathbf{d}\}$. We note that Problem (4.22) and the primal robust satisficing model (4.17) are equivalent. However, unlike Problem (4.17) which may not admit a feasible affine primal recourse \mathbf{y} , Problem (4.22) *always* admits a feasible affine dual recourse for $\boldsymbol{\beta}$. Hence, for this problem, we are not required to come up with an ingenious idea of how to construct a non-affine recourse adaptation that can ensure feasibility. Our objective here is therefore to show that, despite being simpler, the affine dual recourse adaptation of Problem (4.22) is closer to the original Problem (4.17) compared to the previously discussed non-affine primal recourse adaptation of Problem (4.17) itself.

To begin with, we write down the affine recourse approximation of Problem (4.22) as

$$\begin{aligned} \min \quad & k \\ \text{s.t.} \quad & \mathbf{c}^\top \mathbf{x} + \boldsymbol{\rho}^\top \mathbf{f}(\mathbf{x}) + (\boldsymbol{\pi} + \mathbf{\Pi} \boldsymbol{\rho})^\top \mathbf{h} \leq \tau \quad \forall \boldsymbol{\rho} \in \mathcal{P} \\ & -k\mathbf{1} \leq \mathbf{H}^\top (\boldsymbol{\pi} + \mathbf{\Pi} \boldsymbol{\rho}) - \mathbf{F}(\mathbf{x})^\top \boldsymbol{\rho} \leq k\mathbf{1} \quad \forall \boldsymbol{\rho} \in \mathcal{P} \\ & \boldsymbol{\pi} + \mathbf{\Pi} \boldsymbol{\rho} \geq \mathbf{0} \quad \forall \boldsymbol{\rho} \in \mathcal{P} \\ & \mathbf{x} \in \mathcal{X}, \boldsymbol{\pi} \in \mathbb{R}^{n_h}, \mathbf{\Pi} \in \mathbb{R}^{n_h \times n_f}, k \in \mathbb{R}_+ \end{aligned} \quad (4.23)$$

where the dual recourse $\boldsymbol{\beta}$ is restricted to an affine function $\boldsymbol{\pi} + \mathbf{\Pi} \boldsymbol{\rho}$ of $\boldsymbol{\rho}$.

Theorem 21. *Under complete recourse, the affine dual recourse adaptation in Problem (4.23) is a lower bound of Problem (4.20).*

Proof. First of all, we compare the variants of Problems (4.20) and (4.23) when \mathbf{x} is fixed to \mathbf{x}' . We can then abbreviate $\mathbf{f}(\mathbf{x}')$ and $\mathbf{F}(\mathbf{x}')$ to \mathbf{f}' and \mathbf{F}' , respectively. Besides, we let τ' denote the value of $\tau - \mathbf{c}^\top \mathbf{x}'$. It suffices to show that the optimal objective value

of

$$\begin{aligned}
& \min && k \\
& \text{s.t.} && \boldsymbol{\rho}^\top \mathbf{f}' + (\boldsymbol{\pi} + \mathbf{\Pi}\boldsymbol{\rho})^\top \mathbf{h} \leq \tau' && \forall \boldsymbol{\rho} \in \mathcal{P} \\
& && -k\mathbf{1} \leq \mathbf{H}^\top (\boldsymbol{\pi} + \mathbf{\Pi}\boldsymbol{\rho}) - (\mathbf{F}')^\top \boldsymbol{\rho} \leq k\mathbf{1} && \forall \boldsymbol{\rho} \in \mathcal{P} \\
& && \boldsymbol{\pi} + \mathbf{\Pi}\boldsymbol{\rho} \geq \mathbf{0} && \forall \boldsymbol{\rho} \in \mathcal{P} \\
& && \boldsymbol{\pi} \in \mathbb{R}^{n_h}, \mathbf{\Pi} \in \mathbb{R}^{n_h \times n_f}, k \in \mathbb{R}_+
\end{aligned} \tag{4.24}$$

is smaller than or equal to that of

$$\begin{aligned}
& \min && k \\
& \text{s.t.} && \mathbf{d}^\top (\mathbf{q} + \mathbf{Q}\mathbf{z} + \mathbf{q}^\dagger \| \mathbf{z} \|_1) \leq k \| \mathbf{z} \|_1 + \tau' && \forall \mathbf{z} \in \mathcal{Z} \\
& && \mathbf{B}(\mathbf{q} + \mathbf{Q}\mathbf{z} + \mathbf{q}^\dagger \| \mathbf{z} \|_1) \geq \mathbf{f}' + \mathbf{F}'\mathbf{z} && \forall \mathbf{z} \in \mathcal{Z} \\
& && k - \mathbf{d}^\top \mathbf{q}^\dagger \geq 0, \mathbf{B}\mathbf{q}^\dagger \geq \mathbf{0} \\
& && \mathbf{q} \in \mathbb{R}^{n_y}, \mathbf{Q} \in \mathbb{R}^{n_y \times n_z}, \mathbf{q}^\dagger \in \mathbb{R}^{n_y}, k \in \mathbb{R}_+.
\end{aligned} \tag{4.25}$$

If $\tau' < \min_{\mathbf{q}} \{\mathbf{d}^\top \mathbf{q} \mid \mathbf{B}\mathbf{q} \geq \mathbf{f}'\} = \max_{\boldsymbol{\rho} \in \mathcal{P}} \{\boldsymbol{\rho}^\top \mathbf{f}'\}$, then Problems (4.24) and (4.25) are infeasible because their first respective robust constraints cannot be satisfied (recall that $\mathbf{0} \in \mathcal{Z}$ and $\mathbf{h} \geq \mathbf{0}$). Otherwise if $\tau' \geq \min_{\mathbf{q}} \{\mathbf{d}^\top \mathbf{q} : \mathbf{B}\mathbf{q} \geq \mathbf{f}'\}$, they must be feasible thanks to Theorems 19 and 20, which hold when $\mathcal{X} = \{\mathbf{x}'\}$. Henceforth, we assume that τ' is sufficiently large to avoid trivialities.

It suffices to show that, for any $(\mathbf{q}, \mathbf{Q}, \mathbf{q}^\dagger, k)$ feasible in Problem (4.25), we can construct $\boldsymbol{\pi}$ and $\mathbf{\Pi}$ such that $(\boldsymbol{\pi}, \mathbf{\Pi}, k)$ is feasible in Problem (4.24). To achieve this, we specifically consider $\boldsymbol{\pi} = \mathbf{w}^0 \in \mathbb{R}_+^{n_h}$ and $\mathbf{\Pi} = [\mathbf{w}^1, \dots, \mathbf{w}^{n_f}] \in \mathbb{R}_+^{n_h \times n_f}$, where $\{\mathbf{w}^i\}_{i=0}^{n_f}$ satisfy the following conditions.

$$\mathbf{d}^\top \mathbf{q} + \mathbf{h}^\top \mathbf{w}^0 \leq \tau' \tag{4.26a}$$

$$-(k - \mathbf{d}^\top \mathbf{q}^\dagger)\mathbf{1} \leq \mathbf{H}^\top \mathbf{w}^0 - \mathbf{Q}^\top \mathbf{d} \leq (k - \mathbf{d}^\top \mathbf{q}^\dagger)\mathbf{1} \tag{4.26b}$$

$$\mathbf{f}'_i + \mathbf{h}^\top \mathbf{w}^i \leq \mathbf{B}_i \mathbf{q} \quad \forall i \in [n_f] \tag{4.26c}$$

$$-\mathbf{B}_i \mathbf{q}^\dagger \mathbf{1} \leq \mathbf{H}^\top \mathbf{w}^i - (\mathbf{F}')_i^\top + \mathbf{Q}^\top \mathbf{B}_i^\top \leq \mathbf{B}_i \mathbf{q}^\dagger \mathbf{1} \quad \forall i \in [n_f] \tag{4.26d}$$

Note that the existence $\{\mathbf{w}^i\}_{i=0}^{n_h}$ is guaranteed by Proposition 13 and Theorem 20.

We will now show that this choice of $(\boldsymbol{\pi}, \mathbf{\Pi}, k)$ satisfies all constraints in Problem (4.24). By a usual duality argument, the first robust constraint of this problem is satisfied if and only if there exists a vector $\boldsymbol{\nu} \in \mathbb{R}^{n_y}$ such that

$$\boldsymbol{\pi}^\top \mathbf{h} + \boldsymbol{\nu}^\top \mathbf{d} \leq \tau' \quad \text{and} \quad \mathbf{B}\boldsymbol{\nu} \geq \mathbf{f}' + \mathbf{\Pi}^\top \mathbf{h}.$$

Thanks to the inequalities (4.26a) and (4.26c), $\boldsymbol{\nu}$ can be simply chosen as \mathbf{q} .

Similarly, the next two constraints of Problem (4.24), namely $-k\mathbf{1} \leq \mathbf{H}^\top (\boldsymbol{\pi} + \mathbf{\Pi}\boldsymbol{\rho}) - (\mathbf{F}')^\top \boldsymbol{\rho} \leq k\mathbf{1}$, are robustly satisfied for all $\boldsymbol{\rho} \in \mathcal{P}$ if and only if there exist matrices $\boldsymbol{\Phi}, \boldsymbol{\Psi} \in \mathbb{R}^{n_y \times n_z}$ such that

$$\left. \begin{aligned} \mathbf{H}^\top \boldsymbol{\pi} + \boldsymbol{\Phi}^\top \mathbf{d} &\leq k\mathbf{1} \\ \mathbf{B}\boldsymbol{\Phi} &\geq \mathbf{\Pi}^\top \mathbf{H} - \mathbf{F}' \end{aligned} \right\} \quad \text{and} \quad \left\{ \begin{aligned} -\mathbf{H}^\top \boldsymbol{\pi} + \boldsymbol{\Psi}^\top \mathbf{d} &\leq k\mathbf{1} \\ \mathbf{B}\boldsymbol{\Psi} &\geq \mathbf{F}' - \mathbf{\Pi}^\top \mathbf{H}. \end{aligned} \right.$$

In this case, we can choose, $\Phi = \mathbf{q}^\dagger \mathbf{1}^\top - \mathbf{Q}$ and $\Psi = \mathbf{q}^\dagger \mathbf{1}_{n_z}^\top + \mathbf{Q}$. Observe that

$$\begin{aligned} \mathbf{H}^\top \boldsymbol{\pi} + \Phi^\top \mathbf{d} &= \mathbf{H}^\top \mathbf{w}^0 + \mathbf{1}(\mathbf{q}^\dagger)^\top \mathbf{d} - \mathbf{Q}^\top \mathbf{d} \leq k\mathbf{1} \\ \mathbf{B}\Phi - \Pi^\top \mathbf{H} + \mathbf{F}' &= \left[\mathbf{B}_i \mathbf{q}^\dagger \mathbf{1}^\top - \mathbf{B}_i \mathbf{Q} - (\mathbf{w}^i)^\top \mathbf{H} + \mathbf{F}'_i \right]_{i=1}^{n_f} \geq \mathbf{0}, \end{aligned}$$

where the inequalities holds due to the inequalities (4.26b) and (4.26d), as desired. Similarly,

$$\begin{aligned} -\mathbf{H}^\top \boldsymbol{\pi} + \Psi^\top \mathbf{d} &= -\mathbf{H}^\top \mathbf{w}^0 + \mathbf{1}(\mathbf{q}^\dagger)^\top \mathbf{d} + \mathbf{Q}^\top \mathbf{d} \leq k\mathbf{1} \\ \mathbf{B}\Psi + \Pi^\top \mathbf{H} - \mathbf{F}' &= \left[\mathbf{B}_i \mathbf{q}^\dagger \mathbf{1}^\top + \mathbf{B}_i \mathbf{Q} + (\mathbf{w}^i)^\top \mathbf{H} - \mathbf{F}'_i \right]_{i=1}^{n_f} \geq \mathbf{0}. \end{aligned}$$

Finally, the third constraint of (4.24) is trivially satisfied because of the non-negativity of $\boldsymbol{\pi}$, Π and $\boldsymbol{\rho}$. Hence, Problem (4.24) is a lower bound of Problem (4.25), and the theorem follows. \square

4.4.1 Data-driven adaptive conic optimization

We can generalize our earlier results to the data-driven scheme of Long, Sim, and Zhou (2021) where the data comprises Ω samples, and $\hat{\mathbf{z}}^\omega$, $\omega \in [\Omega]$, denotes each known realization of \mathbf{z} . Consistent with the classical data-driven stochastic optimization problem framework, we consider the nominal problem of the form that minimizes the total first stage and the average second stage costs over the Ω realizations as follows:

$$\begin{aligned} Z_0 &= \min \quad \mathbf{c}^\top \mathbf{x} + \frac{1}{\Omega} \sum_{\omega \in [\Omega]} \mathbf{d}^\top \mathbf{y}^\omega \\ \text{s.t.} \quad &\mathbf{B}\mathbf{y}^\omega \succeq_{\mathcal{K}} \mathbf{f}(\mathbf{x}) + \mathbf{F}(\mathbf{x})\hat{\mathbf{z}}^\omega \quad \forall \omega \in [\Omega] \\ &\mathbf{x} \in \mathcal{X}, \mathbf{y}^1, \dots, \mathbf{y}^\Omega \in \mathbb{R}^{n_y}. \end{aligned} \tag{4.27}$$

We assume that an optimal solution of Problem (4.27) exists, and we denote it by $\hat{\mathbf{x}}, \hat{\mathbf{y}}^1, \dots, \hat{\mathbf{y}}^\Omega$. Thus, $Z_0 = \mathbf{c}^\top \hat{\mathbf{x}} + \frac{1}{\Omega} \sum_{\omega \in [\Omega]} \mathbf{d}^\top \hat{\mathbf{y}}^\omega$.

For consistency with the previous adaptive optimization framework in which the nominal uncertainty value is at the origin, for each $\omega \in [\Omega]$, we define the shifted support set

$$\mathcal{Z}_\omega = \{\boldsymbol{\zeta} \in \mathbb{R}^{n_z} \mid \mathbf{H}\boldsymbol{\zeta} \leq \mathbf{h}^\omega\}$$

where $\mathbf{h}^\omega = \mathbf{h} - \mathbf{H}\hat{\mathbf{z}}^\omega$, and the function $g^\omega : \mathcal{X} \times \mathcal{Z}_\omega \mapsto \mathbb{R}$,

$$\begin{aligned} g^\omega(\mathbf{x}, \mathbf{z}) &= \min \quad \mathbf{d}^\top \mathbf{y} \\ \text{s.t.} \quad &\mathbf{B}\mathbf{y} \succeq_{\mathcal{K}} \mathbf{f}^\omega(\mathbf{x}) + \mathbf{F}(\mathbf{x})\mathbf{z} \\ &\mathbf{y} \in \mathbb{R}^{n_y}, \end{aligned} \tag{4.28}$$

where $\mathbf{f}^\omega(\mathbf{x}) = \mathbf{f}(\mathbf{x}) + \mathbf{F}(\mathbf{x})\hat{\mathbf{z}}^\omega$. We also define the joint shifted support set as

$$\bar{\mathcal{Z}} = \mathcal{Z}_1 \times \dots \times \mathcal{Z}_\Omega,$$

and the function $\bar{g} : \mathcal{X} \times \bar{\mathcal{Z}} \mapsto \mathbb{R}$,

$$\bar{g}(\mathbf{x}, (\mathbf{z}^1, \dots, \mathbf{z}^\Omega)) = \frac{1}{\Omega} \sum_{\omega \in [\Omega]} g^\omega(\mathbf{x}, \mathbf{z}^\omega)$$

so that

$$\begin{aligned} Z_0 = \min \quad & \mathbf{c}^\top \mathbf{x} + \bar{g}(\mathbf{x}, (\mathbf{0}, \dots, \mathbf{0})) \\ \text{s.t.} \quad & \mathbf{x} \in \mathcal{X}. \end{aligned} \quad (4.29)$$

We provide a different perspective from Long, Sim, and Zhou (2021) to derive the robust satisficing model without the need of introducing an ambiguity set of uncertain probability distributions. In the data-driven setting, the penalty function, $\bar{p} : \mathbb{R}^{n_z \times \Omega} \mapsto \mathbb{R}$ is also defined over the sample averages as follows

$$\bar{p}(\zeta^1, \dots, \zeta^\Omega) = \frac{1}{\Omega} \sum_{\omega \in [\Omega]} p(\zeta^\omega).$$

Hence, for a chosen target that satisfies $\tau \geq Z_0$, the robust satisficing model along the lines of Problem (4.5) can be expressed as

$$\begin{aligned} \min \quad & k \\ \text{s.t.} \quad & \mathbf{c}^\top \mathbf{x} + \bar{g}(\mathbf{x}, (\mathbf{z}^1, \dots, \mathbf{z}^\Omega)) \leq \tau + k\bar{p}(\mathbf{z}^1, \dots, \mathbf{z}^\Omega), \quad \forall (\mathbf{z}^1, \dots, \mathbf{z}^\Omega) \in \bar{\mathcal{Z}} \\ & \mathbf{x} \in \mathcal{X}, k \in \mathbb{R}_+, \end{aligned} \quad (4.30)$$

or equivalently

$$\begin{aligned} \min \quad & k \\ \text{s.t.} \quad & \mathbf{c}^\top \mathbf{x} + \frac{1}{\Omega} \sum_{\omega \in [\Omega]} (g^\omega(\mathbf{x}, \mathbf{z}^\omega) - kp(\mathbf{z}^\omega)) \leq \tau \quad \forall (\mathbf{z}^1, \dots, \mathbf{z}^\Omega) \in \bar{\mathcal{Z}} \\ & \mathbf{x} \in \mathcal{X}, k \in \mathbb{R}_+, \end{aligned} \quad (4.31)$$

which recovers the data-driven robust satisficing model of Long, Sim, and Zhou (2021). Our result is however more general than that in Long, Sim, and Zhou (2021) since it covers polyhedral penalty functions beyond ℓ_1 -norm, and accommodates second-stage conic optimization problems beyond linear optimization.

Theorem 22. *Under Assumption 2, the approximation of Problem (4.31) via affine dual recourse adaptation is given as:*

$$\begin{aligned} \min \quad & k \\ \text{s.t.} \quad & \mathbf{c}^\top \mathbf{x} + \frac{1}{\Omega} \sum_{\omega \in [\Omega]} v_\omega \leq \tau \\ & \boldsymbol{\rho}^\top \mathbf{f}^\omega(\mathbf{x}) + (\mathbf{h}^\omega)^\top \boldsymbol{\beta}^\omega(\boldsymbol{\rho}) + \eta^\omega(\boldsymbol{\rho}) \leq v_\omega \quad \forall \boldsymbol{\rho} \in \mathcal{P}, \omega \in [\Omega] \\ & \mathbf{M} \left(\mathbf{F}(\mathbf{x})^\top \boldsymbol{\rho} - \mathbf{H}^\top \boldsymbol{\beta}^\omega(\boldsymbol{\rho}) \right) + \mathbf{N} \boldsymbol{\mu}^\omega(\boldsymbol{\rho}) + \mathbf{s} \eta^\omega(\boldsymbol{\rho}) \leq t k \quad \forall \boldsymbol{\rho} \in \mathcal{P}, \omega \in [\Omega] \\ & \boldsymbol{\beta}^\omega(\boldsymbol{\rho}) \geq \mathbf{0}, \eta^\omega(\boldsymbol{\rho}) \geq 0 \quad \forall \boldsymbol{\rho} \in \mathcal{P}, \omega \in [\Omega] \\ & \mathbf{x} \in \mathcal{X}, k \in \mathbb{R}_+, \mathbf{v} \in \mathbb{R}^\Omega, \boldsymbol{\beta}^1, \dots, \boldsymbol{\beta}^\Omega \in \mathcal{L}^{n_f, n_h}, \boldsymbol{\mu}^1, \dots, \boldsymbol{\mu}^\Omega \in \mathcal{L}^{n_f, n_\mu}, \eta^1, \dots, \eta^\Omega \in \mathcal{L}^{n_f, 1} \end{aligned} \quad (4.32)$$

where $\mathcal{P} = \{\boldsymbol{\rho} \in \mathcal{K}^* \mid \mathbf{B}^\top \boldsymbol{\rho} = \mathbf{d}\}$. Additionally, the problem is feasible whenever the target satisfies $\tau \geq Z_0$ and is practicably solvable under Assumption 1.

Proof. First, it follows from the specificity of g^ω in Problem (4.28) that the robust constraint in Problem (4.31) is equivalent to

$$\mathbf{c}^\top \mathbf{x} + \frac{1}{\Omega} \sum_{\omega \in [\Omega]} \left(\max_{\mathbf{z} \in \mathcal{Z}_\omega} \min_{\mathbf{y}} \left\{ \mathbf{d}^\top \mathbf{y} - kp(\mathbf{z}) : \mathbf{B}\mathbf{y} \succeq_{\mathcal{K}} \mathbf{f}^\omega(\mathbf{x}) + \mathbf{F}(\mathbf{x})\mathbf{z} \right\} \right) \leq \tau.$$

Observe that, for each $\omega \in [\Omega]$, the inner minimization (over \mathbf{y}) is strictly feasible and thus we can transform it into a maximization problem via conic duality, that is,

$$\mathbf{c}^\top \mathbf{x} + \frac{1}{\Omega} \sum_{\omega \in [\Omega]} \left(\max_{\boldsymbol{\rho} \in \mathcal{P}} \left\{ \boldsymbol{\rho}^\top \mathbf{f}^\omega(\mathbf{x}) + \max_{\mathbf{z} \in \mathcal{Z}_\omega} \left\{ (\boldsymbol{\rho}^\top \mathbf{F}(\mathbf{x})\mathbf{z} - kp(\mathbf{z})) \right\} \right\} \right) \leq \tau.$$

Next, similarly to the proof of Theorem 18, we will make use of Proposition 12 to transform the inner maximization (over \mathbf{z}^ω for each $\omega \in [\Omega]$) to a minimization problem (over the variables $\boldsymbol{\beta}^\omega$, $\boldsymbol{\mu}^\omega$ and η^ω for each $\omega \in [\Omega]$). As a result, we can express Problem (4.31) as

$$\begin{aligned} \min \quad & k \\ \text{s.t.} \quad & \mathbf{c}^\top \mathbf{x} + \frac{1}{\Omega} \sum_{\omega \in [\Omega]} v_\omega \leq \tau \\ & \boldsymbol{\rho}^\top \mathbf{f}^\omega(\mathbf{x}) + (\mathbf{h}^\omega)^\top \boldsymbol{\beta}^\omega(\boldsymbol{\rho}) + \eta^\omega(\boldsymbol{\rho}) \leq v_\omega & \forall \boldsymbol{\rho} \in \mathcal{P}, \omega \in [\Omega] \\ & \mathbf{M} \left(\mathbf{F}(\mathbf{x})^\top \boldsymbol{\rho} - \mathbf{H}^\top \boldsymbol{\beta}^\omega(\boldsymbol{\rho}) \right) + \mathbf{N} \boldsymbol{\mu}^\omega(\boldsymbol{\rho}) + s \eta^\omega(\boldsymbol{\rho}) \leq t k & \forall \boldsymbol{\rho} \in \mathcal{P}, \omega \in [\Omega] \\ & \boldsymbol{\beta}^\omega(\boldsymbol{\rho}) \geq \mathbf{0}, \eta^\omega(\boldsymbol{\rho}) \geq 0 & \forall \boldsymbol{\rho} \in \mathcal{P}, \omega \in [\Omega] \\ & \mathbf{x} \in \mathcal{X}, k \in \mathbb{R}_+, \mathbf{v} \in \mathbb{R}^\Omega, \boldsymbol{\beta}^1, \dots, \boldsymbol{\beta}^\Omega \in \mathcal{R}^{n_f, n_h}, \boldsymbol{\mu}^1, \dots, \boldsymbol{\mu}^\Omega \in \mathcal{R}^{n_f, n_\mu}, \eta^1, \dots, \eta^\Omega \in \mathcal{R}^{n_f, 1}. \end{aligned}$$

Approximating all recourse variables using affine adaptation results in Problem (4.32), which completes the first half of the proof.

Assume now that $\tau \geq Z_0$ and consider the solution $\mathbf{x} = \hat{\mathbf{x}}$, $\boldsymbol{\beta}^\omega(\boldsymbol{\rho}) = \mathbf{0}$, $\eta^\omega(\boldsymbol{\rho}) = 0$ and $v_\omega = \max_{\boldsymbol{\rho} \in \mathcal{P}} \left\{ \boldsymbol{\rho}^\top (\mathbf{f}^\omega(\hat{\mathbf{x}})) \right\}$ (with $\boldsymbol{\mu}^\omega$ and k to be chosen later), for all $\omega \in [\Omega]$, which robustly satisfies the first constraint of Problem (4.32) since the left-hand side of this constraint evaluates to:

$$\begin{aligned} & \mathbf{c}^\top \hat{\mathbf{x}} + \frac{1}{\Omega} \sum_{\omega \in [\Omega]} \max_{\boldsymbol{\rho} \in \mathcal{P}} \left\{ \boldsymbol{\rho}^\top (\mathbf{f}^\omega(\hat{\mathbf{x}})) \right\} \\ &= \mathbf{c}^\top \hat{\mathbf{x}} + \frac{1}{\Omega} \sum_{\omega \in [\Omega]} \max_{\boldsymbol{\rho} \in \mathcal{P}} \left\{ \boldsymbol{\rho}^\top (\mathbf{f}(\hat{\mathbf{x}}) + \mathbf{F}(\hat{\mathbf{x}})\hat{\mathbf{z}}^\omega) \right\} \\ &= \mathbf{c}^\top \hat{\mathbf{x}} + \frac{1}{\Omega} \sum_{\omega \in [\Omega]} \min_{\mathbf{y}} \left\{ \mathbf{d}^\top \mathbf{y} : \mathbf{B}\mathbf{y} \succeq_{\mathcal{K}} \mathbf{f}(\hat{\mathbf{x}}) + \mathbf{F}(\hat{\mathbf{x}})\hat{\mathbf{z}}^\omega \right\} \\ &= \mathbf{c}^\top \hat{\mathbf{x}} + \frac{1}{\Omega} \sum_{\omega \in [\Omega]} \mathbf{d}^\top \hat{\mathbf{y}}^\omega \leq \tau, \end{aligned}$$

where the last equality follows from the optimality of $(\hat{\mathbf{x}}, \hat{\mathbf{y}}^1, \dots, \hat{\mathbf{y}}^\Omega)$ in Problem (4.27). Besides, the proof of Theorem 19 reveals that there exists $\hat{\boldsymbol{\mu}}$ and $\hat{k} > 0$ such that the constraint (4.15) holds. Hence, by completing the suggested solution with $\boldsymbol{\mu}^\omega(\boldsymbol{\rho}) = \hat{\boldsymbol{\mu}}\hat{k}$, for all $\omega \in [\Omega]$, and $k = \hat{k}$, the remaining constraints of Problem (4.32) are satisfied and

the feasibility argument is completed. \square

We now consider a special, but an important case where each function g^ω , $\omega \in [\Omega]$ evaluates the maximum of n_f biaffine functions and can be expressed as

$$\begin{aligned} g^\omega(\mathbf{x}, \mathbf{z}) = \min \quad & y \\ \text{s.t.} \quad & \mathbf{1}y \geq \mathbf{f}^\omega(\mathbf{x}) + \mathbf{F}(\mathbf{x})\mathbf{z} \\ & y \in \mathbb{R}. \end{aligned} \quad (4.33)$$

Theorem 23. *Suppose each function g^ω , $\omega \in [\Omega]$ is represented as Problem (4.33), then Problems (4.31) and (4.32) are equivalent.*

Proof. Observe that the dual uncertainty set is now a simplex, $\mathcal{P} = \{\boldsymbol{\rho} \in \mathbb{R}_+^{n_f} \mid \mathbf{1}^\top \boldsymbol{\rho} = 1\}$. It has been shown (see for e.g., Zhen, Den Hertog, and Sim, 2018) that if the uncertainty set is a simplex, then the approximation via affine recourse adaption is exact. \square

4.5 Applications and computational studies

In this section, we illustrate the improved performance of the robust satisficing model over the classical robust model with an example for each of the three variants of the problems considered in Sections 4.3 and 4.4, i.e., the quadratic problem with exact reformulation, and the biconvex as well as two-stage linear optimization problems with affine dual adaptation. Our results in Sections 4.5.1 and 4.5.2 were obtained using Mosek 9.2.38 together with YALMIP modeling language (Löfberg, 2004) and MATLAB R2020a, whereas the results in Section 4.5.3 were obtained using Gurobi 9.1.1 with RSome (Robust Stochastic Optimization Made Easy) modeling language (Chen, Sim, and Xiong, 2020) and Python 3.7.7. All experiments were conducted on an Intel Core i7 2.7GHz MacBook with 16GB of RAM.

4.5.1 Growth-optimal portfolios

When the constraint is quadratic and the uncertainty set is ellipsoidal, we demonstrate with a growth-optimal portfolio example that the exact semidefinite reformulation of the robust satisficing model numerically performs better than that of the robust model. Consider an investor who aims to accumulate wealth from trading asset by maximizing a logarithmic utility function. We let x_i , $i \in [n]$, denote the proportion of capital allocated to the i^{th} asset, and we impose the budget constraint $\mathbf{1}^\top \mathbf{x} = 1$ and the non-negativity constraint $\mathbf{x} \geq \mathbf{0}$ to disallow short-selling. We henceforth denote by \mathcal{X} our (simplex) feasible set of portfolios and write down the utility maximization problem as

$$\begin{aligned} \max \quad & \mathbb{E}_{\mathbb{P}} \left[\log(1 + \mathbf{x}^\top \tilde{\mathbf{r}}) \right] \\ \text{s.t.} \quad & \mathbf{x} \in \mathcal{X}, \end{aligned}$$

where $\tilde{\mathbf{r}} \sim \mathbb{P}$ denotes a random vector of asset returns. Assuming that the asset returns are serially independent and identically distributed, the logarithmic utility function is of a particular interest to long-term investors because, if $\mathbb{E}_{\mathbb{P}} [\log(1 + \mathbf{x}^\top \tilde{\mathbf{r}})] > 0$, then (with probability one) \mathbf{x} underlies a fixed-mix strategy that achieves infinite wealth in

the long run. On the other hand, if the expected utility is strictly negative, then the same fixed-mix strategy will eventually lead investors to ruin.

Any optimal solution of the above optimization problem is known as the growth-optimal portfolio. Following Rujeeapaiboon, Kuhn, and Wiesemann (2016), we approximate the logarithmic function using a second-order Taylor expansion around one, resulting in

$$\begin{aligned} \max \quad & \mathbf{x}^\top \boldsymbol{\mu} - \frac{1}{2} \mathbf{x}^\top (\boldsymbol{\Sigma} + \boldsymbol{\mu} \boldsymbol{\mu}^\top) \mathbf{x} \\ \text{s.t.} \quad & \mathbf{x} \in \mathcal{X}, \end{aligned} \quad (4.34)$$

where $\boldsymbol{\mu} \in \mathbb{R}^n$ and $\boldsymbol{\Sigma} \in \mathbb{S}_+^n$ denote the mean vector and the covariance matrix of the asset return distribution \mathbb{P} , respectively. As portfolio optimization problems are very sensitive to the estimation errors in $\boldsymbol{\mu}$, we may robustify Problem (4.34) by seeking a portfolio \mathbf{x} that is robustly optimal in

$$\begin{aligned} \min \quad & \max_{\mathbf{z} \in \mathcal{E}_r} h(\mathbf{x}, \mathbf{z}) \\ \text{s.t.} \quad & \mathbf{x} \in \mathcal{X}, \end{aligned} \quad (4.35)$$

where $\mathbf{z} \in \mathbb{R}^n$ represents an uncertain vector belonging to the ellipsoidal uncertainty set \mathcal{E}_r , $r \geq 0$, which perturbs $\boldsymbol{\mu}$ and $h(\mathbf{x}, \mathbf{z}) = \frac{1}{2} \mathbf{x}^\top (\boldsymbol{\Sigma} + (\boldsymbol{\mu} + \mathbf{z})(\boldsymbol{\mu} + \mathbf{z})^\top) \mathbf{x} - \mathbf{x}^\top (\boldsymbol{\mu} + \mathbf{z})$. The corresponding robust satisficing investment problem can be formulated as

$$\begin{aligned} \min \quad & k \\ \text{s.t.} \quad & h(\mathbf{x}, \mathbf{z}) \leq \tau + k \mathbf{z}^\top \mathbf{z} \quad \forall \mathbf{z} \in \mathbb{R}^n \\ & \mathbf{x} \in \mathcal{X}, k \in \mathbb{R}_+. \end{aligned} \quad (4.36)$$

To facilitate the comparisons between (4.35) and (4.36), we derive their respective robust counterparts in the following propositions.

Proposition 14. For any $r > 0$, Problem (4.35) is equivalent to

$$\begin{aligned} \min \quad & \frac{1}{2} \mathbf{x}^\top \boldsymbol{\Sigma} \mathbf{x} + \frac{x_0}{2} \\ \text{s.t.} \quad & \begin{bmatrix} \lambda \mathbf{I}_n & \mathbf{x} & \mathbf{x} \\ \mathbf{x}^\top & x_0 + 2\mathbf{x}^\top \boldsymbol{\mu} - \lambda r & \mathbf{x}^\top \boldsymbol{\mu} \\ \mathbf{x}^\top & \mathbf{x}^\top \boldsymbol{\mu} & 1 \end{bmatrix} \succeq \mathbf{0} \\ & \mathbf{x} \in \mathcal{X}, x_0 \in \mathbb{R}, \lambda \in \mathbb{R}_+. \end{aligned}$$

Proof. By introducing an epigraph variable $x_0 \in \mathbb{R}$ to denote the uncertain part of the objective function of Problem (4.35), we obtain the following equivalent reformulation

$$\begin{aligned} \min \quad & \frac{1}{2} \mathbf{x}^\top \boldsymbol{\Sigma} \mathbf{x} + \frac{x_0}{2} \\ \text{s.t.} \quad & x_0 \geq \mathbf{x}^\top (\boldsymbol{\mu} + \mathbf{z})(\boldsymbol{\mu} + \mathbf{z})^\top \mathbf{x} - 2\mathbf{x}^\top (\boldsymbol{\mu} + \mathbf{z}) \quad \forall \mathbf{z} \in \mathcal{E}(r) \\ & \mathbf{x} \in \mathcal{X}, x_0 \in \mathbb{R}. \end{aligned}$$

Next, we rewrite the arising robust constraint in an explicit quadratic form

$$\begin{aligned} \begin{bmatrix} z \\ 1 \end{bmatrix}^\top \begin{bmatrix} -\mathbf{x}\mathbf{x}^\top & \mathbf{x} - \mathbf{x}\boldsymbol{\mu}^\top\mathbf{x} \\ \mathbf{x}^\top - \mathbf{x}^\top\boldsymbol{\mu}\mathbf{x}^\top & x_0 + 2\mathbf{x}^\top\boldsymbol{\mu} - \mathbf{x}^\top\boldsymbol{\mu}\boldsymbol{\mu}^\top\mathbf{x} \end{bmatrix} \begin{bmatrix} z \\ 1 \end{bmatrix} \geq 0 \quad \forall z : \begin{bmatrix} z \\ 1 \end{bmatrix}^\top \begin{bmatrix} -\mathbf{I}_n & \mathbf{0} \\ \mathbf{0} & r \end{bmatrix} \begin{bmatrix} z \\ 1 \end{bmatrix} \geq 0 \\ \iff \begin{bmatrix} \lambda\mathbf{I}_n & \mathbf{x} \\ \mathbf{x}^\top & x_0 + 2\mathbf{x}^\top\boldsymbol{\mu} - \lambda r \end{bmatrix} \succeq \begin{bmatrix} \mathbf{x} \\ \mathbf{x}^\top\boldsymbol{\mu} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{x}^\top\boldsymbol{\mu} \end{bmatrix}^\top, \end{aligned}$$

where the equivalence is due to \mathcal{S} -lemma, which holds whenever $r > 0$. Finally, invoking the Schur's complement to linearize the above positive semidefinite constraint gives the desired equivalence. \square

Proposition 15. *Problem (4.36) is equivalent to*

$$\begin{aligned} \min \quad & k \\ \text{s.t.} \quad & \begin{bmatrix} 2k\mathbf{I}_n & \mathbf{x} & \mathbf{x} \\ \mathbf{x}^\top & x_0 + 2\mathbf{x}^\top\boldsymbol{\mu} & \mathbf{x}^\top\boldsymbol{\mu} \\ \mathbf{x}^\top & \mathbf{x}^\top\boldsymbol{\mu} & 1 \end{bmatrix} \succeq \mathbf{0} \\ & \frac{1}{2}\mathbf{x}^\top\boldsymbol{\Sigma}\mathbf{x} + \frac{x_0}{2} \leq \tau \\ & \mathbf{x} \in \mathcal{X}, \quad x_0 \in \mathbb{R}, \quad k \in \mathbb{R}_+. \end{aligned} \tag{4.37}$$

Proof. The proof widely parallels that of Proposition 14 and is therefore omitted. \square

Furthermore, it can be shown that the equally weighted portfolio $\mathbf{x} = \frac{1}{n}\mathbf{1}$ is increasingly close to being optimal in (4.37) as the target τ increases (*i.e.*, as the investor becomes increasingly risk-averse). A similar observation in a data-driven setting can be found in Mohajerin Esfahani and Kuhn (2018) and Long, Sim, and Zhou (2021), among others. We refer to DeMiguel, Garlappi, and Uppal (2007) for the thorough statistical comparison between the equally weighted portfolio and other investment strategies.

Theorem 24. *Denoting by $k^*(\tau)$ the optimal objective value of Problem (4.37) for a given target τ and by $\bar{k}^*(\tau)$ the optimal objective value of the same problem restricted with $\mathbf{x} = \frac{1}{n}\mathbf{1}$, we have that $\lim_{\tau \uparrow \infty} \bar{k}^*(\tau) - k^*(\tau) = 0$.*

Proof. Observe that the positive semidefinite constraint of (4.37) implies that

$$\begin{bmatrix} 2k\mathbf{I}_n & \mathbf{x} \\ \mathbf{x}^\top & 1 \end{bmatrix} \succeq \mathbf{0} \iff 2k\mathbf{I}_n \succeq \mathbf{x}\mathbf{x}^\top \implies 2k\mathbf{1}^\top\mathbf{I}_n\mathbf{1} \geq (\mathbf{1}^\top\mathbf{x})^2 = 1, \tag{4.38}$$

where the equality follows because $\mathbf{x} \in \mathcal{X}$. Therefore, any feasible k must satisfy $k \geq \frac{1}{2n}$.

Next, for any $\delta > 0$, we introduce a matrix $\boldsymbol{\Xi}(\delta) \in \mathbb{S}^{n+1}$ and a scalar $\xi(\delta)$:

$$\boldsymbol{\Xi}(\delta) = \begin{bmatrix} (1+\delta)\mathbf{I}_n & \mathbf{1} \\ \mathbf{1}^\top & n \end{bmatrix} \quad \text{and} \quad \xi(\delta) = \sup_{\mathbf{v}} \left\{ \left(\mathbf{v}^\top \begin{bmatrix} \mathbf{1} \\ \mathbf{1}^\top\boldsymbol{\mu} \end{bmatrix} \right)^2 \left(\mathbf{v}^\top \boldsymbol{\Xi}(\delta) \mathbf{v} \right)^{-1} \mid \|\mathbf{v}\|_2 = 1 \right\}.$$

Observe that for any nonzero vector $(\mathbf{w}, w_{n+1}) \in \mathbb{R}^{n+1}$,

$$\begin{bmatrix} \mathbf{w} \\ w_{n+1} \end{bmatrix}^\top \Xi(\delta) \begin{bmatrix} \mathbf{w} \\ w_{n+1} \end{bmatrix} = \delta \mathbf{w}^\top \mathbf{w} + (\mathbf{w} + \mathbf{1}w_{n+1})^\top (\mathbf{w} + \mathbf{1}w_{n+1}) > 0.$$

Hence, $\Xi(\delta)$ is strictly positive definite, and thus $\xi(\delta)$ is positive and finite because $\{\mathbf{v} \in \mathbb{R}^{n+1} \mid \|\mathbf{v}\|_2 = 1\}$ is compact. Therefore, we have

$$\xi(\delta) \mathbf{v}^\top \Xi(\delta) \mathbf{v} \geq \mathbf{v}^\top \begin{bmatrix} \mathbf{1} \\ \mathbf{1}^\top \boldsymbol{\mu} \end{bmatrix} \begin{bmatrix} \mathbf{1} \\ \mathbf{1}^\top \boldsymbol{\mu} \end{bmatrix}^\top \mathbf{v}$$

for all $\mathbf{v} \in \mathbb{R}^{n+1}$, or equivalently,

$$\xi(\delta) \Xi(\delta) \succeq \begin{bmatrix} \mathbf{1} \\ \mathbf{1}^\top \boldsymbol{\mu} \end{bmatrix} \begin{bmatrix} \mathbf{1} \\ \mathbf{1}^\top \boldsymbol{\mu} \end{bmatrix}^\top.$$

For a fixed $\delta > 0$, consider now a target objective $\tau \geq \frac{1}{2n^2} \mathbf{1}^\top \boldsymbol{\Sigma} \mathbf{1} + \frac{\xi(\delta)}{2n} - \frac{\mathbf{1}^\top \boldsymbol{\mu}}{n}$. As $\xi(\delta)$ is decreasing in $\delta > 0$, this lower bound on τ is increasing as δ decreases. Our next step is to show that $(\mathbf{x}, x_0, k) = \left(\frac{\mathbf{1}}{n}, \frac{\xi(\delta) - 2\mathbf{1}^\top \boldsymbol{\mu}}{n}, \frac{1+\delta}{2n}\right)$ is feasible in Problem (4.37). Observe that

$$\begin{aligned} \xi(\delta) \Xi(\delta) \succeq \begin{bmatrix} \mathbf{1} \\ \mathbf{1}^\top \boldsymbol{\mu} \end{bmatrix} \begin{bmatrix} \mathbf{1} \\ \mathbf{1}^\top \boldsymbol{\mu} \end{bmatrix}^\top &\iff \begin{bmatrix} (1+\delta)\mathbf{I}_n & \mathbf{1} & \mathbf{1} \\ \mathbf{1}^\top & n & \mathbf{1}^\top \boldsymbol{\mu} \\ \mathbf{1}^\top & \mathbf{1}^\top \boldsymbol{\mu} & \xi(\delta) \end{bmatrix} \succeq \mathbf{0} \\ &\iff \begin{bmatrix} 2kn\mathbf{I}_n & n\mathbf{x} & n\mathbf{x} \\ n\mathbf{x}^\top & n & n\mathbf{x}^\top \boldsymbol{\mu} \\ n\mathbf{x}^\top & n\mathbf{x}^\top \boldsymbol{\mu} & nx_0 + 2n\mathbf{x}^\top \boldsymbol{\mu} \end{bmatrix} \succeq \mathbf{0} \end{aligned}$$

where the first equivalence follows from Schur's complement and the definition of $\Xi(\delta)$ and the second follows from the suggested value of (\mathbf{x}, x_0, k) . Dividing both sides of the above inequality by n shows that (\mathbf{x}, x_0, k) satisfies the positive semidefinite constraint in Problem (4.37). Besides, the remaining constraints in Problem (4.37) are trivially satisfied. Therefore, $\bar{k}^*(\tau)$ cannot exceed $\frac{1+\delta}{2n}$. This result together with our earlier observation (4.38) implies $\frac{1}{2n} \leq k^*(\tau) \leq \bar{k}^*(\tau) \leq \frac{1+\delta}{2n}$. By taking the limit as δ approaches zero from above and considering τ that exceeds the prescribed lower bound (which itself increases as δ decreases), the theorem follows. \square

Evaluation and discussion of results:

Our asset universe consists of $n = 8$ assets with the following means and variances

$$\begin{aligned} \boldsymbol{\mu} &= [0.12, 0.16, 0.14, 0.13, 0.15, 0.12, 0.14, 0.15]^\top, \\ \text{diag}(\boldsymbol{\Sigma}) &= [0.18^2, 0.22^2, 0.20^2, 0.16^2, 0.14^2, 0.10^2, 0.14^2, 0.19^2]^\top. \end{aligned}$$

We suppose further that the first four assets (and the last four) are from the same industrial sector and are thus positively correlated with all pairwise correlations equal to 0.1 and that correlations between assets from different sectors are -0.1 . We are now ready

to compare the robust and the robust satisficing investment problems. To this end, for any fixed $r > 0$, which characterizes the radius of the uncertainty set in Problem (4.35), we solve the robust counterpart from Proposition 14. We denote the optimal objective value and the optimal solution by Z_r and \mathbf{x}_r^{rb} , respectively. Intuitively, we can interpret Z_r as the optimal (minimal) worst-case risk. We then solve the robust satisficing problem (4.37) by setting the target risk as $\tau = Z_r$ and denote the optimal solution by \mathbf{x}_r^{st} . Then, compute the *expected shortfall* of both the robust and the robust satisficing solution from

$$\mathbb{E} \left[h(\mathbf{x}_r^{\text{rb}}, \tilde{\mathbf{z}}) - Z_r \mid h(\mathbf{x}_r^{\text{rb}}, \tilde{\mathbf{z}}) > Z_r \right] \quad \text{and} \quad \mathbb{E} \left[h(\mathbf{x}_r^{\text{st}}, \tilde{\mathbf{z}}) - Z_r \mid h(\mathbf{x}_r^{\text{st}}, \tilde{\mathbf{z}}) > Z_r \right]$$

as well as their *probability of ruin*

$$\mathbb{P} \left[\mathbb{E} \left[\log \left(1 + \tilde{\mathbf{r}}^\top \mathbf{x}_r^{\text{rb}} \right) \mid \tilde{\mathbf{r}} \sim \mathcal{N}(\boldsymbol{\mu} + \tilde{\mathbf{z}}, \boldsymbol{\Sigma}) \right] < 0 \right] \quad \text{and} \quad \mathbb{P} \left[\mathbb{E} \left[\log \left(1 + \tilde{\mathbf{r}}^\top \mathbf{x}_r^{\text{st}} \right) \mid \tilde{\mathbf{r}} \sim \mathcal{N}(\boldsymbol{\mu} + \tilde{\mathbf{z}}, \boldsymbol{\Sigma}) \right] < 0 \right]$$

via simulation from 10^5 independent realizations of $\tilde{\mathbf{z}}$ generated from $\mathcal{N}(\mathbf{0}, s\mathbf{I}_n)$, for some $s > 0$ (and 10^3 independent realizations of $\tilde{\mathbf{r}}$ for each realization of $\tilde{\mathbf{z}}$). The obtained results are shown in Figure 4.1, and they are clearly in favour of the robust satisficing solutions. Similar observations can be made for different choices of $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$.

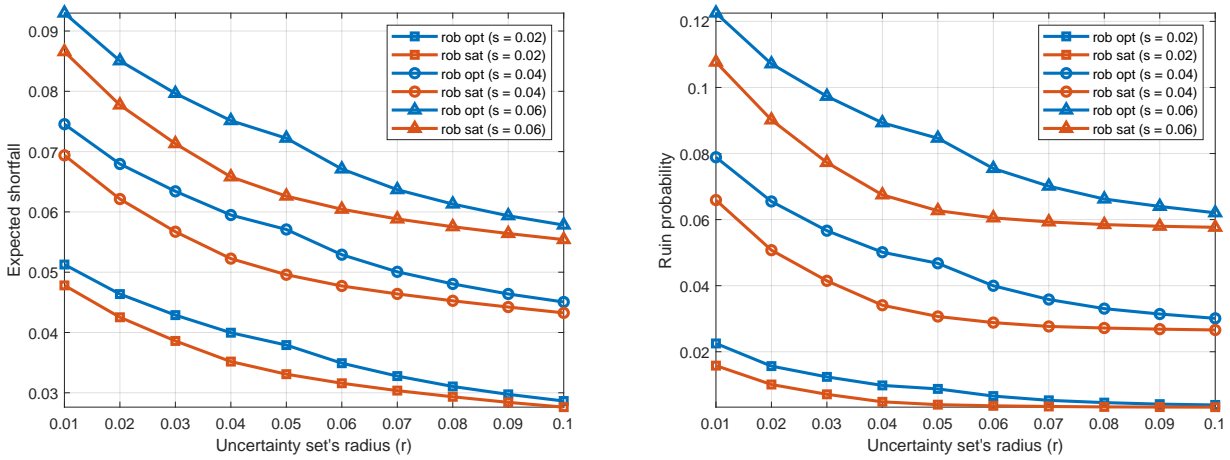


FIGURE 4.1: Expected shortfalls and probabilities of ruin of the robust optimization (rob opt) and the robust satisficing (rob sat) growth-optimal portfolios.

4.5.2 Log-sum-exp optimization

Next, we consider robust optimization and satisficing problems involving biconvex constraints (cf. Example 10). Particularly, we consider a robust optimization problem

$$\begin{aligned} Z_r = \min \quad & \mathbf{1}^\top \mathbf{x} \\ \text{s.t.} \quad & g_i(\mathbf{x}, \mathbf{z}) \leq 0 \quad \forall \mathbf{z} \in \mathcal{U}_r, \quad i \in [m] \\ & \mathbf{x} \in \mathbb{R}^{n_x}, \end{aligned}$$

where $g_i(\mathbf{x}, \mathbf{z}) = \log(\exp((-1 + \mathbf{R}^i \mathbf{z})^\top \mathbf{x}) + \exp((-1 + \mathbf{S}^i \mathbf{z})^\top \mathbf{x}))$ for some matrices $\mathbf{R}^i, \mathbf{S}^i \in \mathbb{R}^{n_x \times n_z}$. Since g_i 's are convex in the uncertain \mathbf{z} , it is typically not possible to derive the exact robust counterpart by the standard duality argument (Ben-Tal and Nemirovski, 1998) and instead one might need to resort to an approximation scheme (see for *e.g.* Roos et al., 2020). For the robust satisficing formulation, we choose the penalty function $p(\zeta) = \|\zeta\|_1$ and hence consider

$$\begin{aligned} \min \quad & \mathbf{1}^\top \mathbf{k} \\ \text{s.t.} \quad & g_i(\mathbf{x}, \mathbf{z}) \leq k_i \|\mathbf{z}\|_1 \quad \forall \mathbf{z} \in \mathcal{Z}, i \in [m] \\ & \mathbf{1}^\top \mathbf{x} \leq \tau \\ & \mathbf{x} \in \mathbb{R}^n, \mathbf{k} \in \mathbb{R}_+^m, \end{aligned}$$

where $\tau \geq Z_0$ is the prescribed target objective. As discussed in Section 4.3, this problem can be solved approximately using affine dual recourse adaptation. In the following, we assume that $\hat{\mathbf{z}} = \mathbf{0}$ so that the nominal problem is bounded, the support set is given by $\mathcal{Z} = \{\mathbf{z} \in \mathbb{R}^{n_z} : \|\mathbf{z}\|_\infty \leq 1\}$, and the uncertainty set is $\mathcal{U}_r = \{\mathbf{z} \in \mathbb{R}^{n_z} : \|\mathbf{z}\|_\infty \leq r\}$, $r \in [0, 1]$.

We can cast the constraint functions g_i 's in our conic framework as

$$\begin{aligned} g_i(\mathbf{x}, \mathbf{z}) = \min \quad & y \\ \text{s.t.} \quad & \begin{bmatrix} -1 \\ -1 \\ 0 \end{bmatrix} y \succeq_{\mathcal{K}} \begin{bmatrix} \mathbf{1}^\top \mathbf{x} \\ \mathbf{1}^\top \mathbf{x} \\ -1 \end{bmatrix} + \begin{bmatrix} -\mathbf{x}^\top \mathbf{R}^i \\ -\mathbf{x}^\top \mathbf{S}^i \\ \mathbf{0}^\top \end{bmatrix} \mathbf{z} \\ & y \in \mathbb{R}, \end{aligned}$$

where the cone \mathcal{K} is given by $\text{cl}(\{\mathbf{v} \in \mathbb{R} \times \mathbb{R} \times \mathbb{R}_{++} : v_3 \log(\exp(v_1/v_3) + \exp(v_2/v_3)) \leq 0\})$, which is representable as an intersection of multiple exponential cones.

Evaluation and discussion of results:

We choose $n_x = m = 20$ and $n_z = 5$. We randomly generate \mathbf{R}^i and \mathbf{S}^i as matrices with sparse density 0.1 whose non-zero elements are independently and uniformly picked from the unit interval. To facilitate the comparison between the robust and the robust satisficing models, for a fixed radius $r \in [0, 1]$ of the robust uncertainty set, we solve the robust log-sum-exp problem *exactly* by enumerating all vertices of the uncertainty set, *i.e.*, we solve

$$\begin{aligned} Z_r = \min \quad & \mathbf{1}^\top \mathbf{x} \\ \text{s.t.} \quad & g_i(\mathbf{x}, \mathbf{z}) \leq 0 \quad \forall \mathbf{z} \in \{-r, +r\}^{n_z} \\ & \mathbf{x} \in \mathbb{R}^{n_x} \end{aligned}$$

and denote the resulting robustly optimal solution by \mathbf{x}_r^{rb} . Subsequently, we solve the robust satisficing problem only *approximately* using affine dual recourse adaptation while setting the target objective τ to Z_r and denote the optimal solution by \mathbf{x}_r^{st} . Finally, we generate 10^5 independent realizations of $\tilde{\mathbf{z}}$ (whose components are independent and drawn uniformly from $[0, 1]$) to compute the *normalized probability of constraint*

violation of \mathbf{x}_r^{rb} and \mathbf{x}_r^{st} :

$$\frac{1}{m} \sum_{i=1}^m \mathbb{P} [g_i(\mathbf{x}_r^{\text{rb}}, \tilde{\mathbf{z}}) > 0] \quad \text{and} \quad \frac{1}{m} \sum_{i=1}^m \mathbb{P} [g_i(\mathbf{x}_r^{\text{st}}, \tilde{\mathbf{z}}) > 0]$$

as well as their *total expected shortfall*:

$$\sum_{i=1}^m \mathbb{E} [g_i(\mathbf{x}_r^{\text{rb}}, \tilde{\mathbf{z}}) | g_i(\mathbf{x}_r^{\text{rb}}, \tilde{\mathbf{z}}) > 0] \quad \text{and} \quad \sum_{i=1}^m \mathbb{E} [g_i(\mathbf{x}_r^{\text{st}}, \tilde{\mathbf{z}}) | g_i(\mathbf{x}_r^{\text{st}}, \tilde{\mathbf{z}}) > 0].$$

Results from a hundred realizations of $\{(\mathbf{R}^i, \mathbf{S}^i)\}_{i=1}^m$ are reported in Figure 4.2, where we see the robust satisficing solutions stochastically dominate the robust solutions in both performance metrics.

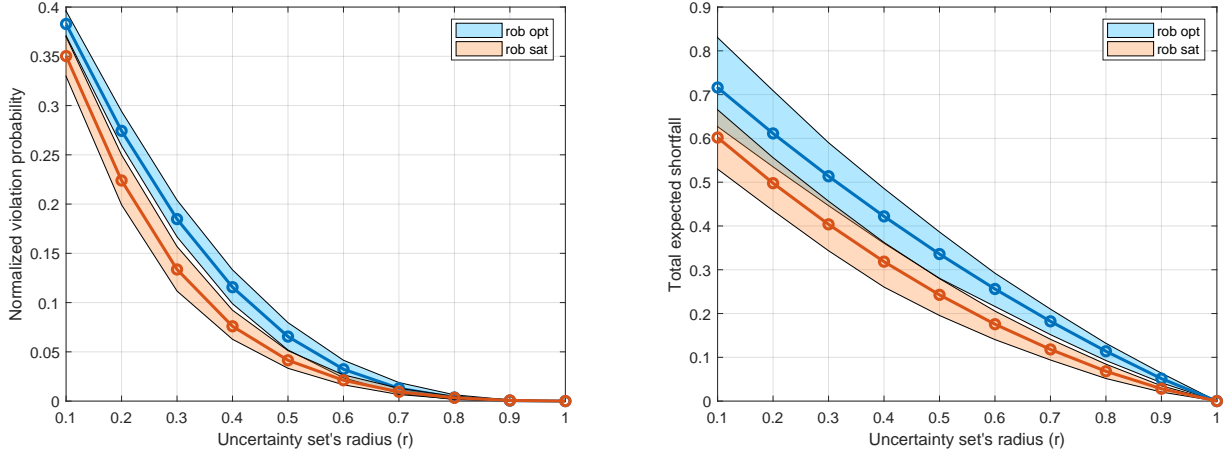


FIGURE 4.2: Normalized probabilities of constraint violation and total expected shortfalls of the robust optimization (rob opt) and the robust satisficing (rob sat) log-sum-exp solutions. Bold lines report mean values, whereas the shaded areas refer to the 10%-90% percentile ranges.

4.5.3 Adaptive network lot-sizing

Next, we present a network lot-sizing example similar to Bertsimas and Ruitter (2016) and Ruitter, Zhen, and Hertog (2018). Suppose that there are n nodes, each of which faces a random demand z_i , $i \in [n]$. Throughout, the support set of \mathbf{z} is assumed to be a hyperrectangle, *i.e.*, $\mathcal{Z} = \{\mathbf{z} \in \mathbb{R}_+^{n_z} \mid \mathbf{z} \leq \bar{\mathbf{z}}\}$. The initial stock $x_i \geq 0$ at each node is to be determined prior to the realization of the random demands. Similarly, we impose that $\mathcal{X} = \{\mathbf{x} \in \mathbb{R}_+^{n_x} \mid \mathbf{x} \leq \bar{\mathbf{x}}\}$. After observing the demand, we can transport stock $y_{ij} \geq 0$ from node i to node j . To ensure that the demands can always be fulfilled, we allow for an emergency order $w_i \geq 0$ to be made at each node. Initial and emergency orders are purchased at the unit costs $c_i \geq 0$ and $\ell_i \geq c_i$, respectively, while the unit transportation costs are denoted by $t_{ij} \geq 0$. It is assumed that t_{ij} is equal to the distance between the two nodes, and hence $t_{ij} = t_{ji}$.

First, we present the robust variant of the lot-sizing problem

$$\begin{aligned}
Z_r = \min \quad & \mathbf{c}^\top \mathbf{x} + x_0 \\
\text{s.t.} \quad & \mathbf{x} + \mathbf{Y}(\mathbf{z})^\top \mathbf{1} - \mathbf{Y}(\mathbf{z})\mathbf{1} + \mathbf{w}(\mathbf{z}) \geq \mathbf{z} & \forall \mathbf{z} \in \mathcal{U}_r \\
& \langle \mathbf{T}, \mathbf{Y}(\mathbf{z}) \rangle + \ell^\top \mathbf{w}(\mathbf{z}) \leq x_0 & \forall \mathbf{z} \in \mathcal{U}_r \\
& \mathbf{Y}(\mathbf{z}) \geq \mathbf{0}, \mathbf{w}(\mathbf{z}) \geq \mathbf{0} & \forall \mathbf{z} \in \mathcal{U}_r \\
& \mathbf{x} \in \mathcal{X}, x_0 \in \mathbb{R}, \mathbf{Y} \in \mathcal{R}^{n,n \times n}, \mathbf{w} \in \mathcal{R}^{n,n},
\end{aligned} \tag{4.39}$$

where $\mathcal{U}_r = \{\mathbf{z} \in \mathbb{R}_+^n \mid \mathbf{z} \leq \bar{\mathbf{z}}, \mathbf{1}^\top \mathbf{z} \leq r\}$ denotes the uncertainty set and the epigraph variable x_0 captures the worst-case transportation and emergency purchase costs. Similar to the proof of Theorem 18, we can dualize Problem (4.39) twice (the first time over the second-stage decisions \mathbf{Y} , \mathbf{w} and the second time over the uncertain demands \mathbf{z}) to obtain an alternative formulation.

Proposition 16. *Problem (4.39) is equivalent to*

$$\begin{aligned}
Z_r = \min \quad & \mathbf{c}^\top \mathbf{x} + x_0 \\
\text{s.t.} \quad & \boldsymbol{\beta}(\boldsymbol{\rho})^\top \bar{\mathbf{z}} + \hat{\boldsymbol{\beta}}(\boldsymbol{\rho})r \leq \boldsymbol{\rho}^\top \mathbf{x} + x_0 & \forall \boldsymbol{\rho} \in \mathcal{P} \\
& \boldsymbol{\beta}(\boldsymbol{\rho}) + \hat{\boldsymbol{\beta}}(\boldsymbol{\rho})\mathbf{1} \geq \boldsymbol{\rho} & \forall \boldsymbol{\rho} \in \mathcal{P} \\
& \boldsymbol{\beta}(\boldsymbol{\rho}) \geq \mathbf{0}, \hat{\boldsymbol{\beta}}(\boldsymbol{\rho}) \geq 0 & \forall \boldsymbol{\rho} \in \mathcal{P} \\
& \mathbf{x} \in \mathcal{X}, x_0 \in \mathbb{R}, \boldsymbol{\beta} \in \mathcal{R}^{n,n}, \hat{\boldsymbol{\beta}} \in \mathcal{R}^{n,1},
\end{aligned} \tag{4.40}$$

where the dual uncertainty set \mathcal{P} is given by $\{\boldsymbol{\rho} \in \mathbb{R}_+^n : \boldsymbol{\rho} \leq \ell, \boldsymbol{\rho}\mathbf{1}^\top - \mathbf{1}\boldsymbol{\rho}^\top \leq \mathbf{T}\}$.

Proof. We can express the robust constraints of Problem (4.39) as

$$\begin{aligned}
& \max_{\mathbf{z} \in \mathcal{U}_r} \min_{\mathbf{Y} \geq \mathbf{0}, \mathbf{w} \geq \mathbf{0}} \left\{ \langle \mathbf{T}, \mathbf{Y} \rangle + \ell^\top \mathbf{w} \mid \mathbf{x} + \mathbf{w} + \mathbf{Y}^\top \mathbf{1} - \mathbf{Y}\mathbf{1} \geq \mathbf{z} \right\} \leq x_0 \\
\iff & \max_{\mathbf{z} \in \mathcal{U}_r} \min_{\mathbf{Y} \geq \mathbf{0}, \mathbf{w} \geq \mathbf{0}} \max_{\boldsymbol{\rho} \geq \mathbf{0}} \left\{ \langle \mathbf{T}, \mathbf{Y} \rangle + \ell^\top \mathbf{w} + \boldsymbol{\rho}^\top (\mathbf{z} - \mathbf{x} - \mathbf{w} + \mathbf{Y}\mathbf{1} - \mathbf{Y}^\top \mathbf{1}) \right\} \leq x_0 \\
\iff & \max_{\mathbf{z} \in \mathcal{U}_r} \max_{\boldsymbol{\rho} \geq \mathbf{0}} \left\{ \boldsymbol{\rho}^\top (\mathbf{z} - \mathbf{x}) + \min_{\mathbf{Y} \geq \mathbf{0}, \mathbf{w} \geq \mathbf{0}} \left\{ \langle \mathbf{Y}, \mathbf{T} + \boldsymbol{\rho}\mathbf{1}^\top - \mathbf{1}\boldsymbol{\rho}^\top \rangle + (\ell - \boldsymbol{\rho})^\top \mathbf{w} \right\} \right\} \leq x_0 \\
\iff & \max_{\mathbf{z} \in \mathcal{U}_r} \max_{\boldsymbol{\rho} \in \mathcal{P}} \left\{ \boldsymbol{\rho}^\top (\mathbf{z} - \mathbf{x}) \right\} \leq x_0 \\
\iff & \max_{\boldsymbol{\rho} \geq \mathbf{0}} \min_{\boldsymbol{\beta} \geq \mathbf{0}, \hat{\boldsymbol{\beta}} \geq 0} \left\{ \boldsymbol{\beta}^\top \bar{\mathbf{z}} + \hat{\boldsymbol{\beta}}r \mid \boldsymbol{\beta} + \hat{\boldsymbol{\beta}}\mathbf{1} \geq \boldsymbol{\rho} \right\} \leq x_0 + \boldsymbol{\rho}^\top \mathbf{x}.
\end{aligned}$$

Treating $\boldsymbol{\rho}$ as uncertainty as well as $\boldsymbol{\beta}$ and $\hat{\boldsymbol{\beta}}$ as dual recourse variables finally completes the proof. \square

Due to the linearity of both formulations, we can solve Problems (4.39) and (4.40) approximately using affine adaptations on the primal and dual recourse, respectively. These approximations however turn out to be equivalent.

Proposition 17. *Problems (4.39) and (4.40) attain the same objective value when solved approximately using affine recourse adaptation.*

Proof. In their Theorem 1, Bertsimas and Ruiter (2016) show an equivalent reformulation of Problem (4.39) which is

$$\begin{aligned}
\min \quad & \mathbf{c}^\top \mathbf{x} + x_0 \\
\text{s.t.} \quad & \boldsymbol{\beta}(\boldsymbol{\rho}, \hat{\rho})^\top \bar{\mathbf{z}} + \hat{\boldsymbol{\beta}}(\boldsymbol{\rho}, \hat{\rho})r \leq \boldsymbol{\rho}^\top \mathbf{x} + \hat{\rho}x_0 & \forall (\boldsymbol{\rho}, \hat{\rho}) \in \hat{\mathcal{P}} \\
& \boldsymbol{\beta}(\boldsymbol{\rho}, \hat{\rho}) + \hat{\boldsymbol{\beta}}(\boldsymbol{\rho}, \hat{\rho})\mathbf{1} \geq \boldsymbol{\rho} & \forall (\boldsymbol{\rho}, \hat{\rho}) \in \hat{\mathcal{P}} \\
& \boldsymbol{\beta}(\boldsymbol{\rho}, \hat{\rho}) \geq \mathbf{0}, \hat{\boldsymbol{\beta}}(\boldsymbol{\rho}, \hat{\rho}) \geq 0 & \forall (\boldsymbol{\rho}, \hat{\rho}) \in \hat{\mathcal{P}} \\
& \mathbf{x} \in \mathcal{X}, x_0 \in \mathbb{R}, \boldsymbol{\beta} \in \mathcal{R}^{n+1,n}, \hat{\boldsymbol{\beta}} \in \mathcal{R}^{n+1,1},
\end{aligned} \tag{4.41}$$

where $\hat{\mathcal{P}} = \{(\boldsymbol{\rho}, \hat{\rho}) \in \mathbb{R}_+^n \times \mathbb{R}_+ \mid \boldsymbol{\rho} \leq \hat{\rho}\boldsymbol{\ell}, \boldsymbol{\rho}\mathbf{1}^\top - \mathbf{1}\boldsymbol{\rho}^\top \leq \hat{\rho}\mathbf{T}, \mathbf{1}^\top \boldsymbol{\rho} + \hat{\rho} = 1\}$. They also argue in their Theorem 2 that the respective affine recourse approximations of Problems (4.39) and (4.41) are equivalent. As a result, it suffices to show that the affine recourse approximations of Problems (4.40) and (4.41) are equivalent.

First, we write down the affine recourse approximation of Problem (4.40) by restricting $\boldsymbol{\beta}(\boldsymbol{\rho})$ and $\hat{\boldsymbol{\beta}}(\boldsymbol{\rho})$ to $\boldsymbol{\beta}^i + \boldsymbol{\beta}^s \boldsymbol{\rho}$ and $\hat{\boldsymbol{\beta}}^i + \hat{\boldsymbol{\beta}}^s \boldsymbol{\rho}$ (where ‘i’ and ‘s’ indicate the intercept and slope of the affine decision rules), respectively, and obtain

$$\begin{aligned}
\min \quad & \mathbf{c}^\top \mathbf{x} + x_0 \\
\text{s.t.} \quad & \bar{\mathbf{z}}^\top \boldsymbol{\beta}^i + r\hat{\boldsymbol{\beta}}^i + (\bar{\mathbf{z}}^\top \boldsymbol{\beta}^s + r\hat{\boldsymbol{\beta}}^s)\boldsymbol{\rho} \leq \boldsymbol{\rho}^\top \mathbf{x} + x_0 & \forall \boldsymbol{\rho} \in \mathcal{P} \\
& \boldsymbol{\beta}^i + \mathbf{1}\hat{\boldsymbol{\beta}}^i + (\boldsymbol{\beta}^s + \mathbf{1}\hat{\boldsymbol{\beta}}^s)\boldsymbol{\rho} \geq \boldsymbol{\rho} & \forall \boldsymbol{\rho} \in \mathcal{P} \\
& \boldsymbol{\beta}^i + \boldsymbol{\beta}^s \boldsymbol{\rho} \geq \mathbf{0}, \hat{\boldsymbol{\beta}}^i + \hat{\boldsymbol{\beta}}^s \boldsymbol{\rho} \geq 0 & \forall \boldsymbol{\rho} \in \mathcal{P} \\
& \mathbf{x} \in \mathcal{X}, x_0 \in \mathbb{R}, \boldsymbol{\beta}^i \in \mathbb{R}^n, \boldsymbol{\beta}^s \in \mathbb{R}^{n \times n}, \hat{\boldsymbol{\beta}}^i \in \mathbb{R}, \hat{\boldsymbol{\beta}}^s \in \mathbb{R}^{1 \times n}.
\end{aligned} \tag{4.42}$$

Next, for Problem (4.41), we first observe that the uncertainty set $\hat{\mathcal{P}}$ requires $\hat{\rho}$ to be linearly dependent on $\boldsymbol{\rho}$. Hence, we can simply ignore the additional uncertain parameter $\hat{\rho}$ and work with the projection of $\hat{\mathcal{P}}$ on $\boldsymbol{\rho}$. By a slight abuse of notation, we will denote this projection by $\hat{\mathcal{P}}$ and note that

$$\hat{\mathcal{P}} = \left\{ \boldsymbol{\rho} \in \mathbb{R}_+^n \mid \boldsymbol{\rho} \leq (1 - \mathbf{1}^\top \boldsymbol{\rho})\boldsymbol{\ell}, \boldsymbol{\rho}\mathbf{1}^\top - \mathbf{1}\boldsymbol{\rho}^\top \leq (1 - \mathbf{1}^\top \boldsymbol{\rho})\mathbf{T} \right\}.$$

Note that as $\hat{\mathcal{P}} \subset \mathbb{R}_+^n$ and as $\boldsymbol{\ell} \geq \mathbf{0}$, it is a necessity that $\mathbf{1}^\top \boldsymbol{\rho} < 1$ for all $\boldsymbol{\rho} \in \hat{\mathcal{P}}$. We are now ready to present the explicit affine recourse approximation of Problem (4.41), which is

$$\begin{aligned}
\min \quad & \mathbf{c}^\top \mathbf{x} + x_0 \\
\text{s.t.} \quad & \bar{\mathbf{z}}^\top \boldsymbol{\beta}^i + r\hat{\boldsymbol{\beta}}^i + (\bar{\mathbf{z}}^\top \boldsymbol{\beta}^s + r\hat{\boldsymbol{\beta}}^s)\boldsymbol{\rho} \leq \boldsymbol{\rho}^\top \mathbf{x} + (1 - \mathbf{1}^\top \boldsymbol{\rho})x_0 & \forall \boldsymbol{\rho} \in \hat{\mathcal{P}} \\
& \boldsymbol{\beta}^i + \mathbf{1}\hat{\boldsymbol{\beta}}^i + (\boldsymbol{\beta}^s + \mathbf{1}\hat{\boldsymbol{\beta}}^s)\boldsymbol{\rho} \geq \boldsymbol{\rho} & \forall \boldsymbol{\rho} \in \hat{\mathcal{P}} \\
& \boldsymbol{\beta}^i + \boldsymbol{\beta}^s \boldsymbol{\rho} \geq \mathbf{0}, \hat{\boldsymbol{\beta}}^i + \hat{\boldsymbol{\beta}}^s \boldsymbol{\rho} \geq 0 & \forall \boldsymbol{\rho} \in \hat{\mathcal{P}} \\
& \mathbf{x} \in \mathcal{X}, x_0 \in \mathbb{R}, \boldsymbol{\beta}^i \in \mathbb{R}^n, \boldsymbol{\beta}^s \in \mathbb{R}^{n \times n}, \hat{\boldsymbol{\beta}}^i \in \mathbb{R}, \hat{\boldsymbol{\beta}}^s \in \mathbb{R}^{1 \times n}.
\end{aligned} \tag{4.43}$$

It remains to show that Problems (4.42) and (4.43) are equivalent. First, we will show that Problem (4.43) is a relaxation of Problem (4.42). To this end, for any feasible solution $\mathbf{X} = (\mathbf{x}, x_0, \boldsymbol{\beta}^i, \boldsymbol{\beta}^s, \hat{\boldsymbol{\beta}}^i, \hat{\boldsymbol{\beta}}^s)$ of Problem (4.42), we will show that $\mathbf{X}' = (\mathbf{x}, x_0, \boldsymbol{\beta}^i, \boldsymbol{\beta}^s - \boldsymbol{\beta}^i \mathbf{1}^\top, \hat{\boldsymbol{\beta}}^i, \hat{\boldsymbol{\beta}}^s - \hat{\boldsymbol{\beta}}^i \mathbf{1}^\top)$ is feasible in Problem (4.43). Note that, as both solutions share the same \mathbf{x} and the same x_0 , they attain the same objective value in their

respective problem.

For any $\rho \in \hat{\mathcal{P}}$, it is readily seen that $\rho/(1 - \mathbf{1}^\top \rho) \in \mathcal{P}$. As a result, the feasibility of X in view of Problem (4.42) implies, for all $\rho \in \hat{\mathcal{P}}$, that

$$\begin{aligned} (1 - \mathbf{1}^\top \rho)(\bar{z}^\top \beta^i + r\hat{\beta}^i) + (\bar{z}^\top \beta^s + \hat{z}\hat{\beta}^s)\rho &\leq \rho^\top \mathbf{x} + (1 - \mathbf{1}^\top \rho)x_0, \\ (1 - \mathbf{1}^\top \rho)(\beta^i + \mathbf{1}\hat{\beta}^i) + (\beta^s + \mathbf{1}\hat{\beta}^s)\rho &\geq \rho, \\ (1 - \mathbf{1}^\top \rho)\beta^i + \beta^s \rho &\geq \mathbf{0}, \\ (1 - \mathbf{1}^\top \rho)\hat{\beta}^i + \hat{\beta}^s \rho &\geq 0. \end{aligned}$$

Rearranging terms in the above four inequalities yields

$$\begin{aligned} \bar{z}^\top \beta^i + r\hat{\beta}^i + \left(\bar{z}^\top (\beta^s - \beta^i \mathbf{1}^\top) + r(\hat{\beta}^s - \hat{\beta}^i \mathbf{1}^\top) \right) \rho &\leq \rho^\top \mathbf{x} + (1 - \mathbf{1}^\top \rho)x_0, \\ \beta^i + \mathbf{1}\hat{\beta}^i + \left((\beta^s - \beta^i \mathbf{1}^\top) + \mathbf{1}(\hat{\beta}^s - \hat{\beta}^i \mathbf{1}^\top) \right) \rho &\geq \rho, \\ \beta^i + (\beta^s - \beta^i \mathbf{1}^\top) \rho &\geq \mathbf{0}, \\ \hat{\beta}^i + (\hat{\beta}^s - \hat{\beta}^i \mathbf{1}^\top) \rho &\geq 0, \end{aligned}$$

for all $\rho \in \hat{\mathcal{P}}$, which in turn implies that X' is indeed feasible in Problem (4.43).

Conversely, for any feasible solution $X = (\mathbf{x}, x_0, \beta^i, \beta^s, \hat{\beta}^i, \hat{\beta}^s)$ of Problem (4.43), one can similarly show that $X' = (\mathbf{x}, x_0, \beta^i, \beta^s + \beta^i \mathbf{1}^\top, \hat{\beta}^i, \hat{\beta}^s + \hat{\beta}^i \mathbf{1}^\top)$ is feasible in Problem (4.42) to conclude that Problem (4.42) is a relaxation of Problem (4.43). To see this, observe that $\rho/(1 + \mathbf{1}^\top \rho) \in \hat{\mathcal{P}}$ for any $\rho \in \mathcal{P}$. As a result, the feasibility of X in view of Problem (4.43) implies, for all $\rho \in \mathcal{P}$, that

$$\begin{aligned} (1 + \mathbf{1}^\top \rho)(\bar{z}^\top \beta^i + r\hat{\beta}^i) + (\bar{z}^\top \beta^s + r\hat{\beta}^s)\rho &\leq \rho^\top \mathbf{x} + x_0, \\ (1 + \mathbf{1}^\top \rho)(\beta^i + \mathbf{1}\hat{\beta}^i) + (\beta^s + \mathbf{1}\hat{\beta}^s)\rho &\geq \rho, \\ (1 + \mathbf{1}^\top \rho)\beta^i + \beta^s \rho &\geq \mathbf{0}, \\ (1 + \mathbf{1}^\top \rho)\hat{\beta}^i + \hat{\beta}^s \rho &\geq 0. \end{aligned}$$

Rearranging the terms in the above inequalities shows that X' is indeed feasible in Problem (4.42) as desired. Therefore, the optimal objective value of Problem (4.42) constitutes both a lower and an upper bound of that of Problem (4.43). The proof is hence completed. \square

For the robust satisficing variant of the problem, we consider

$$\begin{aligned} \min \quad & k \\ \text{s.t.} \quad & \mathbf{x} + \mathbf{Y}(\mathbf{z})^\top \mathbf{1} - \mathbf{Y}(\mathbf{z})\mathbf{1} + \mathbf{w}(\mathbf{z}) \geq \mathbf{z} \quad \forall \mathbf{z} \in \mathcal{Z} \\ & \mathbf{c}^\top \mathbf{x} + \langle \mathbf{T}, \mathbf{Y}(\mathbf{z}) \rangle + \ell^\top \mathbf{w}(\mathbf{z}) \leq \tau + k\|\mathbf{z}\|_1 \quad \forall \mathbf{z} \in \mathcal{Z} \\ & \mathbf{Y}(\mathbf{z}) \geq \mathbf{0}, \mathbf{w}(\mathbf{z}) \geq \mathbf{0} \quad \forall \mathbf{z} \in \mathcal{Z} \\ & \mathbf{x} \in \mathcal{X}, k \in \mathbb{R}_+, \mathbf{Y} \in \mathcal{R}^{n,n \times n}, \mathbf{w} \in \mathcal{R}^{n,n}, \end{aligned} \tag{4.44}$$

where $\tau \geq Z_0 = 0$ is the prescribed target objective. The dualized formulation (4.13) corresponding to this problem is explicitly given below.

Proposition 18. Problem (4.44) is equivalent to

$$\begin{aligned}
& \min && k \\
& \text{s.t.} && (\mathbf{c} - \boldsymbol{\rho})^\top \mathbf{x} + \boldsymbol{\beta}(\boldsymbol{\rho})^\top \bar{\mathbf{z}} \leq \tau && \forall \boldsymbol{\rho} \in \mathcal{P} \\
& && \boldsymbol{\beta}(\boldsymbol{\rho}) + k\mathbf{1} \geq \boldsymbol{\rho} && \forall \boldsymbol{\rho} \in \mathcal{P} \\
& && \boldsymbol{\beta}(\boldsymbol{\rho}) \geq \mathbf{0} && \forall \boldsymbol{\rho} \in \mathcal{P} \\
& && \mathbf{x} \in \mathcal{X}, k \in \mathbb{R}_+, \boldsymbol{\beta} \in \mathcal{R}^{n,n},
\end{aligned} \tag{4.45}$$

where the dual uncertainty set \mathcal{P} is given by $\{\boldsymbol{\rho} \in \mathbb{R}_+^n : \boldsymbol{\rho} \leq \boldsymbol{\ell}, \boldsymbol{\rho}\mathbf{1}^\top - \mathbf{1}\boldsymbol{\rho}^\top \leq \mathbf{T}\}$.

Proof. The proof widely parallels to that of Proposition 16 and is thus omitted. \square

Proposition 19. Problems (4.44) and (4.45) attain the same objective value when solved approximately using affine recourse adaptation.

Proof. First, we can use Theorem 1 in Bertsimas and Ruitter (2016) to argue that Problem (4.44) is equivalent to

$$\begin{aligned}
& \min && k \\
& \text{s.t.} && (\hat{\boldsymbol{\rho}}\mathbf{c} - \boldsymbol{\rho})^\top \mathbf{x} + \bar{\mathbf{z}}^\top \boldsymbol{\beta}(\boldsymbol{\rho}, \hat{\boldsymbol{\rho}}) \leq \hat{\boldsymbol{\rho}}\tau && \forall (\boldsymbol{\rho}, \hat{\boldsymbol{\rho}}) \in \hat{\mathcal{P}} \\
& && \boldsymbol{\beta}(\boldsymbol{\rho}, \hat{\boldsymbol{\rho}}) + k\hat{\boldsymbol{\rho}}\mathbf{1} \geq \boldsymbol{\rho} && \forall (\boldsymbol{\rho}, \hat{\boldsymbol{\rho}}) \in \hat{\mathcal{P}} \\
& && \boldsymbol{\beta}(\boldsymbol{\rho}, \hat{\boldsymbol{\rho}}) \geq \mathbf{0} && \forall (\boldsymbol{\rho}, \hat{\boldsymbol{\rho}}) \in \hat{\mathcal{P}} \\
& && \mathbf{x} \in \mathcal{X}, k \in \mathbb{R}_+, \boldsymbol{\beta} \in \mathcal{R}^{n+1,n},
\end{aligned}$$

where $\hat{\mathcal{P}}$ is the same as that in the proof of Proposition 17. The proof largely follows that of Proposition 17, *i.e.*, one can show that the affine adaptation approximation of the above problem is equivalent to that of (4.45), which in turn implies that the affine recourse approximations of (4.44) and (4.45) are equivalent (see Theorem 2 in Bertsimas and Ruitter, 2016). Details are omitted for the sake of brevity. \square

Evaluation and discussion of results:

We consider a network of $n = 20$ nodes with $\mathcal{X} = \mathcal{Z} = [0, 20]^n$. To ensure suitable variability among the nodes, the components of the initial ordering cost \mathbf{c} and emergency cost $\boldsymbol{\ell}$ are generated uniformly from $[8, 10]$ and $[18, 20]$ respectively. We then select the node locations randomly from $[0, 10]^2$ and accordingly compute the (Euclidean) distance matrix \mathbf{T} . For the evaluation of the robust lot-sizing models, we vary $r \geq 0$ and approximate \mathbf{x}_r^{rb} by solving either solving (4.39) or (4.40) using affine recourse adaptation. Similarly for the robust satisficing models, we vary $\tau \geq 0$ and determine approximate robust satisficing solutions $\mathbf{x}_\tau^{\text{st}}$ from either (4.44) or (4.45). We then compare their respective *first-stage costs* (*i.e.*, $\mathbf{c}^\top \mathbf{x}_r^{\text{rb}}$ and $\mathbf{c}^\top \mathbf{x}_\tau^{\text{st}}$) with the *expected total costs*:

$$\begin{aligned}
& \mathbb{E} \left[\mathbf{c}^\top \mathbf{x}_r^{\text{rb}} + \min_{\mathbf{Y} \geq \mathbf{0}, \mathbf{w} \geq \mathbf{0}} \left\{ \langle \mathbf{Y}, \mathbf{T} \rangle + \boldsymbol{\ell}^\top \mathbf{w} \mid \mathbf{x}_r^{\text{rb}} + \mathbf{Y}^\top \mathbf{1} - \mathbf{Y}\mathbf{1} + \mathbf{w} \geq \bar{\mathbf{z}} \right\} \right], \quad \text{and} \\
& \mathbb{E} \left[\mathbf{c}^\top \mathbf{x}_\tau^{\text{st}} + \min_{\mathbf{Y} \geq \mathbf{0}, \mathbf{w} \geq \mathbf{0}} \left\{ \langle \mathbf{Y}, \mathbf{T} \rangle + \boldsymbol{\ell}^\top \mathbf{w} \mid \mathbf{x}_\tau^{\text{st}} + \mathbf{Y}^\top \mathbf{1} - \mathbf{Y}\mathbf{1} + \mathbf{w} \geq \bar{\mathbf{z}} \right\} \right],
\end{aligned}$$

from a hundred independent realizations of $\bar{\mathbf{z}} = \tilde{\mathbf{z}}^{\text{tot}} \tilde{\mathbf{z}}' / (\mathbf{1}_{n_z}^\top \tilde{\mathbf{z}}')$, where $\tilde{\mathbf{z}}^{\text{tot}}$ representing the total demand is drawn uniformly from $[20\sqrt{n}, 40\sqrt{n}]$ while each component \tilde{z}'_i is

independently and uniformly drawn from $[0, 1]$. This is primarily to enforce possible correlations between the demands.

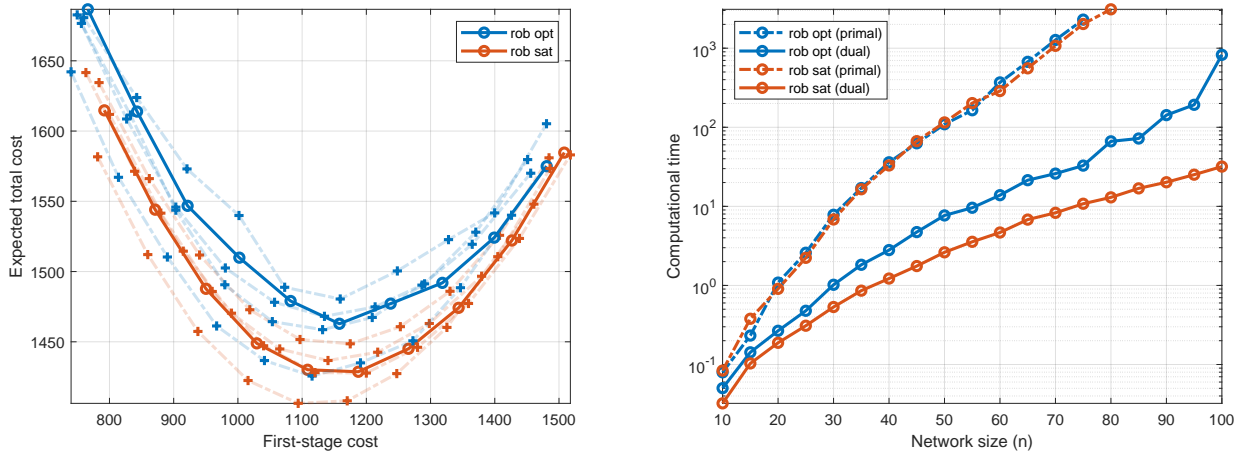


FIGURE 4.3: Costs and computational times (in seconds) of the robust optimization (*rob opt*) and the robust satisficing (*rob sat*) lot-sizing solutions.

Figure 4.3 (left) shows the relative out-of-sample performance of the robust and robust satisficing models by comparing the expected total cost for the same first-stage cost. The experiment is carried out multiple times, each with different (c, ℓ, T) . We arbitrarily highlight the results of a single run in bold curves and show those of another four runs in dashed curves. The expected total cost appears to be minimized when the first-stage cost is around 1,150. When the manager is less committed to making purchases in the first stage, she has to compensate with exorbitant costs in the second stage via transshipment or emergency orders. On the other hand, if the manager is overly committed in the first stage, the total cost could still be high because of the excessive advance purchases. Figure 4.3 (right) compares the computational times required by Gurobi & RSOME in logarithmic scale of the primal robust problem (4.39), dual robust problem (4.40), primal robust satisficing problem (4.44) and dual robust satisficing problem (4.45) by varying the number of nodes $n \in \{10, 15, \dots, 100\}$. The primal models (4.39) and (4.44) cannot be solved within a time limit of one hour when the number of nodes exceed 80. When $n = 100$, the dual robust model (4.40) takes about 15 minutes, whereas the dual robust satisficing model (4.45) takes only about 30 seconds. The better efficiency of the dual approaches was first observed and explained in Bertsimas and Ruiter (2016). Table 4.1 summarizes the number of constraints and decision variables in the robust counterparts of each of the four models discussed in this section: the primal and dual robust models in (4.39), (4.40) and the primal and dual robust satisficing models in (4.44) and (4.45).

	Primal formulation			Dual formulation		
	Constraints		Decision Variables	Constraints		Decision Variables
	Affine	Non-negativity		Affine	Non-negativity	
Robust	$(n+1)(n^2+n+1)$	$(n+1)(n^2+n+1)$	$(2n+1)(n^2+n+1)+1$	$2(n+1)^2$	$2n^2(n+1)$	$2n(n^2+n+1)+(n+3)$
Robust Satisficing	$(n+1)(n^2+n+1)$	$n(n^2+n+1)$	$2n(n^2+n+1)+1$	$(2n+1)(n+1)$	$(2n+1)n^2$	$2n(n^2+n+1)+1$

TABLE 4.1: Number of constraints and decision variables in the robust counterpart formulations of the four lot-sizing models

Comparing the primal and dual models, the number of decision variables are similarly growing as $\mathcal{O}(n^3)$ and the affine constraints in both the primal counterparts grow as $\mathcal{O}(n^3)$ compared to $\mathcal{O}(n^2)$ for the dual counterparts while the dual counterparts admit more non-negativity constraints even though both grow as $\mathcal{O}(n^3)$. This explains the remarkable computational advantage of the dual models over the primal models as demonstrated in Figure 4.3 (right), since non-negativity restrictions are much easier for numerical solvers to handle when compared to affine constraints (see Section 5.3 in Bertsimas and Ruiters, 2016, for an example).

4.6 Summary of Part II and future directions

This section summarizes the results in Part II of this dissertation and provides some useful directions for future research.

Summary:

In summary, this chapter addressed conic uncertain optimization problems in the context of the robust satisficing framework, which seeks to maintain the cost $c^\top x$ below a pre-specified target τ while simultaneously controlling the degree of infeasibility with the robust satisficing parameter k . The constraint function $g(x, z)$ we considered as the optimal value of a conic optimization problem was broad enough to include a wide variety of constraints and problem classes. While quadratic constraints with quadratic uncertainty support and penalty function led to an exact SDP reformulation of the robust constraints, for generic conic uncertain problems with polyhedral support sets and penalty functions, we exploited conic duality under suitable assumptions to derive equivalent dual reformulations which can be approximated with affine recourse adaptation. In both cases, feasibility of the reformulated model is guaranteed when the target is strictly greater than the nominal optimal value Z_0 . The benefits of the dual model are further illustrated in the special case of a non-negative orthant cone, wherein we prove that despite being simpler, the affine recourse approximation of the dual reformulation provides a closer approximation of the original problem when compared to a specific non-affine recourse approximation of the original problem itself. The three numerical examples of growth optimal portfolio selection, log-sum-exp optimization and adaptive lot-sizing demonstrated the improved performance of the robust satisficing framework over classical robust optimization both in terms of both modeling and

computational speed metrics. Thus, the dual formulation provided *tractability, feasibility* and *computational* benefits over the original primal problem.

Future research questions:

We enlist below some future directions of this work:

i) While the double dualized reformulation in (4.13) for generic conic uncertain problems (with polyhedral support sets and penalty functions) is approximately tractable and feasible, it still remains a challenge to interpret the dual recourse variables and code the dual formulation for more complex cones than those considered in this chapter. It would thus be interesting to explore methods and techniques to find tractable primal reformulations that are more readily codable than the double dualized formulation. In spirit, this could be similar to the approach followed in Chapter 3 where we provided a direct primal proof of correctness to show equivalence between the large-size and aggregated linear programs (for the tail probability, weighted tail probability and expected stop-loss functions) instead of examining the dual formulations.

ii) The results in Theorem 17 could be extended to the case of quadratic constraints and penalty function with uncertainty support which is the intersection of finitely many bounded and non-empty ellipsoids instead of a single ellipsoid. Although the robust counterpart with the intersection of ellipsoids is known to be NP-hard (see Section 3.2.2 in Ben-Tal and Nemirovski, 1998), it can be approximated by a single, explicit, semidefinite program by using the approximate S-lemma (see Theorem 2.3 in Ben-Tal, Nemirovski, and Roos, 2002). It would be interesting to see how the quality of approximations with this approach (for the robust satisficing framework) compares with that of the classical robust framework in Theorem 2.4 of Ben-Tal, Nemirovski, and Roos, 2002. Further, properly chosen ellipsoids and intersection of ellipsoids could be used as reasonable approximations to more complicated uncertainty sets.

iii) In Section 4.4.1, the data-driven conic robust satisficing formulation in (4.31) successfully recovered the data-driven robust satisficing model of Long, Sim, and Zhou (2021) without introducing an ambiguity set of uncertain probability distributions. This was achieved by suitably defining the constraint average function \bar{g} and penalty average function \bar{p} . It would be interesting to explore if this approach can be combined with a distributionally robust optimization approach like that in Long, Sim, and Zhou (2021).

iv) The computational speed results in Figure 4.3 (right) for the four lot-sizing models were corroborated in Table 4.1 by delineating the number of decision variables, affine and non-negativity constraints. However, it would be useful to specify how the time complexity grows in (as a function of) the input size of the linear program being employed to solve the robust counterparts of the four models after approximating the dual robust satisficing formulations using affine recourse adaptation.

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Appendix A

A.1 Proof of Theorem 7

Proof. With identical pairwise independent variables, it is straightforward to show that, similar to the probability objective in (2.28), the large-sized linear program (2.50) with the expectation objective is equivalent to the corresponding aggregated linear program proposed by Boros and Prékopa (1989) and Prékopa (1990a):

$$\begin{aligned}
 BP_{pw}(n, k, p) = \max & \quad \sum_{\ell=k+1}^n (\ell - k)v_{\ell} \\
 \text{s.t.} & \quad \sum_{\ell=2}^n \binom{\ell}{2} v_{\ell} = \binom{n}{2} p^2 \\
 & \quad \sum_{\ell=0}^n v_{\ell} = 1 \\
 & \quad \sum_{\ell=1}^n \ell v_{\ell} = np \\
 & \quad v_{\ell} \geq 0, \quad \forall \ell \in [0, n],
 \end{aligned} \tag{A.1}$$

The proof of equivalence is identical to that in the proof of Theorem 4 with the only difference being in the structure of the objective function. The proof of the closed form expression for the tight upper bound in Theorem 7 broadly follows that of the corresponding closed-form in (2.27) for the probability objective function, derived in Boros and Prékopa (1989) by determining valid primal and dual feasible bases which attain the bound.

Denote by $\mathbf{a}_0, \mathbf{a}_1, \dots, \mathbf{a}_n$ the column vectors of the constraint matrix in the linear program (A.1). Corresponding to the three constraints, let $J = \{i, j, \ell\}$ denote the set of subscripts of a basic feasible solution vector (v_i, v_j, v_{ℓ}) and $\mathbf{B} = [\mathbf{a}_i, \mathbf{a}_j, \mathbf{a}_{\ell}]$ denote a basis matrix assuming that the basis columns are placed in the increasing order of their subscripts ($i < j < \ell$). Then from Section 3 in Prékopa (1988), the constraint matrix is a Pascal matrix while the basis matrix \mathbf{B} is a minor of the constraint matrix with every upper triangular element assuming a strictly positive value. From Theorem 4 in the same section, it must be true that the determinant of \mathbf{B} satisfies $|\mathbf{B}| > 0$. We first analyze the necessary conditions on the basis indices i, j, ℓ to guarantee dual feasibility depending on the position of k relative to these indices.

A.1.1 Dual feasibility conditions

Denote by $\mathbf{c}_B^\top = [c_i, c_j, c_\ell]$ the cost vector from the objective in (A.1) corresponding to the basis indices in J and by c_m the cost vector components corresponding to the non-basic indices $m \in [n] \setminus J$. The dual feasibility conditions for the maximization problem in (A.1) are given by:

$$\mathbf{c}_B^\top \mathbf{B}^{-1} \mathbf{a}_m \geq c_m, \quad \forall m \in [n] \setminus J \quad (\text{A.2})$$

From Section 5 in Prékopa (1988), the condition in (A.2) can be reformulated as the non-positivity of the first component of the solution vector

$$\begin{pmatrix} 1 & \mathbf{c}_B^\top \\ 0 & \mathbf{B} \end{pmatrix}^{-1} \begin{pmatrix} c_m \\ \mathbf{a}_m \end{pmatrix}, \quad \forall m \in [n] \setminus J \quad (\text{A.3})$$

which in turn can be formulated using Cramer's rule as:

$$\left| \begin{array}{cc} c_m & \mathbf{c}_B^\top \\ \mathbf{a}_m & \mathbf{B} \end{array} \right| / \left| \begin{array}{c} 1 \\ 0 \end{array} \right| \mathbf{c}_B^\top \leq 0, \quad \forall m \in [n] \setminus J \quad (\text{A.4})$$

Since $|\mathbf{B}| > 0$, the determinant in the denominator is strictly positive and thus we only need to ensure that

$$\left| \begin{array}{cc} c_m & \mathbf{c}_B^\top \\ \mathbf{a}_m & \mathbf{B} \end{array} \right| \leq 0, \quad \forall m \in [n] \setminus J \quad (\text{A.5})$$

From the objective function coefficients in (A.1), the components of the cost vector \mathbf{c}_B^\top and c_m depend on the position of k relative to the basis indices i, j, ℓ . The following four basis types correspond to these positions:

$$\begin{aligned} \text{Basis type 0: } & k \leq i < j < \ell \\ \text{Basis type 1: } & i < j \leq k < \ell \\ \text{Basis type 2: } & i < k \leq j < \ell \\ \text{Basis type 3: } & i < j < \ell \leq k \end{aligned} \quad (\text{A.6})$$

We note that the basis type 0 can hold only for $k = 0$. Otherwise, $k \leq i < j < \ell$ is ruled out since in that case $\mathbf{c}_B^\top = [i - k, j - k, \ell - k]$ and it is easy to show that the determinant in (A.5) would be strictly positive when $c_m = 0$ ($m \leq k - 1$, where $m \in [n] \setminus J$) since

$$\left| \begin{array}{cccc} 0 & i - k & j - k & \ell - k \\ 1 & 1 & 1 & 1 \\ m & i & j & \ell \\ \binom{m}{2} & \binom{i}{2} & \binom{j}{2} & \binom{\ell}{2} \end{array} \right| \xrightarrow{R_1 - R_3 + kR_2} \left| \begin{array}{cccc} k - m & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 \\ m & i & j & \ell \\ \binom{m}{2} & \binom{i}{2} & \binom{j}{2} & \binom{\ell}{2} \end{array} \right| = (k - m)|\mathbf{B}| > 0$$

When $k = 0$, $\mathbf{c}_B^\top = [i, j, \ell]$ and the tight bound from (A.1) is given by the mean:

$$\bar{E}(n, 0, p) = iv_i + jv_j + \ell v_\ell = np$$

Similarly the basis type 3 holds only for $k = n$ with $\bar{E}(n, n, p) = 0$. Otherwise, $i < j < \ell \leq k$ is ruled out since in that case $\mathbf{c}_B^\top = [0, 0, 0]$ and the determinant in (A.5) would be strictly positive when $c_m > 0$ ($m \geq k + 1$, where $m \in [n] \setminus J$). In other words,

for any $p \in (0, 1)$, the maximization problem (A.1) admits an objective function value $\bar{E}(n, k, p) = np$ and $\bar{E}(n, k, p) = 0$ if and only if $k = 0$ and $k = n$ respectively. We now delineate the necessary conditions for bases of types 1 and 2 to be dual feasible.

A) Basis type 1:

We now consider the first basis type ($i < j < k < \ell$) from (A.6). The corresponding cost vector is $c_B^\top = [0, 0, \ell - k]$. From (A.5), we have the determinant inequality

$$\begin{vmatrix} c_m & 0 & 0 & \ell - k \\ 1 & 1 & 1 & 1 \\ m & i & j & \ell \\ \binom{m}{2} & \binom{i}{2} & \binom{j}{2} & \binom{\ell}{2} \end{vmatrix} \leq 0, \quad \forall m \in [n] \setminus J \quad (\text{A.7})$$

i) $m \leq k$

If $m \leq k$, then $c_m = 0$ and from (A.7) we need

$$(-1)^{3+1}(\ell - k) \begin{vmatrix} 1 & 1 & 1 \\ m & i & j \\ \binom{m}{2} & \binom{i}{2} & \binom{j}{2} \end{vmatrix} = (-\frac{1}{2})(\ell - k)(i - m)(j - m)(j - i) \leq 0, \quad \forall m \in [n] \setminus J$$

where the latter expression is from the well-known Vandermonde determinant. Since $i < j < k < \ell$ we need

$$\begin{aligned} (m - i)(m - j) &\geq 0, & \forall m \in [k] \setminus J \\ m \leq i \text{ or } m &\geq j, & \forall m \in [k] \setminus J \\ \text{or } j = i + 1, & & j \in [1, k - 1] \end{aligned} \quad (\text{A.8})$$

where $[k] \setminus J = \{1, \dots, i - 1, i + 2, \dots, k\}$ since the indices i, j satisfy $i + 1 = j < k$. The condition that the indices i, j are consecutive is similar to the third type basis $\{j - 1, j, k\}$ for the probability bound in (2.32) except that the third index k is not included in the basis here, the reason for which will be discussed later in the primal feasibility section of this proof. For this reason, we will henceforward consider only strict inequalities for the conditions in (A.6).

ii) $m > k$

If $m > k$, then $c_m = m - k$ and from (A.7) we have the determinant inequality

$$\begin{vmatrix} m - k & 0 & 0 & \ell - k \\ 1 & 1 & 1 & 1 \\ m & i & j & \ell \\ \binom{m}{2} & \binom{i}{2} & \binom{j}{2} & \binom{\ell}{2} \end{vmatrix} \leq 0, \quad \forall m \in [k + 1, n] \setminus J \quad (\text{A.9})$$

or

$$\begin{aligned}
& \frac{1}{2} [(m-k)(\ell-i)(\ell-j)(j-i) \\
& - (\frac{1}{2})(\ell-k)(i-m)(j-m)(j-i)] \leq 0, \quad \forall m \in [k+1, n] \setminus J \\
& (j-i) \left[\frac{(\ell-i)(\ell-j)}{\ell-k} - \frac{(m-i)(m-j)}{m-k} \right] \leq 0, \quad \forall m \in [k+1, n] \setminus J \\
& \frac{(\ell-i)(\ell-j)}{\ell-k} \leq \frac{(m-i)(m-j)}{m-k}, \quad \forall m \in [k+1, n] \setminus J
\end{aligned} \tag{A.10}$$

where the last inequality is due to $j > i$ and $[k+1, n] \setminus J = \{k+1, \dots, \ell-1, \ell+1, \dots, n\}$. For a given i, j, k (where $i < j < k$), it can be seen that both the functions $\frac{(\ell-i)(\ell-j)}{\ell-k}$ and $\frac{(m-i)(m-j)}{m-k}$ are identical piece-wise linear convex in ℓ and m respectively when $\ell > \max(i, j, k)$, $m > \max(i, j, k)$. Since $i < j < k < \ell$ and $i < j < k < m$, both the functions admit integer minimizers in the range $[k, n]$. Let

$$\underline{m} = \underset{m \in [k+1, n] \setminus J}{\operatorname{argmin}} \frac{(m-i)(m-j)}{m-k}.$$

Then (A.10) is satisfied when the index $\ell = \underline{m}$ where \underline{m} must satisfy:

$$\begin{aligned}
\underline{m} - k &= \frac{(\underline{m}-i)(\underline{m}-j)}{[(\underline{m}-i) + (\underline{m}-j)]} \\
\underline{m} &= k \pm \sqrt{(k-i)(k-j)} \\
&= k + \sqrt{(k-j)(k-i)}
\end{aligned} \tag{A.11}$$

where the negative root is ignored since $m > k$. Since $j = i + 1$, $\sqrt{(k-j)(k-i)}$ is the geometric mean of two consecutive integers, $\underline{m} \notin \mathbb{Z}^+$. The function $\frac{(m-i)(m-j)}{m-k}$ thus admits two consecutive integer minimizers \underline{m}_1 and \underline{m}_2 as follows:

$$\begin{aligned}
k-j &< \sqrt{(k-j)(k-i)} < k-i \\
\underline{m}_1 = \lfloor \underline{m} \rfloor &= k + \left\lfloor \sqrt{(k-j)(k-i)} \right\rfloor = k + k - j = 2k - j \\
\underline{m}_2 = \lceil \underline{m} \rceil &= k + \left\lceil \sqrt{(k-j)(k-i)} \right\rceil = k + k - i = 2k - i
\end{aligned} \tag{A.12}$$

where

$$\underline{m}_2 = \underline{m}_1 + 1, \quad \frac{(\underline{m}_2-i)(\underline{m}_2-j)}{\underline{m}_2-k} = \frac{(\underline{m}_1-i)(\underline{m}_1-j)}{\underline{m}_1-k}.$$

Hence the index ℓ can assume two values $\underline{m}_1, \underline{m}_2$ at which (A.10) is satisfied.

From (A.8) and (A.12), the following two bases of type 1 which we shall call 1A and 1B are dual feasible:

$$\begin{aligned}
\text{Basis type 1A: } & \{i_1, j_1, \ell_{11}\} \quad \text{where } \ell_{11} = 2k - j_1 \quad i_1 = j_1 - 1, \\
\text{Basis type 1B: } & \{i_1, j_1, \ell_{12}\} \quad \text{where } \ell_{12} = 2k - i_1, \quad j_1 = i_1 + 1
\end{aligned} \tag{A.13}$$

where we have added the suffix 1 to all indices to indicate that they belong to the type 1 basis. We observe that $\ell_{12} = \ell_{11} + 1$ and the structure of the feasible bases is such that the indices $\{j_1, k, \ell_{11}\}$ and $\{i_1, k, \ell_{12}\}$ are in arithmetic progression.

B) Basis type 2: We now consider the second basis type ($i < k < j < \ell$) from (A.6). The corresponding cost vector $c_B^\top = [0, j - k, \ell - k]$. From (A.5), we have the determinant inequality

$$\begin{vmatrix} c_m & 0 & j - k & \ell - k \\ 1 & 1 & 1 & 1 \\ m & i & j & \ell \\ \binom{m}{2} & \binom{i}{2} & \binom{j}{2} & \binom{\ell}{2} \end{vmatrix} \leq 0, \quad \forall m \in [n] \setminus J \quad (\text{A.14})$$

a) $m \leq k$

If $m \leq k$, then $c_m = 0$ and from (A.14) we need

$$\begin{aligned} \frac{1}{2} [(j - k)(i - m)(\ell - m)(\ell - i) \\ - (\ell - k)(i - m)(j - m)(j - i)] &\leq 0, \quad \forall m \in [k] \setminus J \\ (i - m) \left[\frac{(\ell - m)(\ell - i)}{\ell - k} - \frac{(j - m)(j - i)}{j - k} \right] &\leq 0, \quad \forall m \in [k] \setminus J \end{aligned} \quad (\text{A.15})$$

where $[k] \setminus J$ is $\{1, \dots, i - 1, i + 1, \dots, k\}$ since $i < k$ and the indices j, ℓ satisfy $\ell > j > k$. Note that the sign of the left hand side of the inequality in (A.15) depends on the relative position of i and m and hence we further partition the interval $[k] \setminus J$ into two parts $[1, i - 1]$ and $[i + 1, k]$.

i) $1 \leq m \leq i - 1, i \geq 1$

If $m \in [1, i - 1]$, then $m < i < k$ and we need the square bracketed term in (A.15) to be non-positive. Since $\ell > j > k \geq m$, a necessary condition for this non-positivity is that $\ell > m$ and $j < m$ should not occur simultaneously *i.e.* $j < m < \ell$ should not be possible which means $\ell = j + 1$. In addition we need

$$\begin{aligned} \frac{(\ell - m)(\ell - i)}{\ell - k} &\leq \frac{(j - m)(j - i)}{j - k}, \quad \forall m \in [1, i - 1] \setminus J \\ \frac{(j + 1 - m)(j + 1 - i)}{j + 1 - k} &\leq \frac{(j - m)(j - i)}{j - k}, \quad \forall m \in [1, i - 1] \setminus J \end{aligned} \quad (\text{A.16})$$

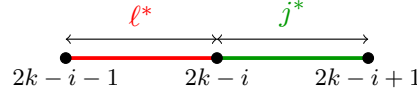
where $[1, i - 1] \setminus J = [1, i - 1]$ since it contains no basic index. Since $\ell > j > \max(i, m, k)$, both $\frac{(j - m)(j - i)}{j - k}$ and $\frac{(\ell - m)(\ell - i)}{\ell - k}$ are piecewise linear convex in j and ℓ respectively. Observe that the functions in (A.10) were convex in ℓ and m for a given (i, j, k) triplet (where $i < j < k$), while those in (A.20) are convex in j and ℓ for a given (i, m, k) triplet for every $m \in [1, i - 1]$. The condition in (A.16) is satisfied if:

$$\begin{aligned} \operatorname{argmin}_{j > k} \min_{m \in [0, i - 1]} \frac{(j + 1 - m)(j + 1 - i)}{j + 1 - k} &\leq \operatorname{argmin}_{j > k} \min_{m \in [0, i - 1]} \frac{(j - m)(j - i)}{j - k} \\ \operatorname{argmin}_{j > k} \frac{(j + 1 - (i - 1))(j + 1 - i)}{j + 1 - k} &\leq \operatorname{argmin}_{j > k} \frac{(j - (i - 1))(j - i)}{j - k} \end{aligned} \quad (\text{A.17})$$

Similar to the analysis in (A.12), the right hand side function in (A.17) admits two minimizers:

$$\begin{aligned} k + \left\lfloor \sqrt{(k - (i - 1))(k - i)} \right\rfloor &= 2k - i \\ k + \left\lceil \sqrt{(k - (i - 1))(k - i)} \right\rceil &= 2k - i + 1 \end{aligned} \quad (\text{A.18})$$

that attain the same function value (where the negative root is ignored since $j > k$) while the left hand side function admits the minimizers $j = 2k - i - 1, 2k - i$.



Minimizers (\star) in terms of j for left and right hand side functions in (A.17), $m < i$

Thus, (A.17) will be satisfied for all j which satisfy:

$$j \leq 2k - i \quad (\text{A.19})$$

where we choose the smaller of the two minimizers in (A.18) (involving the floor function) admitted by the right hand side function.

ii) $i + 1 \leq m \leq k, i < k$

If $m \in [i + 1, k]$, we enforce the necessary conditions for the square bracketed term in (A.15) to be non-negative as follows:

$$\frac{(\ell - m)(\ell - i)}{\ell - k} \geq \frac{(j - m)(j - i)}{j - k} \quad \text{where } j < \ell, \quad \forall m \in [i + 1, k] \setminus J \quad (\text{A.20})$$

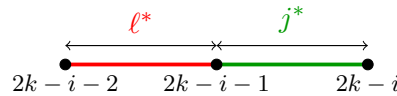
where $[i + 1, k] \setminus J = [i + 1, k]$ since it contains no basic index. The condition in (A.20) is satisfied if:

$$\begin{aligned} \operatorname{argmin}_{j > k} \max_{m \in [i+1, k]} \frac{(j + 1 - m)(j + 1 - i)}{j + 1 - k} &\geq \operatorname{argmin}_{j > k} \max_{m \in [i+1, k]} \frac{(j - m)(j - i)}{j - k} \\ \operatorname{argmin}_{j > k} \frac{(j + 1 - (i + 1))(j + 1 - i)}{j + 1 - k} &\geq \operatorname{argmin}_{j > k} \frac{(j - (i + 1))(j - i)}{j - k} \end{aligned} \quad (\text{A.21})$$

Similar to the analysis in (A.12), the right hand side function in (A.21) admits two minimizers:

$$\begin{aligned} k + \left\lfloor \sqrt{(k - (i + 1))(k - i)} \right\rfloor &= 2k - i - 1 \\ k + \left\lceil \sqrt{(k - (i + 1))(k - i)} \right\rceil &= 2k - i \end{aligned} \quad (\text{A.22})$$

which attain the same function value (where the negative root is ignored since $j > k$) while the left hand side function admits the minimizers $j = 2k - i - 2, 2k - i - 1$. Thus,



Minimizers (\star) in terms of j for left and right hand side functions in (A.21) $m > i$

(A.21) will be satisfied for all j which satisfy:

$$j \geq 2k - i - 1 \quad (\text{A.23})$$

where we choose the smaller of the two minimizers in (A.22) (involving the floor function) admitted by the right hand side function.

Combining both conditions in (A.19) and (A.23), we have:

$$\begin{aligned} 2k - i - 1 &\leq j \leq 2k - i \\ \text{or } 2k - j - 1 &\leq i \leq 2k - j \end{aligned} \quad (\text{A.24})$$

To demonstrate the derivation of the conditions in (A.24) for the basis type 2 when $m \leq k$, we consider a numerical example in Figure A.3 involving $n = 30$ variables with $k = 12$ and a randomly chosen index $i = 7$ where $i < k < j < \ell < n$. The index value i which is part of a primal and dual feasible basis, depends on n, k, p as will be shown in the later part of the proof (see A.41). For now, we assume that there exist $n, k, p, k \in [1, n - 1]$ such that $i = 7$. Figure A.3a considers the case when $m < i$ and plots the left and right hand side functions in (A.17) (where non-integer j have been rounded off to the next highest integer when computing the function value) and shows that the required condition is satisfied when $j \leq 2k - i = 17$ while Figure A.3b plots the same functions when $m > i$ and shows that the required condition in (A.21) is satisfied when $j \geq 2k - i - 1 = 16$. Hence $j = 16, 17$ and corresponding $i = 2k - j = 8, 7$ satisfy the necessary conditions in (A.24).

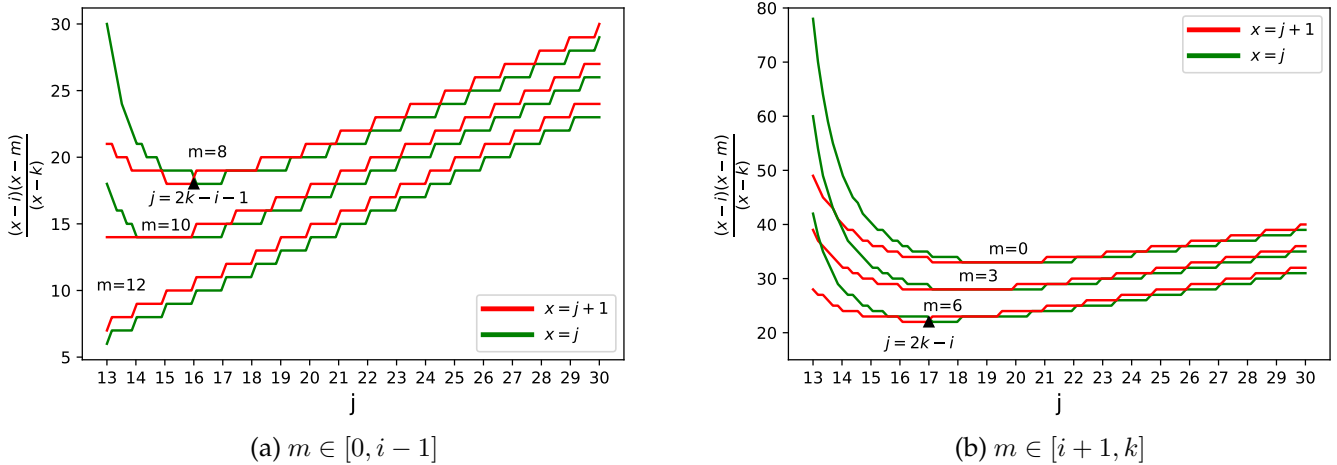


FIGURE A.3: Plots of left and right hand side functions (A.16) with $n = 30$, $k = 12$, $i = 7$

However it is sufficient to consider $j = 16$, $\ell = 17$ for the sake of the proof. In fact it can be shown that considering $j = 17$, $\ell = 18$ will lead to a primal infeasible basis but we skip the proof here. Note that although $i = 7$ was our initial assumption, $i = 8$ is also dual feasible for the same $j = 16$, $\ell = 17$ indices as shown by the second inequality in (A.24). Thus, when $m < k$, the basic index $i \in \{2k - j - 1, 2k - j\}$ can assume two consecutive integer values and along with $\ell = j + 1$, the following two bases of type 2,

which we shall call 2A and 2B are dual feasible:

$$\begin{aligned} \text{Basis type 2A: } & \{i_{21}, j_2, \ell_2\} \text{ where } i_{21} = 2k - \ell_2 \quad j_2 = \ell_2 - 1 \\ \text{Basis type 2B: } & \{i_{22}, j_2, \ell_2\} \text{ where } i_{22} = 2k - j_2, \quad \ell_2 = j_2 + 1 \end{aligned} \quad (\text{A.25})$$

where we have added the suffix 2 to all indices to indicate that they belong to the type 2 basis. We observe that $i_{22} = i_{21} + 1$ and the structure of the feasible bases is such that the indices $\{\ell_2, k, i_{21}\}$ and $\{j_2, k, i_{22}\}$ are in arithmetic progression.

b) $m > k$

If $m > k$, then $c_m = m - k$ and from (A.14) we have the determinant inequality

$$\begin{vmatrix} m-k & 0 & j-k & \ell-k \\ 1 & 1 & 1 & 1 \\ m & i & j & \ell \\ \binom{m}{2} & \binom{i}{2} & \binom{j}{2} & \binom{\ell}{2} \end{vmatrix} \leq 0, \quad \forall m \in [k+1, n] \setminus J \quad (\text{A.26})$$

We enforce the condition that $\ell - j = 1$ from the analysis for $m \leq k$, since we need the condition in (A.14) to be true for all $m \in [n] \setminus J$. With some row and column operations we can reduce the determinant in (A.26) to a simple expression as follows:

$$\begin{aligned} & \begin{vmatrix} m-k & 0 & j-k & \ell-k \\ 1 & 1 & 1 & 1 \\ m & i & j & \ell \\ \binom{m}{2} & \binom{i}{2} & \binom{j}{2} & \binom{\ell}{2} \end{vmatrix} \xrightarrow[\ell-j=1]{C_4-C_3} \begin{vmatrix} m-k & 0 & j-k & 1 \\ 1 & 1 & 1 & 0 \\ m & i & j & 1 \\ \binom{m}{2} & \binom{i}{2} & \binom{j}{2} & j \end{vmatrix} \\ & \xrightarrow[R_4-jR_1]{R_3-R_1} \begin{vmatrix} m-k & 0 & j-k & 1 \\ 1 & 1 & 1 & 0 \\ k & i & k & 0 \\ \binom{m}{2} - j(m-k) & \binom{i}{2} & \binom{j}{2} - j(j-k) & 0 \end{vmatrix} \\ & = (-1)^{4+1} \begin{vmatrix} 1 & 1 & 1 \\ k & i & k \\ \binom{m}{2} - j(m-k) & \binom{i}{2} & \binom{j}{2} - j(j-k) \end{vmatrix} \\ & \xrightarrow{C_1-C_3} \begin{vmatrix} 0 & 1 & 1 \\ 0 & i & k \\ \binom{j}{2} - \binom{m}{2} - j(j-m) & \binom{i}{2} & \binom{j}{2} - j(j-k) \end{vmatrix} \\ & = (k-i)[(j-m)(j+m-1)/2 - j(j-m)] \\ & = (k-i)(j-m)(m-j-1)/2 \\ & = (j-m)(m-\ell)(k-i)/2 \end{aligned}$$

Hence, we need

$$(j-m)(m-\ell)(k-i) \leq 0 \quad \forall m \in [k+1, n] \setminus J$$

or $(m-j)(m-\ell) \geq 0 \quad \forall m \in [k+1, n] \setminus J$

where the last inequality is due to $k > i$ and $[k+1, n] \setminus J$ is $\{k+1, \dots, j-1, j+2, \dots, n\}$ since $i < k$ and the indices j, ℓ satisfy $k < j = \ell - 1$. The condition $(m-j)(m-\ell) \geq 0$ is satisfied for all $m \in \{k+1, \dots, j-1, j+2, \dots, n\}$ since we have $j = \ell - 1$ and thus (A.26) is always satisfied when j, ℓ are consecutive integers.

A.1.2 Primal feasibility conditions

We are now left with the task of finding the conditions under which the dual feasible bases in (A.13) and (A.25) are primal feasible and thus optimal. From the aggregated linear program in (A.1), we have the primal feasibility conditions:

$$v_i = \frac{n(n-1)p^2 - np(j+\ell-1) + j\ell}{(i-j)(i-\ell)} \geq 0, \quad v_j = \frac{n(n-1)p^2 - np(i+\ell-1) + i\ell}{(j-i)(j-\ell)} \geq 0,$$

$$v_\ell = \frac{n(n-1)p^2 - np(i+j-1) + ij}{(\ell-i)(\ell-j)} \geq 0$$

(A.27)

From Section 8.1 in Boros and Prékopa (1989), for basis type 1, $v_{i_1} \geq 0$ and $v_{j_1} \geq 0$ automatically imply that $v_\ell \geq 0$ (where $\ell = \ell_{11}$ or ℓ_{12}) and thus to ensure primal feasibility with $i_1 < j_1 < \ell$, we only need to satisfy:

$$n(n-1)p^2 + np(1-j_1-\ell) + j_1\ell \geq 0,$$

$$n(n-1)p^2 + np(1-i_1-\ell) + i_1\ell \leq 0$$

(A.28)

Similarly for basis type 2, $v_{j_2} \geq 0$ and $v_{\ell_2} \geq 0$ automatically imply that $v_i \geq 0$ (where $i = i_{21}$ or i_{22}) and thus to ensure primal feasibility with $i < j_2 < \ell_2$, we only need to satisfy:

$$n(n-1)p^2 + np(1-i-\ell_2) + i\ell_2 \geq 0,$$

$$n(n-1)p^2 + np(1-i-j_2) + ij_2 \geq 0,$$

(A.29)

a) **Basis type 1:** We first address the primal feasibility of the basis type 1A with $\ell = \ell_{11} = 2k - j_1$, $i_1 = j_1 - 1$. Solving the equations in (A.28) leads to the following four conditions:

$$\ell_1 \geq k - \sqrt{(k-np)^2 + np(1-p)} \quad \text{and} \quad \ell_1 \leq k + \sqrt{(k-np)^2 + np(1-p)}$$

$$\ell_1 \leq k - \frac{1}{2} - \sqrt{(k - \frac{1}{2} - np)^2 + np(1-p)} \quad \text{or} \quad \ell_1 \geq k - \frac{1}{2} + \sqrt{(k - \frac{1}{2} - np)^2 + np(1-p)}$$

(A.30)

However, since $\ell_1 > k$, the left hand side inequalities in the two conditions of (A.30) can be eliminated and thus (A.30) reduces to:

$$k - 1/2 + \sqrt{(k - 1/2 - np)^2 + np(1-p)} \leq \ell_{11} \leq k + \sqrt{(k-np)^2 + np(1-p)} \quad (A.31)$$

By similarly assuming that $\ell = \ell_{12} = 2k - i_1$, $j_1 = i_1 + 1$ from basis type 1B and solving (A.28) with $\ell_1 > k$ leads to:

$$k + \sqrt{(k - np)^2 + np(1 - p)} \leq \ell_{12} \leq k + 1/2 + \sqrt{(k + 1/2 - np)^2 + np(1 - p)} \quad (\text{A.32})$$

(A.31) and (A.32) can be summarized as :

$$\begin{aligned} \beta_1 &\leq \ell_{11} \leq \beta_2 \\ \beta_2 &\leq \ell_{12} \leq \beta_3 \end{aligned} \quad (\text{A.33})$$

where the parameters $\beta_1, \beta_2, \beta_3$ are

$$\begin{aligned} \beta_1(n, k, p) &= k - 1/2 + \sqrt{(k - 1/2 - \mu)^2 + \sigma^2}, \quad \beta_2(n, k, p) = k + \sqrt{(k - \mu)^2 + \sigma^2}, \\ \beta_3(n, k, p) &= k + 1/2 + \sqrt{(k + 1/2 - \mu)^2 + \sigma^2} \end{aligned} \quad (\text{A.34})$$

where $\mu = np$ and $\sigma^2 = np(1 - p)$ are the mean and variance of the sum of n identical pairwise independent variables.

b) Basis type 2: A similar analysis for basis types 2A with $i_{21} = 2k - \ell_2$, $j_2 = \ell_2 - 1$ and 2B with $i_{22} = 2k - j_2$, $\ell_2 = j_2 + 1$ and the conditions in (A.29) leads to:

$$\begin{aligned} k - 1/2 - \sqrt{(k - 1/2 - np)^2 + np(1 - p)} &\leq i_{21} \leq k - \sqrt{(k - np)^2 + np(1 - p)} \\ k - \sqrt{(k - np)^2 + np(1 - p)} &\leq i_{22} \leq k + 1/2 - \sqrt{(k + 1/2 - np)^2 + np(1 - p)} \end{aligned}$$

or

$$\begin{aligned} \gamma_1 &\leq i_{21} \leq \gamma_2 \\ \gamma_2 &\leq i_{22} \leq \gamma_3 \end{aligned} \quad (\text{A.35})$$

where the parameters $\gamma_1, \gamma_2, \gamma_3$ are

$$\begin{aligned} \gamma_1(n, k, p) &= k - 1/2 - \sqrt{(k - 1/2 - \mu)^2 + \sigma^2}, \quad \gamma_2(n, k, p) = k - \sqrt{(k - \mu)^2 + \sigma^2}, \\ \gamma_3(n, k, p) &= k + 1/2 - \sqrt{(k + 1/2 - \mu)^2 + \sigma^2} \end{aligned} \quad (\text{A.36})$$

Henceforward, we drop (n, k, p) while referring to the parameters $\beta_i, \gamma_i, i \in [3]$ for notational convenience.

Observations: For any given (n, k, p) triplet where $n \geq 3$, $p \in (0, 1)$ and $k \in [n]$, we observe that the following conditions are satisfied by the parameters $\beta_i, \gamma_i, i \in [3]$ in (A.34) and (A.36) using elementary algebra:

i)
$$\gamma_1 < \gamma_2 < \gamma_3 < \beta_1 < \beta_2 < \beta_3$$

$$\begin{aligned} \text{ii)} \quad & 0 < \beta_2 - \beta_1 < 1, \quad 0 < \beta_3 - \beta_2 < 1, \quad 0 < \beta_3 - \beta_1 < 2, \\ & 0 < \gamma_3 - \gamma_2 < 1, \quad 0 < \gamma_2 - \gamma_1 < 1, \quad 0 < \gamma_3 - \gamma_1 < 2 \end{aligned} \quad (\text{A.37})$$

$$\text{iii)} \quad \gamma_1 + \beta_1 = 2k - 1, \quad \gamma_2 + \beta_2 = 2k, \quad \gamma_3 + \beta_3 = 2k + 1 \quad (\text{A.38})$$

Using the structure of the type 1 dual feasible basis from (A.13) and the β values from (A.34), we delineate the exact index values of the type 1 bases as follows:

Basis type 1A	Basis type 1B	
$\ell_{11} = \lfloor \beta_2 \rfloor = k + \lfloor \sqrt{(k - \mu)^2 + \sigma^2} \rfloor$	$\ell_{12} = \lceil \beta_2 \rceil = k + \lceil \sqrt{(k - \mu)^2 + \sigma^2} \rceil$	(A.39)
$j_1 = 2k - \ell_{11} = k - \lfloor \sqrt{(k - \mu)^2 + \sigma^2} \rfloor$	$i_1 = 2k - \ell_{12} = k - \lceil \sqrt{(k - \mu)^2 + \sigma^2} \rceil$	
$i_1 = j_1 - 1 = k - \lceil \sqrt{(k - \mu)^2 + \sigma^2} \rceil$	$j_1 = i_2 + 1 = k - \lfloor \sqrt{(k - \mu)^2 + \sigma^2} \rfloor$	

TABLE A.1: Indices of basis type 1 whose primal feasibility depends on n, k, p values

Note that the i_1, j_1 indices are identical in both the bases 1A, 1B in (A.39). While the dual feasibility of both type 1 bases in (A.39) is guaranteed, their primal feasibility depends on the relative position of $\beta_1, \beta_2, \beta_3$ as discussed next. From (A.37), at most two integers can lie between β_1 and β_3 and the following four mutually exclusive and exhaustive conditions are possible:

$$\begin{aligned} (i) \quad & \lceil \beta_1 \rceil = \lfloor \beta_2 \rfloor \text{ and } \lceil \beta_2 \rceil = \lfloor \beta_3 \rfloor, \\ (ii) \quad & \lceil \beta_1 \rceil = \lfloor \beta_2 \rfloor = \lfloor \beta_3 \rfloor, \\ (iii) \quad & \lceil \beta_1 \rceil = \lceil \beta_2 \rceil = \lfloor \beta_3 \rfloor, \\ (iv) \quad & \lfloor \beta_1 \rfloor = \lfloor \beta_2 \rfloor = \lfloor \beta_3 \rfloor \end{aligned} \quad (\text{A.40})$$

Further, exactly one of the four conditions in (A.40) must be true for any given (n, k, p) triplet. Considering the primal feasibility conditions in (A.33), if case (i) occurs, both $\ell_{11} = \lfloor \beta_2 \rfloor$ and $\ell_{12} = \lceil \beta_2 \rceil$ admit integer solutions *i.e.* both bases 1A, 1B are primal and dual feasible. If case (ii) occurs, only ℓ_{11} admits a valid integral solution (*only* basis 1A is primal and dual feasible) while if case (iii) occurs, only ℓ_{12} admits a valid integral solution (*only* basis 1B is primal and dual feasible). Lastly, if case (iv) occurs, both ℓ_{11} and ℓ_{12} do not admit integral solutions and neither basis 1A nor 1B can be primal feasible. In other words, unless

$$x < \beta_1 < \beta_2 < \beta_3 < x + 1,$$

for some $x \in \mathbb{Z}^+$, at least one of ℓ_{11} or ℓ_{12} will have a valid integral solution and *at least* one of the bases 1A, 1B will be primal and dual feasible. Next, using the structure of the type 2 dual feasible basis from (A.25) and the γ values from (A.36), we delineate the exact index values of the type 2 bases as follows:

Basis type 2A	Basis type 2B
$i_{21} = \lfloor \gamma_2 \rfloor = k - \left\lfloor \sqrt{(k - \mu)^2 + \sigma^2} \right\rfloor$	$i_{22} = \lceil \gamma_2 \rceil = k - \left\lfloor \sqrt{(k - \mu)^2 + \sigma^2} \right\rfloor$
$\ell_2 = 2k - i_{21} = k + \left\lfloor \sqrt{(k - \mu)^2 + \sigma^2} \right\rfloor$	$j_2 = 2k - i_{22} = k + \left\lfloor \sqrt{(k - \mu)^2 + \sigma^2} \right\rfloor$
$j_2 = \ell_1 - 1 = k + \left\lfloor \sqrt{(k - \mu)^2 + \sigma^2} \right\rfloor$	$\ell_2 = j_2 + 1 = k + \left\lfloor \sqrt{(k - \mu)^2 + \sigma^2} \right\rfloor$

(A.41)

TABLE A.2: Indices of basis type 2 whose primal feasibility depends on n, k, p values

Note that the j_2, ℓ_2 indices are identical in both the bases 2A, 2B in (A.41). Similar to the analysis for the type 1 bases, unless

$$x < \gamma_1 < \gamma_2 < \gamma_3 < x + 1,$$

for some $x \in \mathbb{Z}^+$, at least one of i_{21} or i_{22} has a valid integral solution and at least one of the bases 2A, 2B will be primal and dual feasible. If $\lfloor \beta_1 \rfloor = \lfloor \beta_2 \rfloor = \lfloor \beta_3 \rfloor$ and $\lceil \gamma_1 \rceil = \lceil \gamma_2 \rceil = \lceil \gamma_3 \rceil$ (case (iv)), none of the four bases 1A, 1B, 2A, 2B will be primal feasible. However, as we will prove in Lemma 25 later, the above conditions are not simultaneously possible and thus at least one of the four bases will always remain primal and dual feasible for any $k \in [n]$. It is also interesting to note that:

$$\begin{aligned} j_2 = \ell_{11} = \lfloor \beta_2 \rfloor &= k + \left\lfloor \sqrt{(k - np)^2 + np(1 - p)} \right\rfloor \\ j_1 = i_{22} = \lceil \gamma_2 \rceil &= k - \left\lfloor \sqrt{(k - np)^2 + np(1 - p)} \right\rfloor \\ j_1 + j_2 = \ell_{11} + i_{22} &= \ell_{12} + i_{21} = 2k \end{aligned}$$

Exclusion of k from dual feasible bases:

It is clear from (A.35) and (A.41) that the basic indices of either type 1 or type 2 can never include k since:

$$(k - \mu)^2 + \sigma^2 \neq 0, \forall p \in (0, 1), \forall k \in [n]$$

Thus, unlike with the extremal distribution for the non-trivial probability bound in cases (b) and (c) (2.31-2.32), where k was part of the basis, the expectation problem does not admit any feasible basis with the index k .

Degeneracy:

It is possible that the parameters $\beta_i, \gamma_i, i \in [3]$ could assume integer values and this can only happen in pairs due to the complementary property in (A.38). In this situation, one or more of the primal decision variables in (A.27) would be zero since $\beta_i, \gamma_i, i \in [3]$ are the roots of the numerators. This leads to degeneracy, the analysis of which is beyond the scope of this proof. Specifically, if $\beta_2, \gamma_2 \in \mathbb{Z}^+$, then $\ell_{11} = \ell_{12} = \ell$ from (A.39) and $i_{21} = i_{22} = i$ from (A.41). In this situation, the indices i_1, j_1 and j_2, ℓ_2 of basis type 1 and 2 respectively can still be arranged to satisfy the consecutive integer requirements

as follows:

$$\begin{aligned}
\text{Basis type 1A: } & \{i_1, j_1, \ell\} \text{ where } j_1 = 2k - \ell \quad i_1 = j_1 - 1, \\
\text{Basis type 1B: } & \{i_1, j_1, \ell\} \text{ where } i_1 = 2k - \ell \quad j_1 = i_1 + 1, \\
\text{Basis type 2A: } & \{i, j_2, \ell_2\} \text{ where } j_2 = 2k - i \quad \ell_2 = j_2 + 1, \\
\text{Basis type 2B: } & \{i, j_2, \ell_2\} \text{ where } \ell_2 = 2k - i \quad j_2 = \ell_2 - 1,
\end{aligned}$$

and all the bases above can be shown to be dual feasible. For example, consider $n = 4$, $k = 2$, $p = 1/2$, then

$$\beta_2 = k + \sqrt{(k - np)^2 + np(1 - p)} = 3, \quad \ell_{11} = \ell_{12} = 3$$

and $\{0, 1, 3\}$, $\{1, 2, 3\}$ are possible type 1 bases while $\{1, 2, 3\}$, $\{1, 3, 4\}$ are possible type 2 bases. However, if $\beta_1, \gamma_1 \in \mathbb{Z}^+$ and/or $\beta_3, \gamma_3 \in \mathbb{Z}^+$, the indices in (A.39) and (A.41) can be used without modification.

Truncation of bases:

Considering the basis type 1, when $k \geq n/2$, it is possible that $i_1 < j_1 < 2k - n$ and thus from (A.39), $\ell_{12} > \ell_{11} = 2k - j_1 > n$ which is an infeasible index. However, since the function $\frac{(\ell-i)(\ell-j)}{\ell-k}$ is convex in ℓ , truncating the index ℓ_{11} to n will not affect the dual feasibility conditions in (A.10). However, the other two indices j_1, i_1 will need to be recomputed by solving for the primal feasibility conditions in (A.28) with $\ell = n$ as follows:

$$j_1 = \left\lceil \frac{np((\ell - 1) - (n - 1)p)}{\ell - np} \right\rceil = \lceil (n - 1)p \rceil, \quad i_1 = j_1 - 1.$$

Similarly considering the basis type 2, when $k < n/2$, it is possible that $\ell_2 > j_2 > 2k$ and thus from (A.41), $i_{21} < i_{22} = 2k - j_2 < 0$ which is an infeasible index. In this case truncating the index i_{22} to zero will not affect the dual feasibility conditions in (A.20) and (A.16). The other two indices j_2, i_2 will need to be recomputed by solving for the primal feasibility conditions in (A.29) with $i = 0$ as follows:

$$j_2 = \left\lceil \frac{np((i - 1) - (n - 1)p)}{i - np} \right\rceil = \lceil 1 + (n - 1)p \rceil = \lceil (n - 1)p \rceil, \quad \ell_2 = j_2 + 1.$$

We thus have the following two possible primal and dual feasible truncated bases, which we shall call 1C and 2C respectively:

$$\begin{aligned}
\text{Truncated Basis 1C: } & i_{31} = j_{31} - 1, \quad j_{31} = \lceil (n - 1)p \rceil, \quad \ell_{31} = n \\
\text{Truncated Basis 2C: } & i_{32} = 0, \quad j_{32} = \lceil (n - 1)p \rceil, \quad \ell_{32} = j_{32} + 1
\end{aligned} \tag{A.42}$$

where we have added the suffix 3 to all indices to indicate that they belong to the truncated type 1 and type 2 bases.

Lemma 25. *At least one of the non-truncated bases 1A, 1B, 1C will be primal and dual feasible if $k \geq np$ while at least one of the non-truncated bases 2A, 2B, 2C will be primal and dual feasible if $k < np$.*

Proof. The proof rests on the fact that

$$\begin{cases} \beta_2 - \beta_1 > 1/2, \\ \beta_3 - \beta_2 > 1/2, \\ \beta_3 - \beta_1 > 1, \end{cases} \quad \text{if } k \geq np \quad \text{and} \quad \begin{cases} \gamma_3 - \gamma_2 > 1/2, \\ \gamma_2 - \gamma_1 > 1/2, \\ \gamma_3 - \gamma_1 > 1 \end{cases} \quad \text{if } k < np \quad (\text{A.43})$$

which is straightforward to verify from the definitions of β_i, γ_i $i \in [3]$ in (A.34) and (A.36). Thus when $k \geq np$, it is not possible that $x < \beta_1 < \beta_2 < \beta_3 < x + 1$, for some $x \in \mathbb{Z}^+$, thus guaranteeing the primal and dual feasibility of *at least* one of the bases 1A, 1B, while if $k < np$, $y < \beta_1 < \beta_2 < \beta_3 < y + 1$, for some $y \in \mathbb{Z}^+$ is not possible thus guaranteeing the primal and dual feasibility of *at least* one of the bases 2A, 2B. However, the non-truncated bases will not always admit valid indices as seen earlier. It is easy to observe from (A.39) and (A.35) that

$$\begin{aligned} \ell_{11} = k + \left\lfloor \sqrt{(k - \mu)^2 + \sigma^2} \right\rfloor &\geq n \quad \text{iff} \quad k > (n + (n - 1)p)/2 \\ i_{22} = k - \left\lfloor \sqrt{(k - \mu)^2 + \sigma^2} \right\rfloor &\leq 0 \quad \text{iff} \quad k < (1 + (n - 1)p)/2. \end{aligned} \quad (\text{A.44})$$

and thus only the truncated bases 1C and 2C are primal and dual feasible in these regions respectively, while from (A.43), *at least* one of the four other bases 1A, 1B, 2A, 2B will be feasible when

$$(1 + (n - 1)p)/2 \leq k \leq (n + (n - 1)p)/2.$$

□

A.1.3 Optimality of bases

We next complete the proof by showing that the objective function values of the aggregated primal linear program (A.1) attained by the four non-truncated bases 1A, 1B, 2A, 2B in (A.39) and (A.41) are equal to each other and that of the corresponding dual linear program and hence optimal whenever *at least* one of them is feasible. Consider the non-truncated bases 1A, 1B, 2A, 2B as described above. Denote by $\bar{E}_P(1A), \bar{E}_P(1B), \bar{E}_P(2A), \bar{E}_P(2B)$ the expectation objective of the primal linear program (A.1) attained by the respective bases and let $\bar{E}_D(1A), \bar{E}_D(1B), \bar{E}_D(2A), \bar{E}_D(2B)$ be the corresponding objective function values of the dual linear program:

$$\begin{aligned} \bar{E}(n, k, p) = \min \quad &\alpha + \beta\mu + \gamma n(n - 1)p^2/2 \\ &\alpha + i\beta + i(i - 1)/2\gamma \geq (i - k)^+, \quad \forall i \in [0, n] \\ &\alpha, \beta, \gamma \text{ free} \end{aligned} \quad (\text{A.45})$$

Lemma 26. *For any $k \in [(1 + (n - 1)p)/2, (n + (n - 1)p)/2]$, where $p \in (0, 1)$, the eight objective function values*

$$\bar{E}_P(1A), \bar{E}_P(1B), \bar{E}_P(2A), \bar{E}_P(2B), \bar{E}_D(1A), \bar{E}_D(1B), \bar{E}_D(2A), \bar{E}_D(2B)$$

attained by the non-truncated bases are equal to each other irrespective of which basis (bases) is (are) feasible and hence the particular basis (bases) which is (are) feasible for a given k is (are) also optimal. Similarly, the truncated bases 1C and 2C are also optimal when $k < (1 +$

$(n-1)p)/2$ and $k > (n + (n-1)p)/2$ respectively since their objective function values satisfy $\bar{E}_P(1C) = \bar{E}_D(1C)$ and $\bar{E}_P(2C) = \bar{E}_D(2C)$ in the specified range of k .

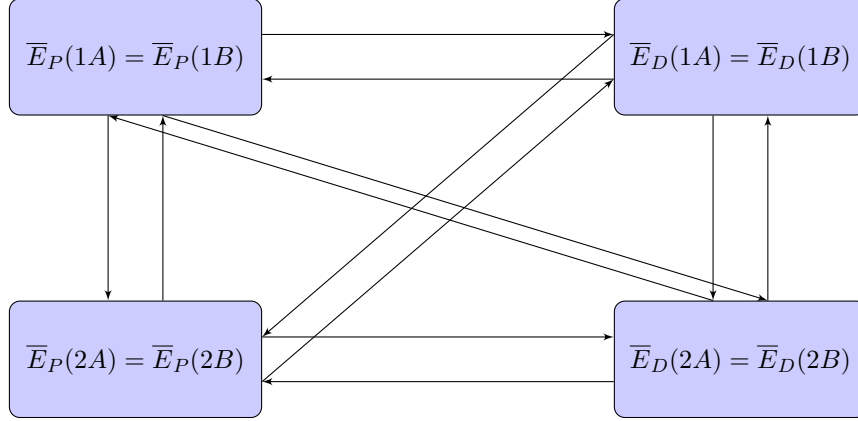


FIGURE A.4: Equality of primal and dual objective function values for non-truncated bases

Proof. From (A.1), the objective function values for the four bases are:

$$\begin{aligned} \bar{E}_P(1A) &= (\ell_{11} - k)V_{\ell_{11}}, & \bar{E}_P(1B) &= (\ell_{12} - k)V_{\ell_{12}} \\ \bar{E}_P(2A) &= np - k - (i_{21} - k)V_{i_{11}}, & \bar{E}_P(2B) &= np - k - (i_{22} - k)V_{i_{22}} \end{aligned} \quad (\text{A.46})$$

To prove that $\bar{E}_P(1A) = \bar{E}_P(1B)$, we recall from in (A.39) that i_1, j_1 indices are identical when $\ell = \ell_{11}$ and $\ell = \ell_{12}$ and the objective function value

$$\begin{aligned} \bar{E}_P(1A) &= (\ell_{11} - k)V_{\ell_{11}} \\ &= \frac{(\ell_{11} - k)}{(\ell_{11} - i_1)(\ell_{11} - j_1)} [n(n-1)p^2 - np(i_1 + j_1 - 1) + i_1 j_1] \\ &= \frac{(\ell_{12} - k)}{(\ell_{12} - i_2)(\ell_{12} - j_2)} [n(n-1)p^2 - np(i_1 + j_1 - 1) + i_2 j_2] \\ &= \bar{E}_P(1B) \end{aligned} \quad (\text{A.47})$$

remains unchanged since $\frac{(\ell_{12}-i)(\ell_{12}-j)}{\ell_{12}-k} = \frac{(\ell_{11}-i)(\ell_{11}-j)}{\ell_{11}-k}$. Equality of $\bar{E}_P(2A)$ and $\bar{E}_P(2B)$ can be similarly proved from (A.35) and (A.46).

To prove that $\bar{E}_P(1A) = \bar{E}_D(1A)$, consider the following dual feasible solution to (A.45) which attains the objective $\bar{E}_P(1A)$:

$$\alpha = \frac{i_1(i_1 + 1)}{2(\ell_{11} - i_1)} \quad \beta = -\frac{i_1}{(\ell_{11} - i_1)}, \quad \gamma = \frac{1}{2(\ell_{11} - i_1)} \quad (\text{A.48})$$

and thus

$$\begin{aligned}
\bar{E}_D(1A) &= \alpha + \beta np + \gamma n(n-1)p^2/2 \\
&= \frac{n(n-1)p^2 - 2i_1 np + i_1(i_1+1)}{2(\ell_{11} - i_1)} \\
&= \left(\frac{1}{2}\right) \frac{n(n-1)p^2 + (1 - i_1 - j_1)np + i_1 j_1}{(\ell_{11} - i_1)} \\
&= \left(\frac{\ell_{11} - k}{\ell_{11} - j_1}\right) \frac{[n(n-1)p^2 + np(1 - i_1 - j_1) + i_1 j_1]}{(\ell_{11} - i_1)} \\
&= \bar{E}_P(1A)
\end{aligned} \tag{A.49}$$

where the third and fourth equalities are due to $j_1 = i_1 + 1$ and $\frac{(\ell_{11}-k)}{(\ell_{11}-j_1)} = \frac{(2k-j_1-k)}{(2k-j_1-j_1)} = 1/2$ respectively and the last equality is due to (A.47). Then using j_1 from left hand column of (A.39) along with $i_1 = j_1 - 1$ and dropping the subscript 1, we derive the second part (case (b)) of the tight bound in Theorem 7 as:

$$\begin{aligned}
\bar{E}_P(1A) &= \frac{n(n-1)p^2 + (j-1)(j-2np)}{2(2(k-j)+1)}, \quad \frac{1+(n-1)p}{2} \leq k \leq \frac{n+(n-1)p}{2}, \\
& \quad j = k - \left\lfloor \sqrt{(k-np)^2 + np(1-p)} \right\rfloor
\end{aligned} \tag{A.50}$$

To prove that $\bar{E}_P(2A) = \bar{E}_D(2A)$, consider the following dual feasible solution to (A.45) which attains the objective $\bar{E}_P(2A)$:

$$\alpha = \frac{i_{21}(i_{21}+1)}{2(j_2 - i_{21})}, \quad \beta = \frac{i_{21}}{(i_{21} - j_2)}, \quad \gamma = \frac{1}{2(j_2 - i_{21})} \tag{A.51}$$

and it can be easily shown that

$$\begin{aligned}
\bar{E}_D(2A) &= \alpha + \beta np + \gamma n(n-1)p^2/2 \\
&= \frac{1}{2} \frac{n(n-1)p^2 - 2i_{21} np + i_{21}(i_{21}+1)}{(j_2 - i_{21})} \\
&= np - k - \left(\frac{1}{2}\right) \left(\frac{n(n-1)p^2 - np(j_2 + \ell_2 - 1) + j_2 \ell_2}{(i_{21} - j_2)}\right) \\
&= np - k - \left(\frac{i_{21} - k}{i_{21} - \ell_2}\right) \left(\frac{n(n-1)p^2 - np(j_2 + \ell_2 - 1) + j_2 \ell_2}{(i_{21} - j_2)}\right) \\
&= np - k - (i_{21} - k)V_{i_{21}} \\
&= \bar{E}_P(2A)
\end{aligned}$$

where the fourth equality is due to $\frac{(i_{21}-k)}{(i_{21}-\ell_2)} = \frac{(i_{21}-k)}{(i_{21}-(2k-i_{21}))} = 1/2$ and the fifth equality follows from the primal variables in (A.27). Then using i_{21} from the left hand column of (A.41) along with $j_2 = 2k - i_{21} - 1$ and dropping the subscript 21, we once again derive the second part of the tight bound in Theorem 7 as:

$$\overline{E}_P(2A) = \frac{[n(n-1)p^2 - 2inp + i(i+1)]}{2(2k - 2i - 1)} \quad \text{where } i = k - \left\lceil \sqrt{(k - np)^2 + np(1-p)} \right\rceil \quad (\text{A.52})$$

where the closed form in (A.52) can be easily shown to be equivalent to the closed form in (A.50) by the transformation $i = j - 1$ thus proving that $\overline{E}_P(1A) = \overline{E}_P(2A)$. The rest of the equivalences in Figure A.4 are proved by transitive relationships and we have thus proved that the non-truncated basic indices 1A, 1B, 2A, 2B from (A.39) and (A.41) achieve the optimal bound irrespective of their feasibility.

It can be independently verified that the truncated basis 1C and 2C indices from (A.42) are also optimal in their respective domains by proving that they attain the third (case (c)) and first (case (a)) parts of the tight bound in Theorem 7 as:

$$\overline{E}_P(1C) = \overline{E}_D(1C) = \frac{(n-k)[n(n-1)p^2 + (j-1)(j-2np)]}{((n-j)^2 + (n-j))}, \quad k > (n + (n-1)p)/2, \quad \text{case (c)}$$

$$\overline{E}_P(2C) = \overline{E}_D(2C) = np \left[1 - k \left(\frac{2j - (n-1)p}{j(j+1)} \right) \right], \quad k < (1 + (n-1)p)/2, \quad \text{case (a)}$$

where $j = \lceil (n-1)p \rceil$. □

Thus we have proved the tight upper bound $\overline{E}(n, k, p)$ in Theorem 7 is always attained by one of the non-truncated or truncated bases depending on the value of k and the proof is thus completed. □

A.2 Extremal distributions

We next provide six different extremal distributions that attain the tight upper bound $\overline{E}(n, k, p)$ under different conditions on k and the relative position of the parameters $\beta_i, \gamma_i, i \in [3]$. Before that, we prove the following lemma (which is a stronger version of Lemma 25) by identifying more detailed conditions under which the non-truncated and truncated bases become optimal. These conditions are then used to delineate the extremal distribution(s) for different values of k .

Lemma 27. *For any given (n, k, p) triplet, where $n \geq 3$, $p \in (0, 1)$ and $k \in [(1 + (n-1)p)/2, (n + (n-1)p)/2]$, at least two of the four non-truncated bases 1A, 1B, 2A, 2B must be optimal. If all the four bases are non-degenerate, exactly two of the four bases 1A, 1B, 2A, 2B must be optimal.*

Proof. From the complementary conditions in (A.38), it is straightforward to observe that when all four bases are non-degenerate i.e. $\beta_i, \gamma_i \notin \mathbb{Z}^+, \forall i \in [3]$ the four mutually exclusive conditions on $\beta_i, i \in [3]$ delineated in (A.40) are equivalent to the following conditions on $\gamma_i, i \in [3]$:

$$\begin{aligned} (i) \quad & \lceil \beta_1 \rceil = \lceil \beta_2 \rceil \text{ and } \lceil \beta_2 \rceil = \lceil \beta_3 \rceil \equiv \lceil \gamma_1 \rceil = \lceil \gamma_2 \rceil = \lceil \gamma_3 \rceil, \\ (ii) \quad & \lceil \beta_1 \rceil = \lceil \beta_2 \rceil = \lceil \beta_3 \rceil \equiv \lceil \gamma_1 \rceil = \lceil \gamma_2 \rceil = \lceil \gamma_3 \rceil, \\ (iii) \quad & \lceil \beta_1 \rceil = \lceil \beta_2 \rceil = \lceil \beta_3 \rceil \equiv \lceil \gamma_1 \rceil = \lceil \gamma_2 \rceil = \lceil \gamma_3 \rceil \\ (iv) \quad & \lceil \beta_1 \rceil = \lceil \beta_2 \rceil = \lceil \beta_3 \rceil \equiv \lceil \gamma_1 \rceil = \lceil \gamma_2 \rceil \text{ and } \lceil \gamma_2 \rceil = \lceil \gamma_3 \rceil \end{aligned} \quad (\text{A.53})$$

From the primal feasibility conditions in (A.33) and (A.35) and the equivalence of conditions in (A.53), it is then straightforward to see that under assumptions of non-degeneracy of all four bases, exactly two non-truncated bases would be optimal for any $k \in [(1 + (n - 1)p)/2, (n + (n - 1)p)/2]$ as shown in Table A.3.

Scenario	Relative Position of $\beta_i, \gamma_i, i \in [3]$	Type 1 basis		Type 2 basis	
		1A	1B	2A	2B
1	$\lceil \beta_1 \rceil = \lfloor \beta_2 \rfloor$ and $\lceil \beta_2 \rceil = \lfloor \beta_3 \rfloor$ and/or $\lceil \gamma_1 \rceil = \lfloor \gamma_2 \rfloor = \lfloor \gamma_3 \rfloor$	✓	✓		
2	$\lceil \beta_1 \rceil = \lfloor \beta_2 \rfloor = \lfloor \beta_3 \rfloor$ and/or $\lceil \gamma_1 \rceil = \lfloor \gamma_2 \rfloor = \lfloor \gamma_3 \rfloor$	✓			✓
3	$\lceil \beta_1 \rceil = \lfloor \beta_2 \rfloor = \lfloor \beta_3 \rfloor$ and/or $\lceil \gamma_1 \rceil = \lfloor \gamma_2 \rfloor = \lfloor \gamma_3 \rfloor$		✓	✓	
4	$\lceil \beta_1 \rceil = \lfloor \beta_2 \rfloor = \lfloor \beta_3 \rfloor$ and/or $\lceil \gamma_1 \rceil = \lfloor \gamma_2 \rfloor$ and $\lceil \gamma_2 \rceil = \lfloor \gamma_3 \rfloor$			✓	✓

TABLE A.3: Optimality of type 1 and 2 non-truncated bases in different scenarios

If *at least* one of the non-truncated bases are degenerate, the equivalence of conditions in (A.53) may break down as seen in the following example:
Suppose $n = 3, k = 3, p = 1/3$, then:

$$\begin{aligned} \beta_1 = 4, \quad \beta_2 = 4.41, \quad \beta_3 = 5 \\ \gamma_1 = 1, \quad \gamma_2 = 1.59, \quad \gamma_3 = 2 \end{aligned} \tag{A.54}$$

and hence conditions (i) and (iv) in (A.53) are violated. However

$$\lceil \beta_1 \rceil = \lfloor \beta_2 \rfloor, \lceil \gamma_1 \rceil = \lfloor \gamma_2 \rfloor \text{ and } \lceil \beta_2 \rceil = \lfloor \beta_3 \rfloor, \lceil \gamma_2 \rceil = \lfloor \gamma_3 \rfloor$$

are still satisfied due to which all four non-truncated bases will be optimal. However, even with the breakdown of the equivalence in (A.53), exactly one of the four conditions for both β_i and γ_i must be true for any given (n, k, p) triplet. Hence, even with degeneracy, *at least* two non-truncated bases will always be optimal. \square

It can be observed that the truncated bases 1C, 2C from (A.42) are simultaneously degenerate in their respective range of k values iff $(n - 1)p \in \mathbb{Z}^+$ and degeneracy among truncated bases can only occur simultaneously. Unlike the non-truncated bases, degeneracy does not impact the feasibility of the truncated bases and thus only the following two scenarios are possible:

Scenario	Range of k	1C	2C
5	$k < \frac{1 + (n-1)p}{2}$	✓	✗
6	$k > \frac{n + (n-1)p}{2}$	✗	✓

TABLE A.4: Feasibility of type 1 and 2 truncated bases in different scenarios

Similar to the proof for the probability objective in Theorem 4, we distribute the aggregated probability mass $v_\ell = \mathbb{P}(\sum_{j=1}^n \tilde{c}_j = \ell)$, $\ell \in [0, n]$, equally, among all scenarios C with exactly ℓ ones as follows:

$$\mathbb{P}(C) = v_\ell / \binom{n}{\ell}, \quad \forall C : \sum_{t=1}^n c_t = \ell, \quad \forall \ell \in [0, n] \quad \text{where} \quad |C : \sum_{t=1}^n c_t = \ell| = \binom{n}{\ell}$$

It is then straightforward to verify that the following distributions attain the bounds for each of the cases (a) – (c) in the statement of Theorem 7 for the specific valid scenarios from Tables A.3 and A.4 for a given (n, k, p) triplet.

I) Case (a), Basis type 1C of the form $\{j-1, j, n\}$, Scenario 5

$$\mathbb{P}(\mathbf{c}) = \begin{cases} \frac{n(n-1)p^2 + (j-1)(j-2np)}{(n-j)^2 + (n-j)}, & \text{if } \sum_{t=1}^n c_t = j-1, \\ \frac{(1-p)(1+(n-1)p-j)}{\binom{n-1}{j}}, & \text{if } \sum_{t=1}^n c_t = j, \\ \frac{n(n-1)p^2 + (j-1)(j-2np)}{(n-j)^2 + (n-j)}, & \text{if } \sum_{t=1}^n c_t = n, \end{cases}$$

where $j = \lceil (n-1)p \rceil < k < (1+(n-1)p)/2$ and all other support points have zero probability.

II) Case (b), $(1+(n-1)p)/2 \leq k \leq (n+(n-1)p)/2$

i) Basis type 1A of the form $\{j-1, j, 2k-j\}$, Scenarios 1, 2

$$\mathbb{P}(\mathbf{c}) = \begin{cases} \frac{n(n-1)p^2 - (2k-1)np + j(2k-j)}{[2(k-j)+1]\binom{n}{j-1}}, & \text{if } \sum_{t=1}^n c_t = j-1, \\ \frac{2(k-1)np - n(n-1)p^2 - (j-1)(2k-j)}{2(k-j)\binom{n}{j}}, & \text{if } \sum_{t=1}^n c_t = j, \\ \frac{n(n-1)p^2 + (j-1)(j-2np)}{2(k-j)[(2(k-j)+1)\binom{n}{2k-j}]}, & \text{if } \sum_{t=1}^n c_t = 2k-j, \end{cases}$$

where $j = k - \lfloor \sqrt{(k - np)^2 + np(1 - p)} \rfloor < k$ and all other support points have zero probability.

ii) Basis type 1B of the form $\{j - 1, j, 2k - j + 1\}$, Scenarios 1, 2

$$\mathbb{P}(\mathbf{c}) = \begin{cases} \frac{n(n-1)p^2 - 2knp + j(2k-j+1)}{[2(k-j)+2] \binom{n}{j-1}}, & \text{if } \sum_{t=1}^n c_t = j-1, \\ \frac{(2k-1)np - n(n-1)p^2 - (j-1)(2k-j+1)}{[2(k-j)+1] \binom{n}{j}}, & \text{if } \sum_{t=1}^n c_t = j, \\ \frac{n(n-1)p^2 + (j-1)(j-2np)}{2(k-j+1)[2(k-j)+1] \binom{n}{2k-j+1}}, & \text{if } \sum_{t=1}^n c_t = 2k-j+1, \end{cases}$$

where $j = k - \lfloor \sqrt{(k - np)^2 + np(1 - p)} \rfloor < k$ and all other support points have zero probability.

iii) Basis type 2A of the form $\{2k - j - 1, j, j + 1\}$, Scenarios 3, 4

$$\mathbb{P}(\mathbf{c}) = \begin{cases} \frac{n(n-1)p^2 + j(j+1-2np)}{2(j-k+1)[2(j-k)+1] \binom{n}{2k-j-1}}, & \text{if } \sum_{t=1}^n c_t = 2k-j-1, \\ \frac{(2k-1)np - n(n-1)p^2 - (j+1)(2k-j-1)}{[2(j-k)-1] \binom{n}{j}}, & \text{if } \sum_{t=1}^n c_t = j, \\ \frac{n(n-1)p^2 - 2(k-1)np + j(2k-j-1)}{2(j-k+1) \binom{n}{j+1}}, & \text{if } \sum_{t=1}^n c_t = j+1, \end{cases}$$

where $j = k + \lfloor \sqrt{(k - np)^2 + np(1 - p)} \rfloor > k$ and all other support points have zero probability.

iv) Basis type 2B of the form $\{2k - j, j, j + 1\}$, Scenarios 2, 4

$$\mathbb{P}(\mathbf{c}) = \begin{cases} \frac{n(n-1)p^2 + j(j+1-2np)}{2(j-k)[2(j-k)+1] \binom{n}{2k-j}}, & \text{if } \sum_{t=1}^n c_t = 2k-j, \\ \frac{2knp - n(n-1)p^2 - (j+1)(2k-j)}{2(j-k) \binom{n}{j}}, & \text{if } \sum_{t=1}^n c_t = j, \\ \frac{n(n-1)p^2 - (2k-1)np + j(2k-j)}{[(2(j-k)+1] \binom{n}{j+1}}, & \text{if } \sum_{t=1}^n c_t = j+1, \end{cases}$$

where $j = k + \lfloor \sqrt{(k - np)^2 + np(1 - p)} \rfloor > k$ and all other support points have zero probability.

III) Case (c), Basis type 2C of the form $\{0, j, j + 1\}$, Scenario 6

$$\mathbb{P}(\mathbf{c}) = \begin{cases} \frac{n(n-1)p^2 + j(j+1-2np)}{j(j+1)}, & \text{if } \sum_{t=1}^n c_t = 0, \\ \frac{p(j - (n-1)p)}{\binom{n-1}{j-1}}, & \text{if } \sum_{t=1}^n c_t = j, \\ \frac{p(1 + (n-1)p - j)}{\binom{n-1}{j}}, & \text{if } \sum_{t=1}^n c_t = j + 1, \end{cases}$$

where $j = \lceil (n-1)p \rceil > k > (n + (n-1)p)/2$ and all other support points have zero probability.