1–38

Submodularity, pairwise independence and correlation gap

Arjun Ramachandra ARJUN.RAMACHANDRA@IIMB.AC.IN
Indian Institute of Management Bangalore

Karthik Natarajan KARTHIK_NATARAJAN@SUTD.EDU.SG
Singapore University of Technology and Design, Singapore

Abstract

In this paper, we provide a characterization of the expected value of monotone submodular set functions with n pairwise independent random inputs. Inspired by the notion of "correlation gap", we study the ratio of the maximum expected value of a function with arbitrary dependence among the random inputs with given marginal probabilities to the maximum expected value of the function with pairwise independent random inputs and the same marginal probabilities. Our results show that the ratio is upper bounded by: (a) $4/3$ for $n = 3$ with general marginal probabilities and any monotone submodular set function (b) $4/3$ for general n with small and large marginal probabilities and any monotone submodular set function and (c) $4k/(4k-1)$ for general n, general identical probabilities and rank functions of k-uniform matroids. The bound is tight in all three cases. This contrasts with the $e/(e-1)$ bound on the correlation gap ratio for monotone submodular set functions with mutually independent random inputs (which is known to be tight in case (b)), and illustrates a fundamental difference in the behavior of submodular functions with weaker notions of independence. These results can be immediately extended beyond pairwise independence to correlated random inputs. We discuss applications in distributionally robust optimization and mechanism design and end the paper with a conjecture.

Keywords: Submodularity, pairwise independence, correlation gap, distributionally robust optimization, mechanism design, linear programming

1. Introduction

Submodular set functions play an important role in machine learning problems Bach (2013); Krause and Jegelka (2013). An important notion which describes the behavior of these functions under random input is the "correlation gap", which was introduced in Agrawal et al. (2012), building on the work of Calinescu et al. (2007). The correlation gap is defined as the ratio of the maximum expected value of a set function with arbitrary dependence among the random inputs with fixed marginal probabilities to the expected value of the function with mutually independent random inputs and the same marginal probabilities. A key result in this area is that for any monotone submodular set function, the correlation gap is always upper bounded by $e/(e-1) \approx 1.582$ and that this bound is tight Calinescu et al. (2007); Agrawal et al. (2012). This result has been applied in many settings including contention resolution schemes Chekuri et al. (2014); Feldman et al. (2021), mechanism design Chawla et al. (2010); Yan (2011), combinatorial prophet inequalities Rubinstein and Singla (2017); Chekuri and Livanos (2021) and distributionally robust optimization Agrawal et al. (2012); Staib et al. (2019). In this paper, we introduce a modification of the notion of correlation gap to set functions with pairwise independent random inputs and derive a new bound of 4/3 for arbitrary monotone submodular set functions in several cases. This adds to a recent result in Ramachandra and Natarajan (2023) where the bound was identified for a specific set function. For structured submodular functions such as rank functions of k-uniform matroids, we prove a further improved upper bound of $4k/(4k-1)$ with identical marginal probabilities.

1.1. Preliminaries

Let $[n] = \{1, 2, \ldots, n\}$ be the ground set and $f : 2^{[n]} \to \mathbb{R}_+$ be a nonnegative set function. The function f is submodular if $f(S) + f(T) \geq f(S \cap T) + f(S \cup T)$ for all $S, T \subseteq [n]$ or equivalently $f(S \cup \{i\}) - f(S) \geq f(T \cup \{i\}) - f(T)$ for all $S \subseteq T \subseteq [n]$, $i \notin T$. The function f is monotone if $f(S) \leq f(T)$ for all $S \subseteq T \subseteq [n]$. We denote the marginal contribution of adding i to S by $f(i|S) = f(S \cup \{i\}) - f(S)$.

Definition 1 (Multilinear extension) *The expected value of a set function f where each input $i \in [n]$ is independently selected with probability x_i is computed as*

$$F(\boldsymbol{x}) = \sum_{S \subseteq [n]} f(S) \prod_{i \in S} x_i \prod_{i \notin S} (1 - x_i), \tag{1}$$

where $F(\boldsymbol{x})$ is referred to as the multilinear extension of f and is defined for any $\boldsymbol{x} \in [0,1]^n$.

Definition 2 (Concave closure) *The maximum expected value of the set function over all joint distributions of the random inputs where each $i \in [n]$ is selected with probability x_i is computed as the optimal value of the following primal-dual pair of linear programs:*

$$\begin{aligned} f^+(\boldsymbol{x}) = \max \quad & \sum_{S} \theta(S) f(S) & = \quad \min \quad & \sum_{i \in [n]} \lambda_i x_i + \lambda_0 \\ s.t \quad & \sum_{S} \theta(S) = 1, & s.t. \quad & \sum_{i \in S} \lambda_i + \lambda_0 \geq f(S), \quad \forall S \subseteq [n]. \\ & \sum_{S : S \ni i} \theta(S) = x_i, \quad \forall i \in [n], & & \\ & \theta(S) \geq 0, \qquad \forall S \subseteq [n], & & \end{aligned} \tag{2}$$

where $f^+(\boldsymbol{x})$ is referred to as the concave closure of f and is defined for any $\boldsymbol{x} \in [0,1]^n$.

Both $F : [0,1]^n \to \mathbb{R}_+$ and $f^+ : [0,1]^n \to \mathbb{R}_+$ define continuous extensions of the set function $f : 2^{[n]} \to \mathbb{R}_+$. The functions satisfy $f(S) = F(1_S) = f^+(1_S)$ for all $S \subseteq [n]$ where 1_S denotes the indicator vector of the set S. The correlation gap is defined as the ratio $f^+(\boldsymbol{x})/F(\boldsymbol{x})$ where we define $0/0 = 1$.

Theorem 3 *[Calinescu et al. (2011); Agrawal et al. (2012)] For any monotone submodular function $f : 2^{[n]} \to \mathbb{R}_+$ and any $\boldsymbol{x} \in [0,1]^n$, $f^+(\boldsymbol{x})/F(\boldsymbol{x}) \leq e/(e-1)$. The upper bound is tight for $f(S) = \min(|S|, 1)$ and $\boldsymbol{x} = (1/n, \ldots, 1/n)$ as $n \uparrow \infty$.*

Remark 4 *Even for $n = 2$, there are instances where violating the assumption of either monotonicity or submodularity leads to an unbounded correlation gap (see Appendix A.1* *for examples). Another important extension of submodular functions is the convex closure (denoted by $f^-(\boldsymbol{x})$) where we minimize over the $\theta(S)$ variables in (2), rather than maximize. The focus of this paper is only on $f^+(\boldsymbol{x})$ and a new continous extension defined with pairwise independence in Section 2.3.*

2. Set functions with pairwise independent random inputs

2.1. Pairwise independence

Given a Bernoulli random vector $\tilde{\boldsymbol{c}} = (\tilde{c}_1, \ldots, \tilde{c}_n)$, mutual independence is defined by the condition $\mathbb{P}(\tilde{c}_i = c_i, \forall i \in [n]) = \prod_{i=1}^n \mathbb{P}(\tilde{c}_i = c_i)$ for all $\boldsymbol{c} \in \{0,1\}^n$. Pairwise independence is a weaker notion of independence where only pairs of random variables are independent. It is defined by the condition $\mathbb{P}(\tilde{c}_i = c_i, \tilde{c}_j = c_j) = \mathbb{P}(\tilde{c}_i = c_i)\mathbb{P}(\tilde{c}_j = c_j)$ for all $(c_i, c_j) \in \{0,1\}^2$, $i \neq j$. While mutual independence implies pairwise independence, the reverse is not true Bernstein (1946). For example, consider a distribution on three random variables that assigns a probability of $1/4$ to each of the scenarios $(0,0,1)$, $(0,1,0)$, $(1,0,0)$ and $(1,1,1)$. The three random variables are pairwise independent but not mutually independent. Another pairwise independent distribution that has the same marginal probabilities of $(1/2, 1/2, 1/2)$ is given by the scenarios $(0,0,0)$, $(0,1,1)$, $(1,0,1)$ and $(1,1,0)$, each occurring with a probability of $1/4$. For general n, constructions of pairwise independent random variables can be found in the works of Geisser and Mantel (1962), Karloff and Mansour (1994) and Koller and Meggido (1994).

2.2. Applications of pairwise independence

One of the motivations for studying constructions of pairwise independent random variables is that there is always a joint distribution that has a low cardinality support (polynomial in n), in contrast to mutual independence (exponential in n). The low cardinality of the distribution has important ramifications in efficiently derandomizing algorithms for combinatorial optimization problems Wigderson (1994); Luby and Wigderson (2005). Pairwise independence is useful in modeling situations where the underlying randomness has zero or close to zero correlations but complex higher-order dependencies. Such behavior has been experimentally observed in cortical neurons in Schneidman et al. (2006), where weak correlations between pairs of neurons coexist with strong collective behavior of multiple neurons. Consequently, approximations based on the assumption of mutual independence are weak.

2.3. A new continuous extension

Inspired by the definition of the concave closure and driven by the need to characterize the behavior of set functions with pairwise independent random inputs, we consider the following continuous extension.

Definition 5 (Upper pairwise independent extension) *The maximum expected value of a set function f over all pairwise independent distributions of the random inputs where each $i \in [n]$ is selected with probability x_i is computed as the optimal value of the following* *primal-dual pair of linear programs:*

$$
\begin{aligned}
f^{++}(\boldsymbol{x}) = \max \quad & \sum_{S} \theta(S) f(S) & \quad = \quad \min \quad & \sum_{i<j\in[n]} \lambda_{ij} x_i x_j + \sum_{i\in[n]} \lambda_i x_i + \lambda_0 \\
s.t \quad & \sum_{S} \theta(S) = 1, & s.t. \quad & \sum_{i<j\in S} \lambda_{ij} + \sum_{i\in S} \lambda_i + \lambda_0 \geq f(S), \\
& \sum_{S:S\ni i} \theta(S) = x_i, \qquad \forall i \in [n], & & \forall S \subseteq [n]. \\
& \sum_{S:S\ni i,j} \theta(S) = x_i x_j, \quad \forall i < j \in [n], & & \\
& \theta(S) \geq 0, \qquad \forall S \subseteq [n], & &
\end{aligned}
\tag{3}
$$

where $f^{++}(\boldsymbol{x})$ is referred to as the upper pairwise independent extension and is defined for any $\boldsymbol{x} \in [0,1]^n$. We define the pairwise independent correlation gap as the ratio $f^{+}(\boldsymbol{x})/f^{++}(\boldsymbol{x})$.

Remark 6 *Clearly $f(S) = f^{++}(1_S)$ for all $S \subseteq [n]$. Instead of maximizing, if we minimize over the $\theta(S)$ variables in (3), we obtain a lower pairwise independent extension (denoted by $f^{--}(\boldsymbol{x})$). In this paper, we only focus on analyzing $f^{++}(\boldsymbol{x})$ for monotone submodular functions and its relation to $f^{+}(\boldsymbol{x})$ and $F(\boldsymbol{x})$. Clearly, $F(\boldsymbol{x}) \leq f^{++}(\boldsymbol{x}) \leq f^{+}(\boldsymbol{x})$ and hence $f^{+}(\boldsymbol{x})/f^{++}(\boldsymbol{x}) \leq f^{+}(\boldsymbol{x})/F(\boldsymbol{x})$.*

We next discuss some technical challenges that arise in the analysis of the pairwise independent correlation gap.

2.4. NP-hardness of computing $f^{+}(\boldsymbol{x})$ and $f^{++}(\boldsymbol{x})$

The proof of the NP-hardness of computing $f^{+}(\boldsymbol{x})$ is provided in Agrawal et al. (2012) and Dughmi (2009). This can be extended to $f^{++}(\boldsymbol{x})$ as shown next.

Lemma 7 *Computing $f^{++}(\boldsymbol{x})$ for a given $\boldsymbol{x} \in [0,1]^n$ and an arbitrary function $f \in \mathcal{F}_n$ is NP-hard.*

Proof The separation problem for the dual linear program in (3) is formulated as:

$$\max_{S\subseteq[n]} f(S) - \sum_{i\in S} \lambda_i - \sum_{i<j\in S} \lambda_{ij}.$$

Given a graph $G = (V, E)$, define for any $S \subseteq V$, the value $f(S)$ as two times the number of edges that have at least one end point in S. For each $i \in V$, let λ_i be the number of edges incident to vertex i and set all λ_{ij} values to be zero. Then the dual separation problem reduces to solving a MAX CUT problem which is NP-hard. From the equivalence of separation and optimization, computing $f^{++}(\boldsymbol{x})$ is in turn NP-hard. ■

2.5. Key contributions

The key contribution of this paper is that despite the NP-hardness of computing $f^+(\boldsymbol{x})$ and $f^{++}(\boldsymbol{x})$, it is possible to prove that the maximum possible value of the ratio $f^+(\boldsymbol{x})/f^{++}(\boldsymbol{x})$ is provably smaller than that of $f^+(\boldsymbol{x})/F(\boldsymbol{x})$ for the following cases:

a) $n = 3$ with general marginal probabilities and any arbitrary monotone submodular set function.

b) general n with small and large marginal probabilities and any arbitrary monotone submodular set function.

c) general n with general identical marginal probabilities and rank functions of k-uniform matroids.

Along the way, for $n = 3$, we derive closed-form expressions for $f^+(\boldsymbol{x})$ and $f^{++}(\boldsymbol{x})$ and analyze cylinder dependence properties of the optimal distributions, which provide useful insights on the interplay between the function values and the marginal probabilities.

While the proof techniques for these cases involve different approaches, a key common step is to carefully construct dual feasible solutions to provide upper bounds on $f^+(\boldsymbol{x})$ and primal feasible distributions to provide lower bounds on $f^{++}(\boldsymbol{x})$. The latter distributions use only the pairwise products of the marginal probabilities $(x_i x_j)$ in contrast to the complete products used in the multilinear extension $F(\boldsymbol{x})$, which is critical in improving the existing upper bound on the ratio. Our results show that by dropping the traditional assumption of mutual independence and assuming pairwise independence instead, we can derive better approximation guarantees for both $f^+(\boldsymbol{x})$ and $f^{++}(\boldsymbol{x})$.

The rest of the paper is structured as follows: Section 2.6 discusses applications in distributionally robust optimization and mechanism design contexts. Section 3.1 highlights the importance and non-triviality of the analysis for $n = 3$, Sections 3.2 and 3.3 list extremal monotone submodular functions and two key inequalities used throughout the proofs for $n = 2, 3$ with general marginal probabilities, Section 3.4 establishes a $4/3$ upper bound for $n = 2$, Section 3.5 derives closed-form expressions of $f^+(\boldsymbol{x})$ and $f^{++}(\boldsymbol{x})$ for $n = 3$ along with a numerical example to highlight the complications involved, Section 3.6 analyzes cylinder dependence properties of the optimal distributions and Section 3.7 establishes a $4/3$ bound for $n = 3$. Section 4 proves a $4/3$ bound for general n with small and large marginal probabilities and extends the result to the n-simplex case and identical probabilities with relaxed conditions. Section 5 proves an improved bound of $4k/(4k-1)$ for rank functions of k-uniform matroids with unrestricted identical probabilities and interprets the results in a mechanism design context. Finally, Section 6 concludes the paper with a summary, possible extensions and a conjecture.

2.6. Applications and related work

In this section, we discuss applications and recent related work.

1. *Distributionally robust optimization*: Using Theorem 3, one can show that the loss in performance by using this approach is bounded by a constant factor for specific optimization problems even if the true joint distribution is not independent Agrawal et al. (2012). In

some instances, the distributionally robust optimization problem given only the marginal distributions of the random variables is itself solvable in polynomial time Meilijson and Nádas (1979); Bertsimas et al. (2004); Mak et al. (2015); Chen et al. (2022). For example, given nonnegative weights $c_1, \ldots, c_n$ and a set $\mathcal{Y} \subseteq \{0,1\}^n$, the deterministic k-sum combinatorial optimization problem for a fixed $k \in [n]$ is formulated as:

$$\min_{\boldsymbol{y} \in \mathcal{Y} \subseteq \{0,1\}^n} \max_{S \subseteq [n]: |S| \leq k} \sum_{i \in S} c_i y_i.$$

For $k = 1$, this reduces to a bottleneck combinatorial optimization problem. Suppose the weights $\tilde{c}_i$ are random where $\tilde{c}_i = c_i$ with probability x_i and $\tilde{c}_i = 0$ with probability $1 - x_i$. Define the set function:

$$f_{\boldsymbol{y}}(S) = \max_{T \subseteq S, |T| \leq k} \sum_{i \in T} c_i y_i, \ \forall S \subseteq [n].$$

For a fixed $\boldsymbol{y} \in \mathcal{Y} \subseteq \{0,1\}^n$, the function $f_{\boldsymbol{y}} : 2^{[n]} \to \mathbb{R}_+$ is a monotone submodular function and the corresponding value of the concave closure $f^+_{\boldsymbol{y}}(\boldsymbol{x})$ is computable in polynomial time Calinescu et al. (2007); Natarajan (2021). The distributionally robust k-sum combinatorial optimization problem is then formulated as:

$$\min_{\boldsymbol{y} \in \mathcal{Y} \subseteq \{0,1\}^n} f^+_{\boldsymbol{y}}(\boldsymbol{x}).$$

The optimal solution for this problem (denoted by $\boldsymbol{y}^+$) can be found in polynomial time under the assumption that optimizing a linear function over $\mathcal{Y}$ is possible in polynomial time. If the random weights are mutually independent, the stochastic optimization problem is formulated as:

$$\min_{\boldsymbol{y} \in \mathcal{Y} \subseteq \{0,1\}^n} F_{\boldsymbol{y}}(\boldsymbol{x}).$$

Using Theorem 3, we obtain a $e/(e-1)$ approximation algorithm for the stochastic optimization problem since:

$$F_{\boldsymbol{y}^+}(\boldsymbol{x}) \leq f^+_{\boldsymbol{y}^+}(\boldsymbol{x}) = \min_{\boldsymbol{y} \in \mathcal{Y} \subseteq \{0,1\}^n} f^+_{\boldsymbol{y}}(\boldsymbol{x}) \leq (e/(e-1)) \min_{\boldsymbol{y} \in \mathcal{Y} \subseteq \{0,1\}^n} F_{\boldsymbol{y}}(\boldsymbol{x}).$$

Now suppose the random weights are pairwise independent. The distributionally robust k-sum combinatorial optimization problem given a fixed marginal probability vector $\boldsymbol{x}$ and assuming pairwise independence is formulated as:

$$\min_{\boldsymbol{y} \in \mathcal{Y} \subseteq \{0,1\}^n} f^{++}_{\boldsymbol{y}}(\boldsymbol{x}).$$

We then obtain a 4/3 approximation algorithm for this problem in the following two cases: (a) for $k = 1$ and general values of $\boldsymbol{x}$, and (b) for general k with small and large values of $\boldsymbol{x}$. Specifically:

$$\min_{\boldsymbol{y} \in \mathcal{Y} \subseteq \{0,1\}^n} f^{++}_{\boldsymbol{y}}(\boldsymbol{x}) \leq f^{++}_{\boldsymbol{y}^+}(\boldsymbol{x}) \leq 4/3 \min_{\boldsymbol{y} \in \mathcal{Y} \subseteq \{0,1\}^n} f^{++}_{\boldsymbol{y}}(\boldsymbol{x}).$$

The precise conditions on the marginal probabilities under which the approximation guarantee in case (b) holds is detailed in Theorem 24 and subsequent corollaries 27 and 28. Thus we obtain improved approximation guarantees for a class of distributionally robust optimization problems where only weaker notions of independence are assumed to hold.

2. *Mechanism design:* In the mechanism design context, where items are to be sold to n unit demand agents with independent random valuations, Yan (2011) show that the performance of a simple mechanism such as sequential posted-price mechanism (SPM) relative to the performance of the optimal mechanism (Myerson's mechanism) can be characterized by showing a connection to the notion of correlation gap. Let x_i be the probability that agent i's valuation exceeds the price offered. The set of agents whose valuation exceeds their offered prices is independent for the SPM and correlated for the optimal mechanism. Hence, computing the expected revenue of SPM and the optimal expected revenue of the Myerson's mechanism corresponds to computing $F(\boldsymbol{x})$ and $f^+(\boldsymbol{x})$ respectively (ensuring that the marginal probabilities are the same in both mechanisms by choosing appropriate offer prices). Since many auction constraints can be modeled using matroids whose weighted rank functions are known to be monotone and submodular, earlier results of Agrawal et al. (2012) (Theorem 3) can be invoked to show that the SPM provides a $(1-1/e)$ approximation to the optimal mechanism. Functions of the form $f(S) = \min(|S|, k)$ are rank functions of k-uniform matroids and can be interpreted as a revenue function in a setting where the seller has only $k \leq n$ items to auction, by considering the minimum of k and the number of agents whose valuation is at least their offered price. For this class of monotone submodular functions, Yan (2011) showed that the SPM provides an improved $\left(1 - \frac{1}{\sqrt{2\pi k}}\right)$ approximation to the optimal mechanism. Building on the interpretation in Yan (2011), when the agent selection for SPM is pairwise independent, the optimal expected revenue with SPM corresponds to computing $f^{++}(\boldsymbol{x})$. Based on the revenue functions employed, in conjunction with the results in this paper, we can thus derive the following improved approximations to the optimal mechanism:

a) a $3/4$ approximation for weighted rank functions of general matroids with small and large values of $\boldsymbol{x}$ (as detailed in Theorem 24 and corollaries 27 and 28)

(b) $1 - 1/(4k)$ approximation to the optimal mechanism for rank functions of k-uniform matroids (k-unit auction) with identical marginal probabilities (from results in Theorem 29).

3. *Properties of the continuous relaxation of the weighted coverage function*: Let $w_1, \dots, w_m$ denote nonnegative weights and $T_1, \dots, T_n$ be subsets of $[m]$. The weighted coverage function $f : 2^{[n]} \to \mathbb{R}_+$ is defined by $f(S) = \sum_{j \in \cup_{i \in S} T_i} w_j$. For each $j \in [m]$, let $U_j = \{i \in [n] \mid j \in T_i\}$ represent the subsets that cover j. The multilinear extension for any $\boldsymbol{x} \in [0,1]^n$ is given by:

$$F(\boldsymbol{x}) = \sum_{j=1}^{m} w_j \mathbb{P}(j \text{ is covered by some } T_i) = \sum_{j=1}^{m} w_j (1 - \prod_{i \in U_j} (1 - x_i)).$$

An upper bound on $F(\boldsymbol{x})$ is obtained by using the concave closure for each individual term:

$$F(\boldsymbol{x}) \leq \sum_{j=1}^{m} w_j f_j^+(\boldsymbol{x}) \text{ where } f_j^+(\boldsymbol{x}) = \min(1, \textstyle\sum_{i \in U_j} x_i).$$

The upper bound can maximized efficiently over a polytope $\mathcal{P} \subseteq [0,1]^n$ in polynomial time using linear optimization or subgradient methods Calinescu et al. (2011); Karimi et al. (2017) to obtain an optimal solution $\boldsymbol{x}^+$. Theorem 3 ensures $F(\boldsymbol{x}^+) \geq (1-1/e)\max_{\boldsymbol{x}\in\mathcal{P}\subseteq[0,1]^n} F(\boldsymbol{x})$. In prior work, pipage rounding has been applied to $\boldsymbol{x}^+$ to find good solutions to the deterministic combinatorial optimization problem while preserving the quality of the approximation in expectation Karimi et al. (2017). In fact, the solution $\boldsymbol{x}^+$ possesses an additional performance guarantee, that is, if we use the upper pairwise independent extension for each individual term then $\sum_{j=1}^{m} w_j f_j^{++}(\boldsymbol{x}^+) \geq 3/4 \sum_{j=1}^{m} w_j \max_{\boldsymbol{x}\in\mathcal{P}\subseteq[0,1]^n} f_j^{++}(\boldsymbol{x})$.

The following theorem states a recent result where $f^{++}(\boldsymbol{x})$ was shown to be computable in closed-form for a specific monotone submodular function.

Theorem 8 *[Ramachandra and Natarajan (2023)] For $f(S) = \min(|S|, 1)$ and any $\boldsymbol{x} \in [0,1]^n$, $f^{++}(\boldsymbol{x}) = \min(1,$
$\sum_{i=1}^{n} x_i(1 - \max_{i\in[n]} x_i) + \max_{i\in[n]} x_i^2)$. In this case, $f^+(\boldsymbol{x})/f^{++}(\boldsymbol{x}) \leq 4/3$ and the upper bound is tight for $\sum_{i=1}^{n} x_i = 1$ and $\max_{i\in[n]} x_i = 1/2$.*

Remark 9 *For the function $f(S) = \min(|S|, 1)$, the ratio $f^+(\boldsymbol{x})/F(\boldsymbol{x})$ attains the $e/(e-1)$ upper bound for specific values of $\boldsymbol{x}$ and n (see Theorem 3). Theorem 8 shows that in contrast, the ratio $f^+(\boldsymbol{x})/f^{++}(\boldsymbol{x})$ is provably smaller in the worst-case for this specific function. In Appendix A.2, we show that the related ratio of $f^{++}(\boldsymbol{x})/F(\boldsymbol{x})$ in the worst-case can be as large as the original $e/(e-1)$ bound. It is thus a natural question to ask if the bound of $4/3$ on the ratio $f^+(\boldsymbol{x})/f^{++}(\boldsymbol{x})$ can be generalized to arbitrary monotone submodular functions.*

In the next two sections, we show that this is indeed true in two cases: (a) small n (specifically $n = 2, 3$) with general marginal probabilities, and (b) general n with small and large marginal probabilities.

2.7. Assumptions and Definitions

Without loss of generality, assume $f(\emptyset) = 0$ and $f([n]) = 1$ since translating and scaling the function by defining $g(S) = (f(S) - f(\emptyset))/(f([n]) - f(\emptyset))$ preserves monotonicity and submodularity. Define the set of functions of interest as follows:

$$\mathcal{F}_n = \{f : 2^{[n]} \to \mathbb{R}_+ \mid f \text{ is monotone submodular}, f(\emptyset) = 0, f([n]) = 1\}.$$

Define a subpolytope of polytope P as a polytope Q, whose extreme points are a subset of the extreme points of P.

3. Upper bound for $n = 3$, general $\boldsymbol{x}$

The goal of this section is to show that for $n = 3$ random inputs, general marginal probabilities and arbitrary monotone submodular set functions, the pairwise independent correlation gap is upper bounded by 4/3. For completeness of exposition and continuity of proof techniques, we begin with proving the result for $n = 2$ and subsequently move to $n = 3$. Our solution technique for small values of n is based on explicitly partitioning the probability space into v regions given by $[0, 1]^n = R_1 \cup R_2 \cup \cdots \cup R_v$, such that we are able to compute $f^+(\boldsymbol{x})$ and $f^{++}(\boldsymbol{x})$ exactly in each region. For $n = 2$, it is straightforward to find $v = 2$ regions such that the probability distributions which attain the bound $f^+(\boldsymbol{x})$ in each of these regions are oblivious to the particular $f \in \mathcal{F}_2$. This is because the worst-case distribution is given by two perfectly negatively dependent random inputs arising from the intrinsic connection between submodular functions and substitutability Topkis (1998). Furthermore for $n = 2$, $f^{++}(\boldsymbol{x})$ is simply $F(\boldsymbol{x})$ and hence $f^+(\boldsymbol{x})/f^{++}(\boldsymbol{x})$ is exactly the original correlation gap.

3.1. Importance and non-triviality of $n = 3$ analysis

The $n = 3$ case is important since since pairwise independence is no longer equivalent to mutual independence. It illustrates a fundamental difference in the behavior of the ratios $f^+(\boldsymbol{x})/F(\boldsymbol{x})$ and $f^+(\boldsymbol{x})/f^{++}(\boldsymbol{x})$ for monotone, submodular functions that is explained by the difference between pairwise and mutual independence Bernstein (1946), which is also the reason why the problem is significantly more challenging as compared to $n = 2$. Perfect negative dependence among three or more random variables is also not well defined Joe (1997) and developing a theory of negative dependence has been a topic of intense research over the past two decades Pemantle (2000); Borcea et al. (2009). The primary challenge lies in computing $f^{++}(\boldsymbol{x})$ and $f^+(\boldsymbol{x})$, since the optimal distributions which attain them are not oblivious to the choice of $f \in \mathcal{F}_3$, as demonstrated in the following example.

Example 1 *Table 1 provides an example of two functions $f_1, f_2 \in \mathcal{F}_3$ where the optimal distributions $\theta^+_*(S)$ and $\theta^{++}_*(S)$ that attain the values $f^+(\boldsymbol{x})$ and $f^{++}(\boldsymbol{x})$ change from f_1 to f_2. Furthermore, for the function f_1, inputs 1 and 2 are perfectly negatively dependent to input 3, making 1 and 2 perfectly positively dependent. This makes the analysis challenging since the optimal distributions in the numerator and the denominator of the ratio $f^+(\boldsymbol{x})/f^{++}(\boldsymbol{x})$ are sensitive to the choice of $f \in \mathcal{F}_n$, in contrast to the multilinear extension $F(\boldsymbol{x})$ and the convex closure $f^-(\boldsymbol{x})$ Dughmi (2009).*

To overcome this challenge in characterizing the optimal distributions, we divide the polytope of monotone submodular functions $\mathcal{F}_3$ into $u = 3$ subpolytopes and for each such subpolytope, the probability space $[0, 1]^3$ is partitioned into $v = 6$ regions. For each subpolytope and partitioning region, we compute $f^+(\boldsymbol{x})$ and $f^{++}(\boldsymbol{x})$ exactly and prove a 4/3 bound over all extremal submodular set functions that are valid in that subpolytope.

3.2. Extremal monotone submodular functions and two key inequalities

This section provides a characterization of the set of extremal monotone submodular functions for $n = 2, 3$ which are used in the subsequent proofs. The set $\mathcal{F}_n$ is a polytope

Table 1: Optimal distributions change with the function for $(x_1, x_2, x_3) = (1/2, 1/2, 1/2)$.

S	$f_1(S)$	$\theta_*^+(S)$	$\theta_*^{++}(S)$	$f_2(S)$	$\theta_*^+(S)$	$\theta_*^{++}(S)$
$\emptyset$	0	0	0	0	0	1/4
$\{1\}$	1/3	0	1/4	1/3	0	0
$\{2\}$	1/2	0	1/4	1/2	1/2	0
$\{3\}$	3/5	1/2	1/4	1/2	0	0
$\{1,2\}$	3/4	1/2	0	3/4	0	1/4
$\{1,3\}$	4/5	0	0	4/5	1/2	1/4
$\{2,3\}$	5/6	0	0	5/6	0	1/4
$\{1,2,3\}$	1	0	1/4	1	0	0
$f^+(\boldsymbol{x})$	-	27/40	-	-	13/20	-
$f^{++}(\boldsymbol{x})$	-	-	73/120	-	-	143/240

contained in $[0,1]^{2^n}$. The extreme points of $\mathcal{F}_n$ define extremal monotone submodular functions and are characterized in Lemma 10 for $n = 2$ and $n = 3$ Shapley (1971); Rosenmuller and Weidner (1974); Kashiwabara (2000). For $n = 3$, we define three subpolytopes which collectively exhaust $\mathcal{F}_3$ (but are not mutually exclusive) and will be useful in computing $f^+(\boldsymbol{x})$ as follows:

$$\mathcal{F}_3^1 = \{f \in \mathcal{F}_3 | f(3|2) \geq f(3|1), f(2|3) \geq f(2|1)\}$$
$$\mathcal{F}_3^2 = \{f \in \mathcal{F}_3 | f(3|1) \geq f(3|2), f(1|3) \geq f(1|2)\}$$
$$\mathcal{F}_3^3 = \{f \in \mathcal{F}_3 | f(2|1) \geq f(2|3), f(1|2) \geq f(1|3)\}$$

and list their extremal set functions in Lemma 10. In addition, we define two subpolytopes which together exhaust $\mathcal{F}_3$ (but are not mutually exclusive) and will be useful in computing $f^{++}(\boldsymbol{x})$ as follows:

$$\mathcal{G}_3^1 = \{f \in \mathcal{F}_3 | f(1|2) + f(2|3) + f(3|1) \leq 1\}, \ \mathcal{G}_3^2 \ = \{f \in \mathcal{F}_3 | f(1|2) + f(2|3) + f(3|1) \geq 1\}$$

Lemma 10 *The extremal set functions in $\mathcal{F}_2$ are given by $\mathcal{E}(\mathcal{F}_2) = \{e_1, e_2, e_3\}$ where:*

$$e_1 = (0,1,0,1), \quad e_2 = (0,0,1,1), \quad e_3 = (0,1,1,1),$$

with the entries of the vector denoting the values $(f(\emptyset), f(1), f(2), f(1,2))$. The extremal set functions in $\mathcal{F}_3$ are given by $\mathcal{E}(\mathcal{F}_3) = \{E_1, E_2, E_3, E_4, E_5, E_6, E_7, E_8\}$ where:

$$E_1 = (0,1,0,0,1,1,0,1), \quad E_2 = (0,0,1,0,1,0,1,1), \quad E_3 = (0,0,0,1,0,1,1,1), \quad E_4 = (0,1,1,0,1,1,1,1),$$
$$E_5 = (0,1,0,1,1,1,1,1), \quad E_6 = (0,0,1,1,1,1,1,1), \quad E_7 = (0,1,1,1,1,1,1,1), \quad E_8 = (0,\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2},1,1,1,1),$$

with the entries of the vector denoting the values $(f(\emptyset),\ f(1),\ f(2),\ f(3),\ f(1,2),\ f(1,3),$ $f(2,3),\ f(1,2,3))$. In addition, the extreme points of the subpolytopes $\mathcal{F}_3^1, \mathcal{F}_3^2, \mathcal{F}_3^3$ are given by $\mathcal{E}(\mathcal{F}_3^1) = \mathcal{E}(\mathcal{F}_3)\backslash\{E_6\}$, $\mathcal{E}(\mathcal{F}_3^2) = \mathcal{E}(\mathcal{F}_3)\backslash\{E_5\}$ and $\mathcal{E}(\mathcal{F}_3^3) = \mathcal{E}(\mathcal{F}_3)\backslash\{E_4\}$ respectively.

Proof See Appendix A.3. ■

3.3. Key Inequalities

The following two inequalities are used in the proofs for $n = 2, 3$ and general $\boldsymbol{x}$:

$$(I_1) \quad \alpha + \beta - 4\alpha\beta \geq 0, \qquad \forall \alpha, \beta \in [0,1], \alpha + \beta \leq 1$$

$$(I_2) \quad 4\alpha + 4\beta - 4\alpha\beta - 3 \geq 0, \quad \forall \alpha, \beta \in [0,1], \alpha + \beta \geq 1.$$

Proof See Appendix A.4. ∎

Figure 1 shows that for (α, β) satisfying the conditions in I_1 and I_2, the plots of $(\alpha + \beta)/(\alpha + \beta - \alpha\beta)$ (left) and $1/(\alpha + \beta - \alpha\beta)$ (right) are upper bounded by 4/3.

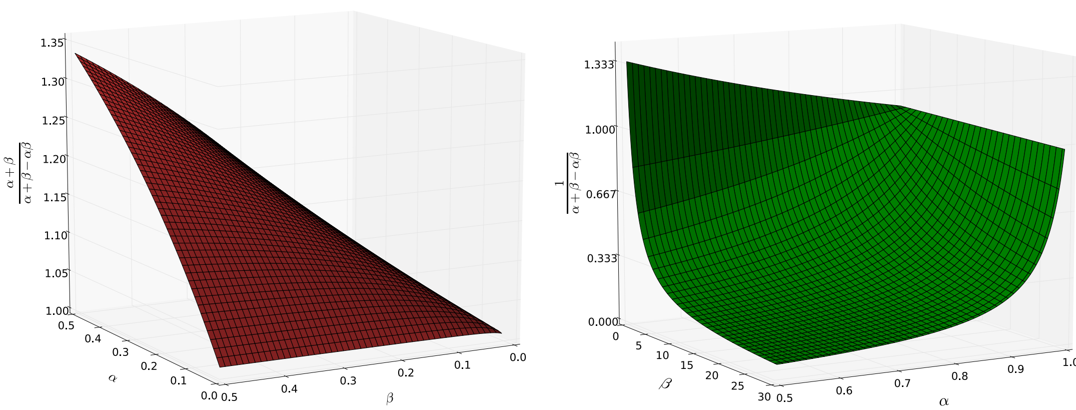

Figure 1: Plot of $\dfrac{\alpha + \beta}{\alpha + \beta - \alpha\beta}$ (left) and $\dfrac{1}{\alpha + \beta - \alpha\beta}$ (right)

3.4. Analysis with $n = 2$

This section first establishes the closed-form expressions for $f^{+}(\boldsymbol{x})$ and $f^{++}(\boldsymbol{x})$ with $n = 2$ before moving on to prove a 4/3 upper bound on their ratio.

Lemma 11 *For any monotone submodular set function* $f : 2^{[2]} \to \mathbb{R}_+$ *and any* $\boldsymbol{x} \in [0,1]^2$,

$$\begin{aligned} f^{+}(\boldsymbol{x}) &= \min\left[f(1)x_1 + f(2)x_2,\ f(1) + f(2) - 1 + (1 - f(2))x_1 + (1 - f(1))x_2\right] \\ f^{++}(\boldsymbol{x}) &= f(1)x_1 + f(2)x_2 + (1 - f(1) - f(2))x_1x_2 \end{aligned}$$

Proof It is straightforward to find $f^{+}(\boldsymbol{x})$ in closed-form based on a partition of the probabilities into $v = 2$ regions (see Figure 2). Table 2 shows the distributions $\theta^{+}_{1,*}(S)$ and $\theta^{+}_{2,*}(S)$ for the primal linear program (2) that are optimal in regions R_1 and R_2 respectively.

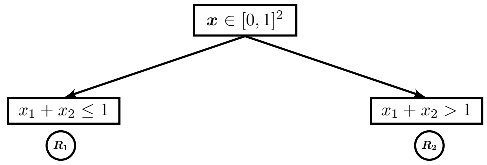

Figure 2: Partition of $[0,1]^2$ into $v = 2$ regions

Table 2: Optimal distributions for $f^+(\boldsymbol{x})$ and $f^{++}(\boldsymbol{x})$

S	$\theta^+_{1,*}(S)$	$\theta^+_{2,*}(S)$	$\theta^{++}(S)$
$\emptyset$	$1 - x_1 - x_2$	0	$(1-x_1)(1-x_2)$
$\{1\}$	x_1	$1 - x_2$	$x_1(1-x_2)$
$\{2\}$	x_2	$1 - x_1$	$x_2(1-x_1)$
$\{1,2\}$	0	$x_1 + x_2 - 1$	$x_1 x_2$
Region	R_1	R_2	$[0,1]^2$

Here the optimal distributions are oblivious to the specific choice of $f \in \mathcal{F}_2$. The optimality can be verified by noting that $(\lambda_0, \lambda_1, \lambda_2) = (0, f(1), f(2))$ is dual feasible in R_1, $(\lambda_0, \lambda_1, \lambda_2) = (f(1) + f(2) - 1, 1 - f(2), 1 - f(1))$ is dual feasible in R_2 and the dual objective values match the primal objective values for $\theta^+_{1,*}(S)$ and $\theta^+_{2,*}(S)$ in these regions respectively. The upper pairwise independent extension with $n = 2$ reduces to $f^{++}(\boldsymbol{x}) = F(\boldsymbol{x}) = x_1(1-x_2)f(1) + x_2(1-x_1)f(2) + x_1x_2$, where the distribution $\theta^{++}(S)$ is once again oblivious to the specific choice of $f \in \mathcal{F}_2$. ■

The next lemma establishes a 4/3 bound for $n = 2$. While this result follows as a special case of a general result in Chekuri et al. (2014) (see Lemma 4.10), we provide an alternative proof that builds the techniques needed for proving our main result with $n = 3$.

Lemma 12 (Chekuri et al. (2014)) *For any set function $f : 2^{[2]} \to \mathbb{R}_+$ and any $\boldsymbol{x} \in [0,1]^2$:*

$$f^+(\boldsymbol{x})/f^{++}(\boldsymbol{x}) \leq 4/3.$$

Proof For $n = 2$, $f^{++}(\boldsymbol{x}) = F(\boldsymbol{x})$ and the proof simply reduces to showing that the original correlation gap is itself upper bounded by $4/3$. Let $\delta = 4F(\boldsymbol{x}) - 3f^+(\boldsymbol{x})$. For $x_1 + x_2 \leq 1$ (region R_1), $f^+(\boldsymbol{x}) = x_1 f(1) + x_2 f(2)$. In this case $\delta = x_1 f(1) + x_2 f(2) + 4x_1x_2(1 - f(1) - f(2))$. The minimum value of this expression over all functions in $\mathcal{F}_2$ is attained at one of the extremal set functions e_1, e_2 or e_3. This gives the expression $\delta = \min(x_1, x_2, x_1 + x_2 - 4x_1x_2)$. Using the inequality I_1, we get the desired result in R_1. For $x_1 + x_2 > 1$ (region R_2), $f^+(\boldsymbol{x}) = (1-x_2)f(1) + (1-x_1)f(2) + x_1 + x_2 - 1$. In this case, $\delta = (4x_1 + 3x_2 - 4x_1x_2 - 3)f(1) + (3x_1 + 4x_2 - 4x_1x_2 - 3)f(2) + 4x_1x_2 - 3x_1 - 3x_2 + 3$. The minimum value of this expression over all functions in $\mathcal{F}_2$ is attained at one of the extremal set functions e_1, e_2 or e_3 which gives the expression $\delta = \min(x_1, x_2, 4x_1 + 4x_2 - 4x_1x_2 - 3)$. Using the inequality I_2, we get the desired result in R_2. ■

Lemma 12 shows that for all monotone submodular functions defined on two inputs:

$$f^+(\boldsymbol{x})/f^{++}(\boldsymbol{x}) = f^+(\boldsymbol{x})/F(\boldsymbol{x}) \leq 4/3.$$

The bound is tight when $f(S) = \min(|S|, 1)$ and $\boldsymbol{x} = (1/2, 1/2)$. For clarity, Figure 3 shows the plots when $f(S) = \min(|S|, 1)$ ($f^+(\boldsymbol{x}) = \min(x_1 + x_2, 1)$ and $f^{++}(\boldsymbol{x}) = x_1 + x_2 - x_1x_2$). The two functions are most seperated at $\boldsymbol{x} = (1/2, 1/2)$ where $f^+(\boldsymbol{x}) = 1$ and $f^{++}(\boldsymbol{x}) = 0.75$.

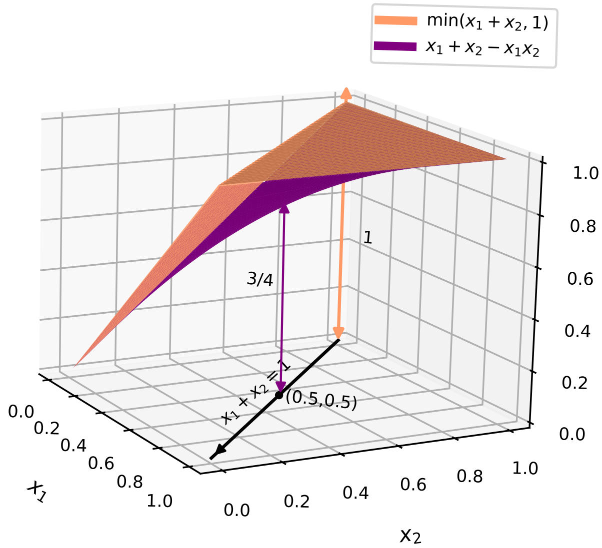

Figure 3: Plots of $f^{+}(\boldsymbol{x}) = \min(x_1 + x_2, 1)$ and $f^{++}(\boldsymbol{x}) = x_1 + x_2 - x_1 x_2$

Our goal is to show that the 4/3 bound continues to hold for $n = 3$, when pairwise independence and mutual independence begin to differ. As mentioned earlier, obtaining a handle on $f^{+}(\boldsymbol{x})$ and $f^{++}(\boldsymbol{x})$ is significantly more demanding in moving from $n = 2$ to $n = 3$, due to the non-oblivious nature of the optimal distributions (Table 1). This is demonstrated by the complicated nature of the closed-form expressions for $f^{+}(\boldsymbol{x})$ and $f^{++}(\boldsymbol{x})$ derived next. While the closed-forms in themselves are not the focus of this paper, their proofs of optimality will he helpful in proving the 4/3 bound and consequently, we include them here before proceeding to the main result for $n = 3$.

3.5. Closed-form expressions for $f^{+}(\boldsymbol{x})$ and $f^{++}(\boldsymbol{x})$ with $n = 3$

In preparation for deriving $f^{+}(\boldsymbol{x})$, Table 3 lists few feasible dual solutions to the linear program in (2), along with the corresponding submodular subpolytopes ($\mathcal{F}_3^k,\ k \in [3]$) where feasibility occurs. Here $\boldsymbol{\lambda}_i = (\lambda_{i0}, \lambda_{i1}, \lambda_{i2}, \lambda_{i3}),\ i \in [14]$ is the i^{th} dual feasible solution vector and the dual objective $\overline{f}^{+}(\boldsymbol{x}) = \lambda_{i0} + \sum_{j=1}^{3} \lambda_{ij} x_j$ provides a valid upper bound on $f^{+}(\boldsymbol{x})$ for each dual solution. . Note that $\boldsymbol{\lambda}_1$ and $\boldsymbol{\lambda}_{14}$ are feasible solutions in the entire polytope of submodular functions $\mathcal{F}_3$, while the remaining solutions $\boldsymbol{\lambda}_2 - \boldsymbol{\lambda}_{13}$ are feasible in exactly one of $\mathcal{F}_3^k,\ k \in [3]$. The feasibility of the dual solutions can be easily verified by using submodularity of the set function f and the conditions satisfied by the specific submodular subpolytopes $\mathcal{F}_3^k,\ k \in [3]$ (Lemma 10).

Table 3: Feasible dual solutions of the linear program in (2)

For $\mathcal{F}_3$:	
	$\boldsymbol{\lambda}_1 = (0, f(1), f(2), f(3)),$
For $\mathcal{F}_3^1$:	
	$\boldsymbol{\lambda}_2 = (f(2) - f(2\|3), f(1) - f(2) + f(2\|3), f(2\|3), f(3\|2)),$
	$\boldsymbol{\lambda}_3 = (f(1) - f(1\|3), f(1\|3), f(2\|3), f(3\|1)),$
	$\boldsymbol{\lambda}_4 = (f(2) - f(2\|1), f(1\|2), f(2\|1), f(3\|2)),$
	$\boldsymbol{\lambda}_5 = (f(2,3) - f(3\|1) - f(2\|1), f(2\|1) + f(1,3) - f(2,3), f(2\|1), f(3\|1)),$
For $\mathcal{F}_3^2$:	
	$\boldsymbol{\lambda}_6 = (f(1) - f(1\|3), f(1\|3), f(2) - f(1) + f(1\|3), f(3\|1)),$
	$\boldsymbol{\lambda}_7 = (f(2) - f(2\|3), f(1\|3), f(2\|3), f(3\|2)),$
	$\boldsymbol{\lambda}_8 = (f(2) - f(2\|1), f(1\|2), f(2\|1), f(3\|1)),$
	$\boldsymbol{\lambda}_9 = (f(1,3) - f(1\|2) - f(3\|2), f(1\|2), f(1\|2) + f(2,3) - f(1,3), f(3\|2)),$
For $\mathcal{F}_3^3$:	
	$\boldsymbol{\lambda}_{10} = (f(1) - f(1\|2), f(1\|2), f(2\|1), f(3) - f(2) + f(2\|1)),$
	$\boldsymbol{\lambda}_{11} = (f(2) - f(2\|3), f(1\|2), f(2\|3), f(3\|2)),$
	$\boldsymbol{\lambda}_{12} = (f(3) - f(3\|1), f(1\|3), f(2\|1), f(3\|1)),$
	$\boldsymbol{\lambda}_{13} = (f(1,2) - f(1\|3) - f(2\|3), f(1\|3), f(2\|3), f(2\|3) + f(1,3) - f(1,2)),$
For $\mathcal{F}_3$:	
	$\boldsymbol{\lambda}_{14} = (f(1,2) + f(1,3) + f(2,3) - 2, 1 - f(2,3), 1 - f(1,3), 1 - f(1,2)),$

Lemma 13 *For any monotone submodular set function $f : 2^{[3]} \to \mathbb{R}_+$ and any $\boldsymbol{x} \in [0,1]^3$, the concave closure can be written as*

$$f^+(\boldsymbol{x}) = \sum_{k=1}^{3} \mathbb{1}_{f \in \mathcal{S}_3^k} \left[\min \left(\min_{i \in \{4k-2, 4k-1, 4k, 4k+1\}} \left(\lambda_{i0} + \sum_{j=1}^{3} \lambda_{ij} x_j \right), \zeta \right) \right]. \tag{4}$$

where $\mathbb{1}$ is the indicator function, $\mathcal{S}_3^k = \mathbb{1}_{f \in \mathcal{F}_3^k \setminus \bigcup_{j<k} \mathcal{F}_3^j}$, $k \in [3]$, $\zeta = \min_{\ell = 1,14} \left(\lambda_{\ell 0} + \sum_{j=1}^{3} \lambda_{\ell j} x_j \right)$ and the λ values are obtained from the dual feasible solutions in Table 3.

Proof The proof of optimality follows by constructing for each dual solution in Table 3 (feasible for a specific submodular subpolytope), a corresponding primal distribution (feasible in a particular region of the probability space) that attains the same objective value as the dual solution. Table 4 shows the optimal regions $R_j,\ j \in [14]$ of the probability space $[0,1]^3$ and the polytope of submodular functions for each dual solution. For each $\mathcal{F}_3^k,\ k \in [3]$, there are four probability regions that neatly partition the space $\boldsymbol{x} : 1 < x_1 + x_2 + x_3 < 2$ (although the partitioning regions change with k). Along with the small and large probability regions R_1 and R_{14} (which are valid for any $f \in \mathcal{F}_3$), the entire probability space $[0,1]^3$ is partitioned. We note that, since the marginal probabilities are not ordered, it is possible that $x_1 + x_2 > 1$ and $x_1 + x_3 \leq 1$ (region R_4) and correspondingly $x_1 + x_2 > 1,\ x_2 + x_3 \leq 1$ in R_8 and $x_1 + x_3 > 1,\ x_2 + x_3 \leq 1$ in R_{12}. We will prove the result for $f \in \mathcal{F}_3^1$ and the proof for $f \in \mathcal{F}_3^2, \mathcal{F}_3^3$ follows from symmetry. For $f \in \mathcal{F}_3^1$, using the dual feasible solution $\boldsymbol{\lambda_2}$, we can rewrite the objective of the dual linear program in (2) as $\overline{f_2}^+(\boldsymbol{x}) = \lambda_{20} + \sum_{j=1}^{3} \lambda_{2j} x_j = f(\{1\})x_1 + f(\{2\})(1 - x_1 - x_3) + f(\{3\})(1 - x_1 - x_2) + f(\{2,3\})(x_1 + x_2 + x_3 - 1)$ where $\overline{f_2}^+(\boldsymbol{x})$ is an upper bound on $f^+(\boldsymbol{x})$.

Table 4: Optimal regions of probability space and submodular subpolytope for each dual solution

Dual Solution	Optimal for $\boldsymbol{x}$ satisfying	Region of $\mathcal{F}_3$
$\boldsymbol{\lambda_1}$	$R_1 : x_1 + x_2 + x_3 \leq 1$	$\mathcal{F}_3$
$\boldsymbol{\lambda_2}$	$R_2 : 1 < x_1 + x_2 + x_3 < 2,\ x_1 + x_2 \leq 1,\ x_1 + x_3 \leq 1$	
$\boldsymbol{\lambda_3}$	$R_3 : 1 < x_1 + x_2 + x_3 < 2,\ x_1 + x_2 \leq 1,\ x_1 + x_3 > 1$	$\mathcal{F}_3^1$
$\boldsymbol{\lambda_4}$	$R_4 : 1 < x_1 + x_2 + x_3 < 2,\ x_1 + x_2 > 1,\ x_1 + x_3 \leq 1$	
$\boldsymbol{\lambda_5}$	$R_5 : 1 < x_1 + x_2 + x_3 < 2,\ x_1 + x_2 > 1,\ x_1 + x_3 > 1$	
$\boldsymbol{\lambda_6}$	$R_6 : 1 < x_1 + x_2 + x_3 < 2,\ x_1 + x_2 \leq 1,\ x_2 + x_3 \leq 1$	
$\boldsymbol{\lambda_7}$	$R_7 : 1 < x_1 + x_2 + x_3 < 2,\ x_1 + x_2 \leq 1,\ x_2 + x_3 > 1$	$\mathcal{F}_3^2$
$\boldsymbol{\lambda_8}$	$R_8 : 1 < x_1 + x_2 + x_3 < 2,\ x_1 + x_2 > 1,\ x_2 + x_3 \leq 1$	
$\boldsymbol{\lambda_9}$	$R_9 : 1 < x_1 + x_2 + x_3 < 2,\ x_1 + x_2 > 1,\ x_2 + x_3 > 1$	
$\boldsymbol{\lambda_{10}}$	$R_{10} : 1 < x_1 + x_2 + x_3 < 2,\ x_1 + x_3 \leq 1,\ x_2 + x_3 \leq 1$	
$\boldsymbol{\lambda_{11}}$	$R_{11} : 1 < x_1 + x_2 + x_3 < 2,\ x_1 + x_3 \leq 1,\ x_2 + x_3 > 1$	$\mathcal{F}_3^3$
$\boldsymbol{\lambda_{12}}$	$R_{12} : 1 < x_1 + x_2 + x_3 < 2,\ x_1 + x_3 > 1,\ x_2 + x_3 \leq 1$	
$\boldsymbol{\lambda_{13}}$	$R_{13} : 1 < x_1 + x_2 + x_3 < 2,\ x_1 + x_3 > 1,\ x_2 + x_3 > 1$	
$\boldsymbol{\lambda_{14}}$	$R_{14} : x_1 + x_2 + x_3 \geq 2$	$\mathcal{F}_3$

When $x_1 + x_2 \leq 1,\ x_1 + x_3 \leq 1,\ x_1 + x_2 + x_3 > 1$ (region R_2), it is possible to construct a feasible joint distribution of the primal linear progam in (2) supported on the sets $\{1\}, \{2\}, \{3\}, \{2, 3\}$ with probabilities $x_1, 1 - x_1 - x_3, 1 - x_1 - x_2$ and $x_1 + x_2 + x_3 - 1$ respectively. The primal objective attains the upper bound $\overline{f_2}^+(\boldsymbol{x})$ which is thus optimal. Similarly, for $\boldsymbol{\lambda_3}, \boldsymbol{\lambda_4}, \boldsymbol{\lambda_5}$, we can write:

$$\overline{f_3}^+(\boldsymbol{x}) = f(\{1\})(1 - x_3) + f(\{3\})(1 - x_1 - x_2) + f(\{1,3\})(x_1 + x_3 - 1) + f(\{2,3\})x_2,$$
$$\overline{f_4}^+(\boldsymbol{x}) = f(\{1\})(1 - x_2) + f(\{2\})(1 - x_1 - x_3) + f(\{1,2\})(x_1 + x_2 - 1) + f(\{2,3\})x_3,$$
$$\overline{f_5}^+(\boldsymbol{x}) = f(\{1\})(2 - x_1 - x_2 - x_3) + f(\{1,2\})(x_1 + x_2 - 1) + f(\{1,3\})(x_1 + x_3 - 1) + f(\{2,3\})(1 - x_1)$$

which are optimal for $\boldsymbol{x} \in R_3, R_4, R_5$ respectively. Further for $\boldsymbol{\lambda_1}$ and $\boldsymbol{\lambda_{14}}$, we have

$$\begin{aligned} \overline{f_1}^+(\boldsymbol{x}) &= f(\{1\})x_1 + f(\{2\})x_2 + f(\{3\})x_3 \\ \overline{f_{14}}^+(\boldsymbol{x}) &= f(\{1,2\})(1-x_3) + f(\{1,3\})(1-x_2) + f(\{2,3\})(1-x_1) \\ &\quad + f(\{1,2,3\})(x_1+x_2+x_3-2) \end{aligned}$$

which are optimal for $\boldsymbol{x} \in R_1, R_{14}$ respectively. Note that the regions $R_1, R_2, R_3, R_4, R_5, R_{14}$ partition the probability space $[0,1]^3$ and hence the result is proved for all $\boldsymbol{x} \in [0,1]^3$ and $f \in \mathcal{F}_3^1$ by considering the minimum over the corresponding six dual solutions. By symmetry, it is straightforward to establish the optimal solutions for $f \in \mathcal{F}_3^2$ and $f \in \mathcal{F}_3^3$ in the respective regions R_6 to R_9 and R_{10} to R_{13}, while the regions R_1 and R_{14} remain common to both. Note that the sets $\mathcal{S}_3^k = \mathbb{1}_{f \in \mathcal{F}_3^k \setminus \underset{j<k}{\cup} \mathcal{F}_3^j}$, $k \in [3]$ form a partition of the set $\mathcal{F}_3$ (unlike the subpolytopes $\mathcal{F}_3^k$ which have common functions). This ensures that the indicator function turns on exactly once for a given $f \in \mathcal{F}_3$ and chooses the corresponding minimum of dual solutions. Finally, we note that the closed-form expression for $f^+(\boldsymbol{x})$ in (4) can be extended to non-monotone submodular functions since the outlined dual feasible solutions in Table 3 do not depend on the monotonicity of f. ■

Corollary 14 *[Concavity] $f^+(\boldsymbol{x})$ (as derived in (4)) is concave in $\boldsymbol{x}$.*

Proof Concavity follows by noting that the for any $f \in \mathcal{F}_3$, the indicator function switches on for exactly one $k \in [3]$ and that the dual objective $\overline{f}^+(\boldsymbol{x})$ is linear in the marginal probability vector $\boldsymbol{x}$. Considering the minimum of six linear pieces must preserve concavity. ■

Lemma 15 *For any monotone submodular set function $f : 2^{[3]} \to \mathbb{R}_+$ and any $\boldsymbol{x} \in [0,1]^3$, the upper pairwise independent extension can be written as*

$$f^{++}(\boldsymbol{x}) = h(\boldsymbol{x}) + \max_{\omega \in \{\underline{\omega},\, \overline{\omega}\}} \left[(g_2 - g_1)\,\omega\right]. \tag{5}$$

where $\underline{\omega} = \max\left[(1-x_{k^\star})(1-x_{i^\star}-x_{j^\star}),\ 0\right]$, $\overline{\omega} = \min\left[\prod_{i=1}^{3} x_i + \prod_{i=1}^{3}(1-x_i),\ (1-x_{j^\star})(1-x_{k^\star})\right]$,

$x_{i^\star} \le x_{j^\star} \le x_{k^\star}$ *are the ordered marginal probabilities,*

$g_1 = 1 + f(1) + f(2) + f(3)$, $\quad g_2 = f(1,2) + f(1,3) + f(2,3)$ *and*

$$h(\boldsymbol{x}) = \sum_{i=1}^{3} x_i f(i) - \sum_{1 \le i < j \le 3} x_i x_j \left[f(i) + f(j) - f(i,j)\right] - (g_2 - g_1)\left[\prod_{i=1}^{3} x_i + \prod_{i=1}^{3}(1-x_i)\right]$$

Proof The proof follows by characterizing all pairwise independent joint distributions with $n = 3$ random variables (see Table 5) which can be derived by solving the system of 7 equations with 8 variables along with the non-negativity constraints from the primal linear program in (3).

Table 5: Pairwise independent distributions for $n = 3$.

S	$\theta^{++}(S)$
$\emptyset$	ω
$\{1\}$	$-\omega + (1 - x_2)(1 - x_3)$
$\{2\}$	$-\omega + (1 - x_1)(1 - x_3)$
$\{3\}$	$-\omega + (1 - x_1)(1 - x_2)$
$\{1, 2\}$	$\omega + (x_1 + x_2 - 1)(1 - x_3)$
$\{1, 3\}$	$\omega + (x_1 + x_3 - 1)(1 - x_2)$
$\{2, 3\}$	$\omega + (x_2 + x_3 - 1)(1 - x_1)$
$\{1, 2, 3\}$	$-\omega + \prod_{i=1}^{3} x_i + \prod_{i=1}^{3}(1 - x_i)$

We denote the free parameter by ω, where $\omega \in [0, 1]$ since from Table 5, ω defines the joint probability of not including any element in S. Using the fact that $0 \leq \theta^{++}(S) \leq 1$, we have $\underline{\omega}(\boldsymbol{x}) \leq \omega \leq \overline{\omega}(\boldsymbol{x})$, where

$$\underline{\omega}(\boldsymbol{x}) = \max\left[\max_{\{i,j,k\}\in[3],\, i\neq j\neq k}(1 - x_i)(1 - x_j - x_k),\ 0\right] = \max\left[(1 - x_{k^\star})(1 - x_{i^\star} - x_{j^\star}),\ 0\right],$$

$$\overline{\omega}(\boldsymbol{x}) = \min\left[\prod_{i=1}^{3} x_i + \prod_{i=1}^{3}(1 - x_i),\ \min_{1\leq i<j\leq 3}(1 - x_i)(1 - x_j)\right] = \min\left[\prod_{i=1}^{3} x_i + \prod_{i=1}^{3}(1 - x_i),\ (1 - x_{j^\star})(1 - x_{k^\star})\right].$$

For notational convenience, we drop the dependence on $\boldsymbol{x}$ and use $\underline{\omega}, \overline{\omega}$ henceforth. The exact value of ω chosen in the optimal distribution depends on the particular region of the probability space $[0, 1]^3$ and the set function considered. More specifically, if $g_1 \geq g_2$, we choose the lower bound $\underline{\omega}$ while, if $g_2 > g_1$, we choose a upper bound $\overline{\omega}$. For example if $x_i + x_j \geq 1$ for $(i, j) : 1 \leq i < j \leq 3$ and $g_1 \geq g_2$, the optimal ω would be chosen as zero, while if $x_i + x_j \leq 1$ for $(i, j) : 1 \leq i < j \leq 3$ and $g_2 > g_1$, the optimal ω would be chosen as $\prod_{i=1}^{3} x_i + \prod_{i=1}^{3}(1 - x_i)$. Note that the choice of ω ensures that at least one of the decision variables $\theta(S)$ is zero. The distributions in Table 5 can also be derived from Derriennic and Kłopotowski (2000) (Theorem 1) by considering $\mathbb{P}(\tilde{c}_i = 1) = x_i,\ i = 1, 2, 3$ instead of $\mathbb{P}(\tilde{c}_i = 0) = x_i$. Finally, we note that monotonicity and submodularity are sufficient but not necessary conditions to derive the closed-form expression for $f^{++}(\boldsymbol{x})$ and the result can be extended to arbitrary set functions. ■

Note that we can re-write the closed-form expression in (5) as

$$f^{++}(\boldsymbol{x}) = \sum_{k=1}^{2} \mathbb{1}_{f\in\mathcal{T}_3^k}\ \underline{f_k}^{++}(\boldsymbol{x}) = \max(\underline{f_1}^{++}(\boldsymbol{x}),\ \underline{f_2}^{++}(\boldsymbol{x})),$$

where $\mathcal{T}_3^k = \mathbb{1}_{f\in\mathcal{G}_3^k\setminus\bigcup_{j<k}\mathcal{G}_3^j}$, $k \in [2]$ form a partition of the set $\mathcal{F}_3$ and $\underline{f_1}^{++}(\boldsymbol{x}) = h(\boldsymbol{x}) + (g_2 - g_1)\,\underline{\omega}$, $\underline{f_2}^{++}(\boldsymbol{x}) = h(\boldsymbol{x}) + (g_2 - g_1)\,\overline{\omega}$ are valid lower bounds on $f^{++}(\boldsymbol{x})$. These bounds are generated from the two primal feasible distributions $\theta^{++}(S)$ with $\omega = \underline{\omega}$ (when $f \in \mathcal{T}_3^1$) and $\omega = \overline{\omega}$ (when $f \in \mathcal{T}_3^2$) respectively. We have intentionally cast the closed-form expression for $f^{++}(\boldsymbol{x})$ as the maximum of primal feasible solutions (unlike $f^{+}(\boldsymbol{x})$ in (4) which is expressed as minimum of dual feasible solutions), since, for our main result described in Theorem 19, it suffices to use lower bounds on $f^{++}(\boldsymbol{x})$. With the closed-forms for $f^{+}(\boldsymbol{x})$ and $f^{++}(\boldsymbol{x})$ for $n = 3$ now established, the following example highlights the challenges in computing them.

Example 2 *In this example, we consider $n = 3$ random inputs with fixed marginal probabilities $\boldsymbol{x} = (0.3, 0.4, 0.5)$ and 500 randomly generated instances of $f(1)$ and $f(2,3)$ (ensuring submodularity), while fixing all other function values at $f(\emptyset) = 0, f(3) = 0.974, f(2) = 0.029, f(1,3) = 1, f(1,2) = 0.055, f([3]) = 1$. This random variation of $f(1)$ and $f(2,3)$ generates each instance of f from exactly one of three subpolytopes $\mathcal{F}_3^k,\ k \in [3]$ that define $f^+(\boldsymbol{x})$ and exactly one of two subpolytopes $\mathcal{G}_3^k,\ k \in [2]$ that define $f^{++}(\boldsymbol{x})$. Figure 4*

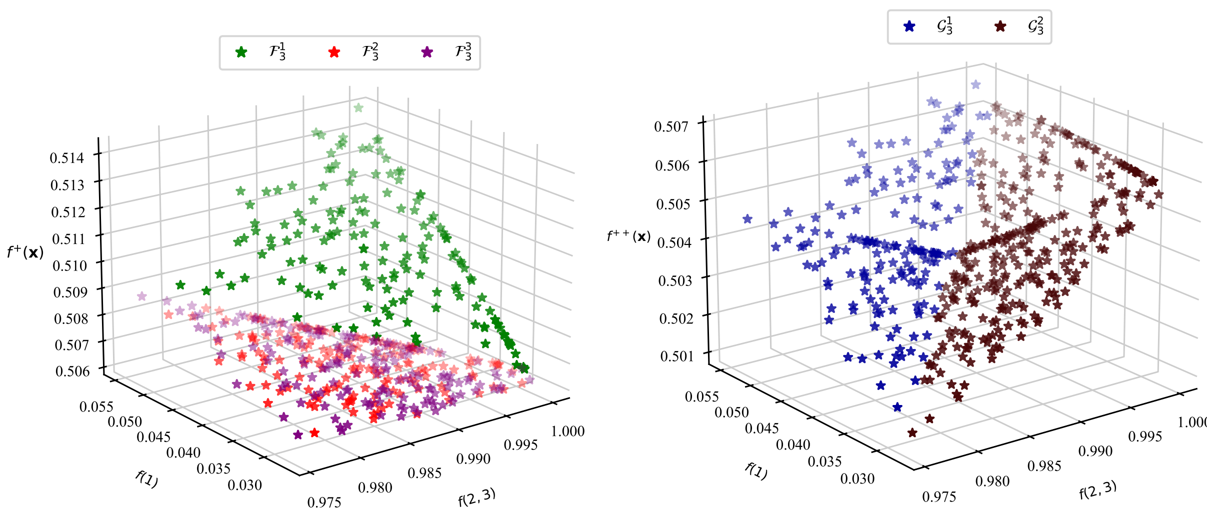

Figure 4: Scatter plots of $f^+(\boldsymbol{x})$ (left) and $f^{++}(\boldsymbol{x})$ (right) for $\boldsymbol{x} = (0.3, 0.4, 0.5)$.

demonstrates that the optimal distributions that attain $f^+(\boldsymbol{x})$ (left) and $f^{++}(\boldsymbol{x})$ (right) are not oblivious to changes in the function values. Even with fixed marginal probabilities, the optimal distributions change as f moves across subpolytopes, highlighting the challenge with $n = 3$, unlike $n = 2$, where there was no such change. Our proof technique overcomes this challenge by careful choices of $f^+(\boldsymbol{x})$ and $f^{++}(\boldsymbol{x})$ for a given probability region, ensuring that the distributions which attain them are oblivious to changes in f as long as the marginal probabilities are restricted to the concerned region.

3.6. Cylinder dependency for $n = 3$

We now highlight some insightful characteristics of the extremal distributions induced by $f^+(\boldsymbol{x})$ and $f^{++}(\boldsymbol{x})$. Note that since both $f^+(\boldsymbol{x})$ and $f^{++}(\boldsymbol{x})$ involve maximizing the expected value of $f(S)$, submodularity attempts to induce negative dependence to the maximum extent possible, depending on the chosen marginal probabilities. When computing $f^{++}(\boldsymbol{x})$, the pairwise independence constraints impose an addditional challenge by forcing the inputs to be uncorrelated. The extent of negative dependence induced can be captured through the notion of cylinder dependence. Negative cylinder dependence Pemantle (2000); Borcea et al. (2009) is a property which captures "perfect" negative dependence or negative dependence among every pair, triplet, quadruplet and so on of the random variables. It is formally defined as :

$$\mathbb{E}\Big[\prod_{i\,\in\,S}\tilde{c}_i\Big] \leq \prod_{i\in S}\mathbb{E}\,[\tilde{c}_i], \quad \forall S \subseteq [n]$$

$$\text{or} \qquad \mathbb{P}(\tilde{c}_i = 1, \forall i \in S) - \prod_{i\in S} x_i \leq 0, \quad \forall S \subseteq [n].$$

Corollary 16 *[Cylinder dependence for $f^+(\boldsymbol{x})$] For any $f \in \mathcal{F}_3$, when the marginal probabilities are small or large* i.e. $x_1 + x_2 + x_3 \leq 1$ *($\boldsymbol{x} \in R_1$) or $x_1 + x_2 + x_3 \geq 2$ ($\boldsymbol{x} \in R_{14}$), the optimal distribution induced by $f^+(\boldsymbol{x})$ exhibits negative cylinder dependency. Additionally, the triplet in the optimal distribution exhibits negative dependence for any $\boldsymbol{x} \in [0,1]^n$.*

Proof The proof can be found in Appendix A.5. ■

In fact, it can be shown that when $\boldsymbol{x} \in R_1$ or $\boldsymbol{x} \in R_{14}$, the optimal distribution admits a countermonotonic random vector (see Theorem 3.7 in Joe (1997)).

Corollary 17 *[Cylinder dependence for $f^{++}(\boldsymbol{x})$] For any $\boldsymbol{x} \in [0,1]^3$, the optimal distribution that attains $f^{++}(\boldsymbol{x})$ exhibits negative cylinder dependency when $f(1,2) + f(1,3) + f(2,3) \geq 1 + f(1) + f(2) + f(3)$ and positive cylinder dependency otherwise.*

Proof The proof can be found in Appendix A.6. ■

Remark 18 *Corollary 16 shows that while it is easy to induce negative cylinder dependency for small and large marginal probabilities ($\boldsymbol{x} \in R_1, R_{14}$), the situation is more complicated for the moderate range of probabilities ($\boldsymbol{x} \in R_1 - R_{14}$), where the optimal distributions are not oblivious to the chosen submodular function $f \in \mathcal{F}_3$. In these latter regions, it is not possible for every pair of inputs to be negatively correlated at optimality. When $f \in \mathcal{F}_3^1$, Table 6 shows the sign of correlation between pairs of random inputs induced by the optimal distribution corresponding to each region of the partitioned probability space.*

Table 6: Correlation sign table for the optimal distributions that attain $f^+(\boldsymbol{x})$ for $f \in \mathcal{F}_3^1$.

Region	(x_1, x_2)	(x_1, x_3)	(x_2, x_3)
R_1	$-$	$-$	$-$
R_2	$-$	$-$	$\pm$
R_3	$-$	$-$	$+$
R_4	$-$	$-$	$+$
R_5	$-$	$-$	$\pm$
R_{14}	$-$	$-$	$-$

For example, when $\boldsymbol{x} \in R_2$ and $f \in \mathcal{F}_3^1$, the optimal distribution is supported on the sets $\{1\}, \{2\}, \{3\}, \{2,3\}$ with probabilities $x_1, 1 - x_1 - x_3, 1 - x_1 - x_2$ and $x_1 + x_2 + x_3 - 1$ which implies that the pairs (x_1, x_2) and (x_1, x_3) are negatively correlated while (x_2, x_3) can be either positively or negatively correlated depending on whether $x_1 + x_2 + x_3 - 1 - x_2x_3 = x_1 - (1 - x_2)(1 - x_3)$ is non-negative or non-positive. The situation is further complicated *by the dependence of the optimal distribution on the subpolytope in which the considered submodular function lies. The interaction between the subpolytopes and moderate probability regions induces a variety of correlation structures in the optimal distributions and provides a glimpse into the increased challenges involved with $n = 3$ as compared to $n = 2$. Our solution approach takes this into account by designating unique feasible distributions for each region, ensuring that it is sufficient to prove the $4/3$ bound for the extreme points of the submodular subpolytopes.*

We are now ready to establish our main result for $n = 3$.

3.7. Main result with $n = 3$

Theorem 19 *For any monotone submodular function $f : 2^{[3]} \to \mathbb{R}_+$ and any $\boldsymbol{x} \in [0,1]^3$:*

$$f^+(\boldsymbol{x})/f^{++}(\boldsymbol{x}) \leq 4/3.$$

Proof It is sufficient to verify the inequality $4\underline{f}^{++}(\boldsymbol{x}) - 3f^+(\boldsymbol{x}) \geq 0$ for all $f \in \mathcal{F}_3$ and all $\boldsymbol{x} \in [0,1]^3$ where $\underline{f}^{++}(\boldsymbol{x})$ is a valid lower bound on $f^{++}(\boldsymbol{x})$. In other words, we show that

$$\min_{f \in \mathcal{F}_3} \min_{\boldsymbol{x} \in [0,1]^3} [4\underline{f}^{++}(\boldsymbol{x}) - 3f^+(\boldsymbol{x})] \geq 0$$

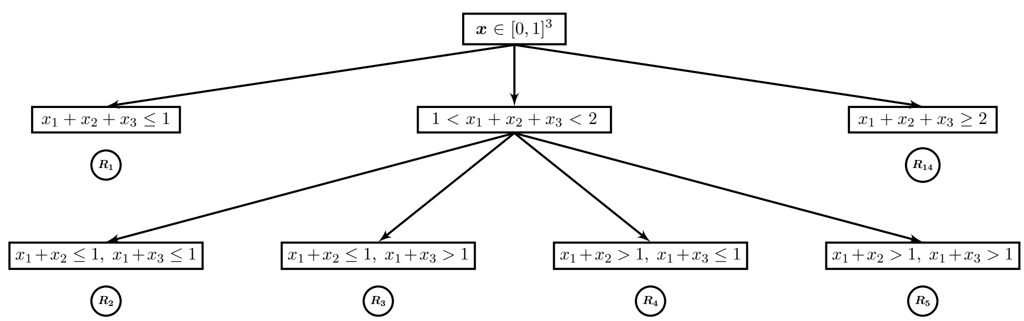

Figure 5: Partition of $[0,1]^3$ into $v = 6$ regions when $f \in \mathcal{F}_3^1$

We outline the main steps of the proof next:

1. For each $f \in \mathcal{F}_3^k,\ k \in [3]$, consider the six regions which partition the probability space $[0,1]^3$ from Table 4. These include the four regions exclusive to $\mathcal{F}_3^k$ and two common regions R_1, R_{14}. For example, Figure 5 shows the corresponding regions when $f \in \mathcal{F}_3^1$.

2. For each partitioning region, compute $f^+(\boldsymbol{x})$ from Lemma 13 by using the corresponding dual solutions from Table 4. Fix the lower bound $\underline{f_1}^{++}(\boldsymbol{x})$ for regions R_1, R_2, R_3, R_4 and $\underline{f_2}^{++}(\boldsymbol{x})$ for region R_{14}. For R_5, we further partition the region into two parts (see Appendix A.7) and fix one of the two lower bounds in each part. The key idea is that for all marginal probability vectors $\boldsymbol{x}$ in a given region, $f^+(\boldsymbol{x})$ and $\underline{f}^{++}(\boldsymbol{x})$ are expressed in terms of a single piece and not as the minimum or maximum of multiple linear pieces as seen in (4) and (5). This is critical to ensure that $4\underline{f}^{++}(\boldsymbol{x}) - 3f^+(\boldsymbol{x})$ is linear in the function values f (it would otherwise be convex in f) for a fixed $\boldsymbol{x}$, which in turn ensures that it suffices to consider extremal set functions alone.

3. Verify the inequality

$$\min_{f\in\mathcal{E}(\mathcal{F}_3^k)} \min_{\boldsymbol{x}\in[0,1]^3} [4\underline{f}^{++}(\boldsymbol{x}) - 3f^{+}(\boldsymbol{x})] \geq 0$$

region-wise for all six regions, where $\mathcal{E}(\mathcal{F}_3^k)$ is the set of extremal set functions of $\mathcal{F}_3^k$ (Lemma 10).

4. Repeat the earlier steps for each $k \in [3]$.

We next prove the result for $f \in \mathcal{F}_3^1$ for the low and high probability regions (R_1 and R_{14}) while the proof for the moderate probability regions (R_2, R_3, R_4 and R_5) can be found in the appendix. The proof for $f \in \mathcal{F}_3^2, \mathcal{F}_3^3$ follows by symmetry, and we do not include it in the paper. Notice that the first six extremal set functions $E_1 - E_6$ satisfy $g_1 = g_2$ and hence we have for all $\boldsymbol{x} \in [0,1]^3$ and for all $f \in \mathcal{E}(\mathcal{F}_3) \setminus \{E_7, E_8\}$,

$$\underline{f_1}^{++}(\boldsymbol{x}) = \underline{f_2}^{++}(\boldsymbol{x}) = f^{++}(\boldsymbol{x}) = \sum_{i=1}^{3} x_i f_i - \sum_{1\leq i<j\leq 3} x_i x_j \left[f(i) + f(j) - f(i,j)\right].$$

Consider $f \in \mathcal{F}_3^1$ and let $\delta = 4f^{++}(\boldsymbol{x}) - 3f^{+}(\boldsymbol{x})$. Recall from Lemma 10 that $\mathcal{F}_3^1$ has seven extremal set functions $E_1, E_2, E_3, E_4, E_5, E_7$ and E_8, at each of which, we verify that $\delta \geq 0$.

(a) Region R_1: Choose $\underline{f_1}^{++}(\boldsymbol{x}) = h(\boldsymbol{x}) + (g_2 - g_1)\underline{\omega}$ where $\underline{\omega} = (1 - x_{k^\star})(1 - x_{i^\star} - x_{j^\star})$, since $x_i + x_j \leq 1$ for $i \neq j$ in R_1. Using $\boldsymbol{\lambda}_1$, we obtain $f^{+}(\boldsymbol{x}) = x_1 f(1) + x_2 f(2) + x_3 f(3)$. For $E_1 = (0,1,0,0,1,1,0,1)$ we obtain $f^{+}(\boldsymbol{x}) = f^{++}(\boldsymbol{x}) = x_1$ and:

$$\delta = 4x_1 - 3x_1 = x_1 \geq 0$$

Similar computations for E_2 and E_3 give $\delta = x_2 \geq 0$ and $\delta = x_3 \geq 0$. For $E_4 = (0,1,1,0,1,1,1,1)$, we obtain:

$$\begin{aligned}\delta &= 4(x_1 + x_2 - x_1x_2) - 3(x_1 + x_2)\\ &= x_1 + x_2 - 4x_1x_2\\ &\geq 0 \text{ [using } I_1 \text{ since } x_1 + x_2 \leq 1 \text{ in } R_1 \text{ by setting } \alpha = x_1, \beta = x_2].\end{aligned}$$

Similar computation for E_5 gives $\delta = x_1 + x_3 - 4x_1x_3$ which is nonnegative since $x_1 + x_3 \leq 1$ in region R_1. For E_7, we have $g_1 = g_2 + 1$, $h(\boldsymbol{x}) = 1$, $\underline{f_1}^{++}(\boldsymbol{x}) = 1 - \underline{\omega}$, $f^{+}(\boldsymbol{x}) = \sum_{i=1}^{3} x_i$

$$\begin{aligned}\text{and}\quad \delta &= 4(1 - (1 - x_{k^\star})(1 - x_{i^\star} - x_{j^\star})) - 3(x_1 + x_2 + x_3)\\ &= x_1 + x_2 + x_3 - 4x_{k^\star}(x_{i^\star} + x_{j^\star})\\ &\geq 0 \text{ [using } I_1 \text{ since } x_1 + x_2 + x_3 \leq 1 \text{ in } R_1 \text{ by setting } \alpha = x_{i^\star} + x_{j^\star}, \beta = x_{k^\star}].\end{aligned}$$

For E_8, we have $g_2 = g_1 + 1/2,\ h(\boldsymbol{x}) = \sum_{i=1}^{3} x_i - \frac{1}{2}\big(1 + \sum_{1\le i<j\le 3} x_i x_j\big)$

$\underline{f_1}^{++}(\boldsymbol{x}) = \sum_{i=1}^{3} x_i - \frac{1}{2}\big(1 + \sum_{1\le i<j\le 3} x_i x_j - \underline{\omega}\big) = \frac{1}{2}\big(\sum_{i=1}^{3} x_i - x_{i^\star} x_{j^\star}\big),\ f^{+}(\boldsymbol{x}) = \frac{1}{2}\sum_{i=1}^{3} x_i$

$$\begin{aligned} \text{and} \quad \delta &= \tfrac{1}{2}\left[4\big(\sum_{i=1}^{3} x_i - x_{i^\star}x_{j^\star}\big) - 3\big(\sum_{i=1}^{3} x_i\big)\right] \\ &= \tfrac{1}{2}\left[(x_{i^\star} + x_{j^\star} - 4x_{i^\star}x_{j^\star}) + x_{k^\star}\right] \\ &\ge 0 \ [\text{ using } I_1 \text{ since } x_{i^\star} + x_{j^\star} \le 1 \text{ in } R_1 \text{ by setting } \alpha = x_{i^\star}, \beta = x_{j^\star}]. \end{aligned}$$

(b) Region R_{14}: Choose $\underline{f_2}^{++}(\boldsymbol{x}) = h(\boldsymbol{x}) + (g_2 - g_1)\overline{\omega}$ where $\overline{\omega} = (1 - x_{j^\star})(1 - x_{k^\star})$ since $x_i + x_j \ge 1$ for $i \ne j$ in R_{14}. Using $\boldsymbol{\lambda}_{14}$, we obtain $f^{+}(\boldsymbol{x}) = x_1 + x_2 + x_3 - 2 + (1 - x_3)f(1,2) + (1 - x_2)f(1,3) + (1 - x_1)f(2,3)$. For $E_1 = (0,1,0,0,1,1,0,1)$, we obtain $f^{+}(\boldsymbol{x}) = f^{++}(\boldsymbol{x}) = x_1$ and:

$$\delta = 4x_1 - 3x_1 = x_1 \ge 0$$

Similarly, for E_2 and E_3, we have $\delta = x_2$ and $\delta = x_3$ which are nonnegative. For $E_4 = (0,1,1,0,1,1,1,1)$, we have $f^{+}(\boldsymbol{x}) = 1$, $f^{++}(\boldsymbol{x}) = x_1 + x_2 - x_1 x_2$ and thus:

$$\begin{aligned} \delta &= 4(x_1 + x_2 - x_1 x_2) - 3 \\ &\ge 0 \ [\text{using } I_2 \text{ since } x_1 + x_2 > 1 \text{ in } R_{14} \text{ by setting } \alpha = x_1, \beta = x_2]. \end{aligned}$$

Similar computations for E_5 gives $\delta = 4x_1 + 4x_3 - 4x_1x_3 - 3$ which is nonnegative since $x_1 + x_3 > 1$ in region R_{14}. For E_7, we have $\underline{f_2}^{++}(\boldsymbol{x}) = 1 - \overline{\omega},\ f^{+}(\boldsymbol{x}) = 1$ and

$$\begin{aligned} \delta &= 4(x_{i^\star} + x_{j^\star} - x_{i^\star}x_{j^\star}) - 3 \\ &\ge 0 \ [\text{using } I_2 \text{ since } x_{i^\star} + x_{j^\star} \ge 1 \text{ in } R_{14} \text{ by setting } \alpha = x_{i^\star}, \beta = x_{j^\star}]. \end{aligned}$$

Finally, for E_8, we have $\underline{f_2}^{++}(\boldsymbol{x}) = \sum_{i=1}^{3} x_i - \frac{1}{2}\big(1 + \sum_{1\le i<j\le 3} x_i x_j - \overline{\omega}\big),\ f^{+}(\boldsymbol{x}) = 1$ and

$$\begin{aligned} \delta &= 4\Big[\sum_{i=1}^{3} x_i - \tfrac{1}{2}\big(1 + \sum_{1\le i<j\le 3} x_i x_j - \overline{\omega}\big)\Big] - 3 \\ &= 4\big[x_{i^\star} + \tfrac{1}{2}(x_{j^\star} + x_{k^\star}) - x_{i^\star}\tfrac{1}{2}(x_{j^\star} + x_{k^\star})\big] - 3 \\ &\ge 0 \quad [\text{using } I_2 \text{ since } x_{i^\star} + \tfrac{1}{2}(x_{j^\star} + x_{k^\star}) \ge 1 \text{ in } R_{14} \text{ by setting } \alpha = x_{i^\star}, \beta = \tfrac{1}{2}(x_{j^\star} + x_{k^\star})] \end{aligned}$$

Hence, $\delta \ge 0$ for all $f \in \mathcal{F}_3^1$ and marginal probabilities defined by regions R_1 and R_{14}. The proof for the remaining four regions $R_2 - R_5$ is more involved and can be found in Appendix A.7.

■

Remark 20 *For $n = 3$, consider the function $f(S) = \min(|S|, 1)$ with marginal probabilities $\boldsymbol{x} = (1/3, 1/3, 1/3)$. Here $f^{+}(\boldsymbol{x}) = 1$ and $F(\boldsymbol{x}) = 19/27$ which gives $f^{+}(\boldsymbol{x})/F(\boldsymbol{x}) = 27/19 \approx 1.421$. Theorem 19 shows in contrast, the ratio $f^{+}(\boldsymbol{x})/f^{++}(\boldsymbol{x})$ can never be larger than $4/3 \approx 1.333$ for all functions $f \in \mathcal{F}_3$. This illustrates that even for $f \in \mathcal{F}_3$, the upper pairwise independent bound is closer to the concave closure than the multilinear extension.*

The next lemma shows an immediate extension of the results for $n = 2, 3$ to sums of monotone submodular functions defined on disjoint ground sets of size at most three.

Corollary 21 *Let $f = f_1 + \ldots + f_m : 2^{[n_1 + \ldots + n_m]} \to \mathbb{R}_+$, where the set functions f_i are monotone submodular functions defined on disjoint ground sets of size $n_i \leq 3$. Then $f^+(\boldsymbol{x})/f^{++}(\boldsymbol{x}) \leq 4/3$ for all $\boldsymbol{x} \in [0,1]^n$.*

Proof The proof can be found in Appendix A.8. ■

4. Upper bound for general n, small $\boldsymbol{x}$

Our technique of analysis for general n is based on a recent construction of two pairwise independent distributions in Ramachandra and Natarajan (2023), that were shown to be optimal (by attaining $f^{++}(\boldsymbol{x})$) for the submodular functions $f(S) = \min(|S|, 1)$ and $f(S) = \min\big(\big|[n] \setminus S\big|, 1\big)$, as stated in Lemmas 22 and 23. The focus of this section is to show that these distributions suffice to prove a 4/3 upper bound for all functions in $\mathcal{F}_n$ when the marginal probabilities are small and large.

Lemma 22 *[Ramachandra and Natarajan (2023)] For any $\boldsymbol{x} \in [0,1]^n$, sort the values as $0 \leq x_1 \leq \ldots \leq x_n \leq 1$. Suppose $\sum_{i=1}^{n-1} x_i \leq 1$. Then there always exists a pairwise independent distribution with the marginal probability vector $\boldsymbol{x}$ of the form shown in Table 7 (left). Specifically, the joint probabilities are given by: (a) $\theta(\emptyset) = (1 - \sum_{i=1}^{n-1} x_i)(1 - x_n)$, (b) $\theta(i) = x_i(1 - x_n)$ for all $i < n$, (c) $\theta(S) = 0$ for all other S with $n \notin S$, and (d) $\theta(S) \geq 0$ for all $S \ni n$ such that $\sum_{S:n \in S} \theta(S) = x_n$, $\sum_{S:i,n \in S} \theta(S) = x_i x_n$ for $i < n$, $\sum_{S:i,j,n \in S} \theta(S) = x_i x_j$ for all $i < j < n$.*

Lemma 23 *[Ramachandra and Natarajan (2023)] Suppose $\sum_{i=2}^{n} x_i \geq n - 2$. Then there always exists a pairwise independent distribution with the marginal probability vector $\boldsymbol{x}$ of the form shown in Table 7 (right). Specifically, the joint probabilities are given by: (a) $\theta([n]) = x_1 \left(\sum_{i=2}^{n} x_i - (n-2)\right)$, (b) $\theta([n] \setminus \{i\}) = x_1(1 - x_i)$ for all $i > 1$, (c) $\theta(S) = 0$ for all other S with $1 \in S$, and (d) $\theta(S) \geq 0$ for all $1 \notin S$ such that $\sum_{S:1 \notin S} \theta(S) = 1 - x_1$, $\sum_{S:1,i \notin S} \theta(S) = (1 - x_1)(1 - x_i)$ for $i > 1$, $\sum_{S:1,i,j \notin S} \theta(S) = (1 - x_i)(1 - x_j)$ for all $1 < i < j$.*

This brings us to the main results of this section.

Theorem 24 *For any monotone submodular function $f : 2^{[n]} \to \mathbb{R}_+$ and any $\boldsymbol{x} \in [0,1]^n$ where $0 \leq x_1 \leq \ldots \leq x_n \leq 1$, we have $f^+(\boldsymbol{x})/f^{++}(\boldsymbol{x}) \leq 4/3$ under the assumption that*

i) $\sum_{i=1}^{n-1} x_i \leq 1$ and $x_n \leq 1/4$ (small probabilities)

ii) $\sum_{i=2}^{n} x_i \geq n - 2$ and $x_1 \geq 3/4$ (large probabilities)

Proof For small probabilities (i), to compute the lower bound on $f^{++}(\boldsymbol{x})$, we use the pairwise independent distribution provided in Lemma 22. This distribution is feasible when $\sum_{i=1}^{n-1} x_i \leq 1$ and was shown to be optimal in Ramachandra and Natarajan (2023) for the set function $f(S) = \min(|S|, 1)$. Despite the non-optimality of this distribution for arbitrary

Table 7: Pairwise independent distributions with $\sum_{i=1}^{n-1} x_i \le 1$ (left) and $\sum_{i=2}^{n} x_i \ge n-2$ (right).

S	$\theta(S)$	S	$\theta(S)$
$\emptyset$	$\left(1-\sum_{i=1}^{n-1} x_i\right)(1-x_n)$	$[n]$	$x_1\left(\sum_{i=2}^{n} x_i-(n-2)\right)$
$\{1\}$	$x_1(1-x_n)$	$[n]\setminus\{2\}$	$x_1(1-x_2)$
$\{2\}$	$x_2(1-x_n)$	$[n]\setminus\{3\}$	$x_1(1-x_3)$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$\{n-1\}$	$x_{n-1}(1-x_n)$	$[n]\setminus\{n\}$	$x_1(1-x_n)$
All other S with $n \notin S$	0	All other S with $1 \in S$	0
All S with $n \in S$	$\theta(S)$	All S with $1 \notin S$	$\theta(S)$

set functions, it is sufficient to prove our result. For general functions $f \in \mathcal{F}_n$, from the non-decreasing property of f, we have $f(S) \ge f(n)$ for all $S \ni n$. This implies that:

$$f^{++}(\boldsymbol{x}) \ge \underline{f}^{++}(\boldsymbol{x}) = \sum_{i=1}^{n-1} x_i(1-x_n)f(i) + x_n f(n).$$

For the upper bound, we use the dual feasible solution $\lambda_0 = 0$ and $\lambda_i = f(i)$ for all $i \in [n]$. This is feasible for the dual linear program in (2) for all functions $f \in \mathcal{F}_n$ and gives:

$$f^{+}(\boldsymbol{x}) \le \overline{f}^{+}(\boldsymbol{x}) = \sum_{i=1}^{n} x_i f(i).$$

Together we get

$$\begin{aligned}
\delta &= 4\underline{f}^{++}(\boldsymbol{x}) - 3\overline{f}^{+}(\boldsymbol{x}) \\
&= 4\sum_{i=1}^{n-1} x_i(1-x_n)f(i) + 4x_n f(n) - 3\sum_{i=1}^{n} x_i f(i) \\
&= \sum_{i=1}^{n-1} x_i(1-4x_n)f(i) + x_n f(n) \\
&\ge 0 \quad [\text{since } x_n \le 1/4].
\end{aligned} \tag{6}$$

Next, for the large probabilities case (ii), generate $\underline{f}^{++}(\boldsymbol{x})$ from the distribution in Lemma 23 as

$$\underline{f}^{++}(\boldsymbol{x}) = \sum_{i=2}^{n} x_1(1-x_i)f([n]\setminus\{i\}).$$

where we ignore the part of the distribution with $1 \notin S$ in Table 7 (right) since $f(S) \ge f(\emptyset) = 0$ for all $S : 1 \notin S$ (from the non-decreasing property of f). For the upper bound, we use the dual feasible solution $\lambda_0 = \sum_{i=1}^n f([n]\setminus\{i\}) - (n-1)$ and $\lambda_i = 1 - f([n]\setminus\{i\})$ for all $i \in [n]$. This is dual feasible for the linear program in (2) for all functions $f \in \mathcal{F}_n$ since

$$\begin{aligned}
\textstyle\sum_{i\in S}\lambda_i + \lambda_0 &= \textstyle\sum_{i\in S}\ [1 - f([n]\setminus\{i\})] + [\sum_{i=1}^n f([n]\setminus\{i\}) - (n-1)] \\
&= |S| - \textstyle\sum_{i\in S} f([n]\setminus\{i\}) + \left[\sum_{i\in S\cup S^c} f([n]\setminus\{i\}) - (n-1)\right] \quad \text{[where } S^c = [n]\setminus S] \\
&= \textstyle\sum_{i\in S^c} f([n]\setminus\{i\}) + [|S| - (n-1)]] \\
&\geq [f(S) + |S^c| - 1] + [|S| - (n-1)] \quad \text{[using submodularity of f].} \\
&= f(S) \ \ \forall S \subseteq [n].
\end{aligned}$$

The upper bound can be derived as:

$$\overline{f}^+(\boldsymbol{x}) = \sum_{i=1}^n (1-x_i) f([n]\setminus\{i\}) + \left[\sum_{i=1}^n x_i - (n-1)\right].$$

Together we get

$$\begin{aligned}
\delta &= 4\underline{f}^{++}(\boldsymbol{x}) - 3\overline{f}^+(\boldsymbol{x}) \\
&= 4\left[\sum_{i=2}^n x_1(1-x_i) f([n]\setminus\{i\}) + x_1\left(\sum_{i=2}^n x_i - (n-2)\right)\right] \\
&\quad -3\left[\sum_{i=1}^n (1-x_i) f([n]\setminus\{i\}) + \sum_{i=1}^n x_i - (n-1)\right] \\
&= 4\left[\sum_{i=2}^n x_1(1-x_i) f([n]\setminus\{i\}) + x_1\left(\sum_{i=2}^n x_i - (n-2)\right)\right] \\
&\quad -3\left[\sum_{i=2}^n (1-x_i) f([n]\setminus\{i\}) + \left(\sum_{i=2}^n x_i - (n-2)\right) - (1-x_1)(1 - f([n]\setminus\{1\}))\right] \\
&\geq (4x_1 - 3)\left[\sum_{i=2}^n (1-x_i) f([n]\setminus\{i\}) + \left(\sum_{i=2}^n x_i - (n-2)\right)\right] \quad \text{[since } 0 \leq f([n]\setminus\{1\}) \leq 1]. \\
&\geq 0 \quad \text{[since } \sum_{i=2}^n x_i \geq n-2 \text{ and } x_1 \geq 3/4].
\end{aligned}$$

■

Remark 25 *For the function $f(S) = \min(|S|, 1)$ and $\boldsymbol{x} = (1/n, \ldots, 1/n)$, the correlation gap $f^+(\boldsymbol{x})/F(\boldsymbol{x}) \uparrow e/(e-1)$ as $n \uparrow \infty$. Theorem 24 shows that in the regime of small and large marginal probabilities, for any value of n, the maximum value of the ratio $f^+(\boldsymbol{x})/f^{++}(\boldsymbol{x})$ is provably smaller for arbitrary $f \in \mathcal{F}_n$.*

Remark 26 *We note that the dual solutions used to compute $\overline{f}^{+}(\boldsymbol{x})$ for both cases in the proof of Theorem 24 are feasible for all $f \in \mathcal{F}_n$. This advantage is lost in the moderate probability regions where these two upper bounds are no longer sufficient to prove the bound. Hence, there is a need to look at subpolytopes of $\mathcal{F}_n$ (where better bounds can be obtained), which leads to complications with several subcases (as was observed even in the $n = 3$ case). The challenge in computing $\overline{f}^{+}(\boldsymbol{x})$ for the general n case with moderate probabilities is reflective of earlier results that countermotonic random vectors for $n \geq 3$ can exist if and only if the marginal probabilities are small or large (see Theorem 3.7 in Joe (1997)). Consequently, extending the results in Theorem 24 to the moderate probability regions appears to be non-trivial, even with identical marginal probabilities.*

The next two extensions for general n explore cases where it is possible to do away with the $x_n \leq 1/4$ condition in Theorem 24, specifically, when the marginal probabilities are in the n-simplex and are identical respectively.

Corollary 27 (n-simplex) *Assume $\boldsymbol{x} \in [0,1]^n : \sum_{i=1}^{n} x_i \leq 1$ where $0 \leq x_1 \leq \ldots \leq x_n \leq 1$. Then $f^{+}(\boldsymbol{x})/f^{++}(\boldsymbol{x}) \leq 4/3$ under the assumption that $f : 2^{[n]} \to \mathbb{R}_+$ is a monotone submodular function that satisfies:*

i) $f(n) = \max_{i \in [n]} f(i)$

ii) $f(i) = f_u$, $\forall i \in [n]$ *where* f_u *is a constant*

Corollary 28 (Identical probabilities) *Assume $x_i = x \in [0,1]$ for all $i \in [n]$ where $x \leq 1/(n-1)$ or $x \geq (n-2)/(n-1)$. Then $f^{+}(\boldsymbol{x})/f^{++}(\boldsymbol{x}) \leq 4/3$ for any monotone submodular function $f : 2^{[n]} \to \mathbb{R}_+$.*

Proof The proofs can be found in Appendix A.9. ∎

5. Upper bound for rank functions of k-uniform matroids

This section shows that a further tightening of the $4/3$ bound is possible when structured submodular functions are considered for any n with unrestricted identical marginal probabilities. Functions of the form $f(S) = \min(|S|, k)$ are rank functions of k-uniform matroids and have been studied in the context of mechanism design (see Yan (2011)), where it has been shown that the bound on the correlation gap is asymptotically $1/\left(1 - \frac{1}{\sqrt{2\pi k}}\right)$, which is tight with identical probabilities $\boldsymbol{x} = (k/n, \ldots, k/n)$ as $n \uparrow \infty$. With identical pairwise independent random inputs, Theorem 29 shows that this bound can be further improved to $4k/(4k-1)$ for any n and $k \in [n]$.

Theorem 29 *Consider the submodular set function $f(S) = \min(|S|, k)$ where $k \in [n]$. Assume $x_i = x$ for all $i \in [n]$. Then $f^{+}(\boldsymbol{x})/f^{++}(\boldsymbol{x}) \leq 4k/(4k-1)$ for any $x \in [0,1]$ and any $k \in [n]$. Further, this bound is attained when $k = n/2$ (n even) and $x = 1/2$.*

Proof With identical marginal probabilities, both $f^+(\boldsymbol{x})$ and $f^{++}(\boldsymbol{x})$ can be exactly computed as described next. We first note that the submodular function $f(S) = \min(|S|, k)$ can be re-written as $\min(|S|, k) = |S| - (|S| - k)^+$ for any $S \subseteq [n]$ and $k \in [n]$, where $z^+ = \max(z, 0)$ is the positive part of a real number and $(|S| - k)^+$ is a supermodular function. Hence, we have:

$$\max_{\theta} \mathbb{E}_{\theta}\big[\min(|S|, k)\big] = \sum_{i=1}^{n} x_i - \min_{\theta} \mathbb{E}_{\theta}\big[(|S| - k)^+\big], \quad \forall k \in [n].$$

The tight lower bound on $\mathbb{E}\big[(|S| - k)^+\big]$ with univariate marginal information and pairwise independence can be computed in closed form as $(np - k)^+$ and $\max((np - k)^+,$ $p\,[(np - k) + (1 - p)])$ respectively (see Theorem 15 and Corollary 3 in Ramachandra (2021)). Note that the univariate bound corresponds to the Jensen's bound while the pairwise independent bound involves an additional term $p\,[(np - k) + (1 - p)]$ which is tight when $(n - 1)p \leq k \leq 1 + (n - 1)p$. It suffices to prove the result for this interval since the ratio $f^+(\boldsymbol{x})/f^{++}(\boldsymbol{x})$ will be trivially one everywhere else. In this interval, we have $f^+(\boldsymbol{x}) = np - (np - k)^+ = \min(np, k)$ while $f^{++}(\boldsymbol{x}) = np - p\,[(np - k) + (1 - p)] = p\,[(n - 1)(1 - p) + k]$. Since the univariate bound depends on np, the proof follows by further splitting the interval $[(n - 1)p,\ 1 + (n - 1)p]$ for k into two sub intervals on either side of np. For convenience, we denote the intervals in terms of p rather than k.

i) $(k - 1)/(n - 1) \leq p \leq k/n$: In this case we have $f^+(\boldsymbol{x}) = np$ and hence:

$$\begin{aligned} f^+(\boldsymbol{x})/f^{++}(\boldsymbol{x}) &= \frac{np}{p\,[(n - 1)(1 - p) + k]} \\ &\leq \frac{n}{(n - 1)(1 - k/n) + k} \\ &= \frac{n^2}{n(n - 1) + k} \\ &= \frac{1}{1 - [(n - k)/n^2]} \\ &\leq \frac{4k}{4k - 1} \end{aligned}$$

where the second inequality follows from $p \leq k/n$ and the last equality follows from the fact that $(n - k)/n^2$ is maximized at $n = 2k$.

ii) $k/n \leq p \leq k/(n-1)$: In this case we have $f^+(\boldsymbol{x}) = k$ and hence:

$$\begin{aligned} f^+(\boldsymbol{x})/f^{++}(\boldsymbol{x}) &= \frac{k}{[(n-1+k)p-(n-1)p^2]} \\ &\leq \frac{k}{\min\limits_{p \in \left\{\frac{k}{n}, \frac{k}{(n-1)}\right\}} [(n-1+k)p-(n-1)p^2]} \\ &= \frac{k}{[(n-1+k)(k/n)-(n-1)(k/n)^2]} \\ &= \frac{1}{1-[(n-k)/n^2]} \\ &\leq \frac{4k}{4k-1} \end{aligned}$$

where the second inequality follows from the fact that the expression in the denominator, $g(p) = (n-1+k)p-(n-1)p^2$ is concave in p and thus minimized at one of the end-points of the interval $\left[\frac{k}{n}, \frac{k}{(n-1)}\right]$, while the third inequality follows from $p = k/n$ being the minimizer of $g(p)$. The last inequality follows due to the same reason as in the previous case.

It is clear that in both the above cases the bound of $4k/(4k-1)$ is attained when the number of random inputs n is even, $k = n/2$ and $x = 1/2$. ■

Remark 30 *We note that the $4k/(4k-1)$ strictly improves on the $4/3$ bound for $k \geq 2$ and retrieves the results in Ramachandra and Natarajan (2023) for $k = 1$. Compared to the results in Corollary 28, by restricting the submodular functions to rank functions of uniform matroids, we gain on two fronts: first, the conditions on the identical probability can be completely relaxed to $x \in [0,1]$ and more importantly, the $4/3$ bound can be tightened.*

6. Conclusions, extensions and a conjecture

In this paper, we provided a new definition of correlation gap for set functions with pairwise independent random inputs and proved a 4/3 upper bound in several cases for monotone submodular set functions. They key takeaway from this paper is that despite the NP-hardness of computing $f^+(\boldsymbol{x})$ and $f^{++}(\boldsymbol{x})$, it is possible to characterize improved upper bounds on their ratio (as compared to exisiting bounds with mutual independence) in several cases by a careful choice of dual feasible solutions for $f^+(\boldsymbol{x})$ and primal feasible distributions for $f^{++}(\boldsymbol{x})$. Specifically, the results in this paper in conjunction with Ramachandra and Natarajan (2023) show that the bound of 4/3 holds in the following cases: (a) for $f(S) = \min(|S|, 1)$ for all n and all $\boldsymbol{x} \in [0,1]^n$, (b) $n = 3$ for all $f \in \mathcal{F}_n$ and all $\boldsymbol{x} \in [0,1]^n$, (c) for small and large marginal probabilities $\boldsymbol{x}$ for all n and all $f \in \mathcal{F}_n$. With rank functions of k-uniform matroids, improved bounds of $4k/(4k-1)$ can be obtained for all n, any $k \in [2, n]$ and for all identical probabilities $x \in [0,1]$. The proof technique for the $n = 3$ case tackled the challenge of general probabilities and arbitrary set functions by explicitly partitioning the probability space into regions and dividing the polytope of submodular functions into subpolytopes, designating unique feasible distributions for each region and subpolytope and finally proving the bound for extreme points of the submodular subpolytope. Along the way, we highlighted the importance and non-triviality of the $n = 3$ case by deriving closed-form expressions for the optimal expected values and analyzing cylinder dependence properties of the optimal distributions. For the general n case, it was sufficient to consider two existing feasible pairwise independent distributions to prove the result for sufficiently small and large probabilities and any arbitrary set function. Applications of our results in distributionally robust optimization and mechanism design were demonstrated.

The results in this paper can be immediately extended beyond pairwise independence to correlated Bernoulli random inputs (where some or all of the inputs could be positively correlated, negatively correlated or uncorrelated) which would induce a larger class of distributions in the ambiguity set used for computing $f^{++}(\boldsymbol{x})$. As a result of this relaxation, $f^{++}(\boldsymbol{x})$ would increase while $f^{+}(\boldsymbol{x})$ remains unchanged and the ratio can only decrease further, retaining the $4/3$ or $4k/(4k-1)$ upper bounds. Despite the limitations of the proof techniques and results in this paper, we believe they open the door to understanding the behavior of submodular set functions with random inputs subjected to weaker notions of independence, which has hitherto been largely unexplored. Specifically, this brings us to the following conjecture:

Conjecture 31 *For any $n \geq 2$, any $\boldsymbol{x} \in [0,1]^n$ and any monotone submodular function $f : 2^{[n]} \to \mathbb{R}_+$ the pairwise independent correlation gap satisfies $f^{+}(\boldsymbol{x})/f^{++}(\boldsymbol{x}) \leq 4/3$.*

Appendix A. Appendix

A.1. Example of unbounded correlation gap with non-monotone or non-submodular functions

Let $n = 2$ and $(f(\emptyset), f(1), f(2), f(1,2)) = (0, \eta, 0, 0)$ and $(x_1, x_2) = (\epsilon, 1-\epsilon)$. For any $\eta > 0$, this function is non-monotone submodular where $f^{+}(\boldsymbol{x}) = \eta\epsilon$ and $F(\boldsymbol{x}) = \eta\epsilon^2$. As $\epsilon \downarrow 0$, $f^{+}(\boldsymbol{x})/F(\boldsymbol{x}) \uparrow \infty$ Rubinstein and Singla (2017). Let $(f(\emptyset), f(1), f(2), f(1,2)) = (0, 0, 0, \eta)$ and $(x_1, x_2) = (\epsilon, \epsilon)$. For any $\eta > 0$, this function is monotone but not submodular where $f^{+}(\boldsymbol{x}) = \eta\epsilon$ and $F(\boldsymbol{x}) = \eta\epsilon^2$. As $\epsilon \downarrow 0$, $f^{+}(\boldsymbol{x})/F(\boldsymbol{x}) \uparrow \infty$.

A.2. Bound on $f^{++}(\boldsymbol{x})/F(\boldsymbol{x})$

For monotone submodular functions, we have $1 \leq f^{++}(\boldsymbol{x})/F(\boldsymbol{x}) \leq f^{+}(\boldsymbol{x})/F(\boldsymbol{x}) \leq e/(e-1)$. We construct an example where the ratio $f^{++}(\boldsymbol{x})/F(\boldsymbol{x})$ can be as large as $f^{+}(\boldsymbol{x})/F(\boldsymbol{x})$ and equal $e/(e-1)$. Let $f(S) = \min(|S|, 1)$ with $\boldsymbol{x} = (1/n, \ldots, 1/n)$. The value $f^{+}(\boldsymbol{x}) = 1$ is attained by the distribution supported on n points where $\theta(i) = 1/n$ for all $i \in [n]$ (all other probabilities are zero). Furthermore $F(\boldsymbol{x}) = 1 - (1 - 1/n)^n$. Now consider a distribution supported on $n + 2$ points where $\theta(\emptyset) = 1/n - 1/n^2$, $\theta(i) = 1/n - 1/n^2$ for all $i \in [n]$ and $\theta([n]) = 1/n^2$. It is easy to see this distribution is pairwise independent and the marginal probabilities are given by $\boldsymbol{x} = (1/n, \ldots, 1/n)$. Hence, $f^{++}(\boldsymbol{x}) \geq 1 - 1/n + 1/n^2$ Ramachandra and Natarajan (2023). As $n \uparrow \infty$, we get $f^{++}(\boldsymbol{x})/F(\boldsymbol{x}) \geq e/(e-1)$ and hence the bound is attained.

A.3. Proof of Lemma 10

The polytope $\mathcal{F}_2$ is given by the values of the vector $(f(\emptyset), f(1), f(2), f(1,2))$ satisfying the following linear constraints:

$$f(1) + f(2) \geq 1, 0 \leq f(1) \leq 1, 0 \leq f(2) \leq 1, f(\emptyset) = 0, f(1,2) = 1.$$

The polytope $\mathcal{F}_3$ is given by the values of the vector $(f(\emptyset),\ f(1),\ f(2),\ f(3),\ f(1,2),\ f(1,3),\ f(2,3),\ f(1,2,3))$ satisfying the following linear constraints:

$$\begin{aligned}
&f(1) + f(2) \geq f(1,2), f(1) + f(3) \geq f(1,3), f(2) + f(3) \geq f(2,3),\\
&f(1,2) + f(1,3) \geq f(1) + 1, f(1,2) + f(2,3) \geq f(2) + 1,\\
&f(1,3) + f(2,3) \geq f(3) + 1, f(1) \leq f(1,2), f(2) \leq f(1,2),\\
&f(1) \leq f(1,3), f(3) \leq f(1,3), f(2) \leq f(2,3), f(3) \leq f(2,3),\\
&f(1,2) \leq 1, f(1,3) \leq 1, f(2,3) \leq 1, f(1) \geq 0, f(2) \geq 0, f(3) \geq 0,\\
&f(\emptyset) = 0, f(1,2,3) = 1.
\end{aligned}$$

One can find all the extreme points of the polytope $\mathcal{F}_n$ by solving for every set of 2^n linearly independent active constraints. If the corresponding solution satisfies the remaining linear constraints describing $\mathcal{F}_n$, it is an extreme point of the polytope. For $n = 2$ and 3 it is easy to do this by enumeration. In practice this can also be verified by using the open-source software *polymake* Assarf et al. (2017) which finds all the extreme points. For the subpolytopes $\mathcal{F}_3^1$, $\mathcal{F}_3^2$ and $\mathcal{F}_3^3$, we simply add new inequalities to the set $\mathcal{F}_3$. It can be verified that the extreme points of these subpolytopes exclude E_6, E_5 and E_4 (respectively) from $\mathcal{E}(\mathcal{F}_3)$.

A.4. Proofs of inequalities

Inequality I_1 holds for values of α and β satisfying $1 \geq \alpha, \beta \geq 0$ and $\alpha + \beta \leq 1$ since:

$$\alpha + \beta - 4\alpha\beta = \underbrace{(1 - \alpha - \beta)}_{\geq 0}\underbrace{(\alpha + \beta)}_{\geq 0} + (\alpha - \beta)^2 \geq 0.$$

Inequality I_2 holds for values of α and β satisfying $1 \geq \alpha, \beta \geq 0$ and $\alpha + \beta \geq 1$ since:

$$4\alpha + 4\beta - 4\alpha\beta - 3 = \underbrace{(3 - \alpha - \beta)}_{\geq 0}\underbrace{(\alpha + \beta - 1)}_{\geq 0} + (\alpha - \beta)^2 \geq 0.$$

A.5. Proof of Corollary 16

For $n = 3$, we only need to verify the property for all pairs and the single triplet. Table 8 shows the optimal distributions that attain $f^+(\boldsymbol{x})$ for $\boldsymbol{x} \in R_1, R_{14}$.

Table 8: Optimal distributions that attain $f^+(\boldsymbol{x})$ for $\boldsymbol{x} \in R_1, R_{14}$.

S	$\theta_1^+(S)$	$\theta_{14}^+(S)$
$\emptyset$	$1-(x_1+x_2+x_3)$	0
$\{1\}$	x_1	0
$\{2\}$	x_2	0
$\{3\}$	x_3	0
$\{1,2\}$	0	$1-x_3$
$\{1,3\}$	0	$1-x_2$
$\{2,3\}$	0	$1-x_1$
$\{1,2,3\}$	0	$x_1+x_2+x_3-2$

For $x_1+x_2+x_3 \leq 1$, we have from $\theta_1^+(S)$

$$\begin{aligned}
\mathbb{P}(\tilde{c}_i=1,\tilde{c}_j=1)-\mathbb{P}(\tilde{c}_i=1,)\mathbb{P}(\tilde{c}_j=1) &= 0-x_ix_j \quad \text{for } 1\leq i<j\leq 3\\
&\leq 0\\
\text{and}\quad \mathbb{P}(\tilde{c}_1=1,\tilde{c}_2=1,\tilde{c}_3=1)-\prod_{i=1}^{3}\mathbb{P}(\tilde{c}_i=1) &= 0-x_1x_2x_3\\
&\leq 0
\end{aligned}$$

which in fact exhibits perfect negative dependence. For $x_1+x_2+x_3\geq 2$, we have from $\theta_{14}^+(S)$

$$\begin{aligned}
\mathbb{P}(\tilde{c}_i=1,\tilde{c}_j=1)-\mathbb{P}(\tilde{c}_i=1,)\mathbb{P}(\tilde{c}_j=1) &= [(1-x_k)+(x_1+x_2+x_3-2)]-x_ix_j\\
&\qquad [\text{where } k\neq i,j \text{ for } 1\leq i<j\leq 3]\\
&= x_i+x_j-1-x_ix_j\\
&= -(1-x_i)(1-x_j)\\
&\leq 0
\end{aligned}$$

and

$$\begin{aligned}
\mathbb{P}(\tilde{c}_1=1,\tilde{c}_2=1,\tilde{c}_3=1)-\prod_{i=1}^{3}\mathbb{P}(\tilde{c}_i=1) &= (x_1+x_2+x_3-2)-x_1x_2x_3\\
&= (x_1+x_2-1-x_1x_2)+(x_3+x_1x_2-1-x_1x_2x_3)\\
&= -(1-x_1)(1-x_2)-(1-x_3)(1-x_1x_2)\\
&\leq 0
\end{aligned}$$

and hence negative cylinder dependency is established for both regions R_1 and R_{14}. Finally, it is straightforward to see that for all other regions R_2-R_{13}, the triplet in the optimal distributions that attain $f^+(\boldsymbol{x})$ exhibits perfect negative dependence since $\mathbb{P}(\tilde{c}_1=1,\tilde{c}_2=1,\tilde{c}_3=1)=0$ in these regions.

A.6. Proof of Corollary 17

The proof follows from Lemma 15 by plugging in $\underline{\omega}$ or $\overline{\omega}$ depending on whether $g_1\geq g_2$ or $g_2>g_1$. Note that since the distribution in Table 5 satisfies pairwise independence, we only need to check dependency for the triplet. When $g_1 \geq g_2$, we have

$$\begin{aligned}
\mathbb{P}(\tilde{c}_1 = 1, \tilde{c}_2 = 1, \tilde{c}_3 = 1) \\
- \prod_{i=1}^{3} \mathbb{P}(\tilde{c}_i = 1) &= \prod_{i=1}^{3}(1 - x_i) - \overline{\omega} \\
&= \begin{cases} -x_1 x_2 x_3, & \text{if } \overline{\omega} = \prod_{i=1}^{3} x_i + \prod_{i=1}^{3}(1 - x_i) \\ -x_{k^\star}(1 - x_{i^\star})(1 - x_{j^\star}), & \text{if } \overline{\omega} = (1 - x_{i^\star})(1 - x_{j^\star}) \end{cases} \\
&\leq 0
\end{aligned}$$

Similarly, when $g_2 > g_1$, we have

$$\begin{aligned}
\mathbb{P}(\tilde{c}_1 = 1, \tilde{c}_2 = 1, \tilde{c}_3 = 1) \\
- \prod_{i=1}^{3} \mathbb{P}(\tilde{c}_i = 1) &= \prod_{i=1}^{3}(1 - x_i) - \underline{\omega} \\
&= \begin{cases} \prod_{i=1}^{3}(1 - x_i), & \text{if } \underline{\omega} = 0 \\ x_{j^\star} x_{k^\star}(1 - x_{i^\star}), & \text{if } \underline{\omega} = (1 - x_{i^\star})(1 - x_{j^\star} - x_{k^\star}) \end{cases} \\
&\geq 0
\end{aligned}$$

A.7. Completing the proof of Theorem 19

We complete the proof for $f \in \mathcal{F}_3^1$ in the regions R_2, R_3, R_4 and R_5 (moderate probabilities) by proving the inequality one by one for the extremal submodular functions in $\mathcal{E}(\mathcal{F}_3^k)$ while ensuring that the choice of $f^+(\boldsymbol{x})$ and $\underline{f_1}^{++}(\boldsymbol{x})$ remains fixed for each region. For $E_1 = (0, 1, 0, 0, 1, 1, 0, 1)$, each of the dual solutions $\boldsymbol{\lambda}_i,\ i = 2, 3, 4, 5$ gives $f^+(\boldsymbol{x}) = x_1$ while $f^{++}(\boldsymbol{x}) = x_1$ and we have $\delta = 4x_1 - 3x_1 = x_1 \geq 0$. Similar computations for E_2 and E_3 give $\delta = x_2 \geq 0$ and $\delta = x_3 \geq 0$. For $E_4 = (0, 1, 1, 0, 1, 1, 1, 1)$, we get $f^+(\boldsymbol{x}) = \min(x_1 + x_2, 1)$ while $f^{++}(\boldsymbol{x}) = x_1 + x_2 - x_1 x_2$ and thus we have for R_2, R_3

$$\begin{aligned}
\delta &= 4(x_1 + x_2 - x_1 x_2) - 3(x_1 + x_2) \\
&= x_1 + x_2 - 4x_1 x_2 \\
&\geq 0 \text{ [using } I_1 \text{ since } x_1 + x_2 \leq 1 \text{ in } R_2, R_3].
\end{aligned}$$

while for R_4, R_5

$$\begin{aligned}
\delta &= 4(x_1 + x_2 - x_1 x_2) - 3 \\
&\geq 0 \text{ [using } I_2 \text{ since } x_1 + x_2 > 1 \text{ in } R_4, R_5].
\end{aligned}$$

Similar computations for E_5 gives $\delta = x_1 + x_3 - 4x_1 x_3 \geq 0$ in regions R_2, R_4 and $\delta = 4(x_1 + x_3 - x_1 x_3) - 3 \geq 0$ in regions R_3, R_5.

For E_7, each of the dual solutions $\boldsymbol{\lambda}_i,\ i = 2, 3, 4, 5$ gives $f^+(\boldsymbol{x}) = 1$. Partition R_5 into two regions $R_{51} = \{\boldsymbol{x} \in R_5 : x_2 + x_3 \leq 1\},\ R_{52} = \{\boldsymbol{x} \in R_5 : x_2 + x_3 > 1\}$. For regions R_2, R_3, R_4 and R_{51}, choose $\underline{f_1}^{++}(\boldsymbol{x}) = h(\boldsymbol{x}) + (g_2 - g_1)\underline{\omega} = 1 - \underline{\omega}$ where $\underline{\omega} = (1 - x_{k^\star})(1 - x_{i^\star} - x_{j^\star})$

(since there is at least one pair of random inputs whose marginal probabilities add up to at most one) and thus

$$\begin{aligned}\delta &= 4(1-(1-x_{k^\star})(1-x_{i^\star}-x_{j^\star}))-3\\&= 4(x_1+x_2+x_3-x_{k^\star}(x_{i^\star}+x_{j^\star}))-3\\&\geq 0 \text{ [using } I_2 \text{ since } x_1+x_2+x_3>1 \text{ in } R_2,R_3,R_4,R_{51} \text{ by setting } \alpha=x_{k^\star},\beta=x_{i^\star}+x_{j^\star}].\end{aligned}$$

For region R_{52}, choose $\underline{f_2}^{++}(\boldsymbol{x})=h(\boldsymbol{x})+(g_2-g_1)\overline{\omega}=1-\overline{\omega}$ where $\overline{\omega}=(1-x_{j^\star})(1-x_{k^\star})$ and

$$\begin{aligned}\delta &= 4(1-(1-x_{j^\star})(1-x_{k^\star}))-3\\&= 4(x_{j^\star}+x_{k^\star}-x_{j^\star}x_{k^\star})-3\\&\geq 0 \text{ [using } I_2 \text{ since } x_{j^\star}+x_{k^\star}>1 \text{ in } R_{52} \text{ by setting } \alpha=x_{j^\star},\beta=x_{k^\star}].\end{aligned}$$

For E_8, each of the dual solutions $\boldsymbol{\lambda}_i,\ i=2,3,4,5$ gives $f^+(\boldsymbol{x})=\frac{1}{2}\sum_{i=1}^{3}\ x_i$. For regions R_2,R_3,R_4 and R_{51}, choose $\underline{f_1}^{++}(\boldsymbol{x})=\sum_{i=1}^{3}x_i-\frac{1}{2}\big(1+\sum_{1\leq i<j\leq 3}x_ix_j-\underline{\omega}\big)=\frac{1}{2}\big(\sum_{i=1}^{3}x_i-x_{i^\star}x_{j^\star}\big)$ and thus

$$\begin{aligned}\delta &= \tfrac{1}{2}\left[4(\sum_{i=1}^{3}x_i-x_{i^\star}x_{j^\star})-3(\sum_{i=1}^{3}x_i)\right]\\&= \tfrac{1}{2}\left[(x_{i^\star}+x_{j^\star}-4x_{i^\star}x_{j^\star})+x_{k^\star}\right]\\&\geq 0 \text{ [using } I_1 \text{ since } x_{i^\star}+x_{j^\star}\leq 1 \text{ in } R_1,R_2,R_3,R_{51} \text{ by setting } \alpha=x_{i^\star},\beta=x_{j^\star}].\end{aligned}$$

For region R_{52}, choose $\underline{f_2}^{++}(\boldsymbol{x})=h(\boldsymbol{x})+(g_2-g_1)\overline{\omega}$ where $\overline{\omega}=(1-x_{j^\star})(1-x_{k^\star})$ and thus

$$\begin{aligned}\delta &= 4[\sum_{i=1}^{3}x_i-\tfrac{1}{2}\big(1+\sum_{1\leq i<j\leq 3}x_ix_j-\overline{\omega}\big)]-3\tfrac{1}{2}(\sum_{i=1}^{3}x_i)\\&= 4[x_{i^\star}+\tfrac{1}{2}(x_{j^\star}+x_{k^\star})-x_{i^\star}\tfrac{1}{2}(x_{j^\star}+x_{k^\star})]-3\tfrac{1}{2}(\sum_{i=1}^{3}x_i)\\&\geq 4[x_{i^\star}+\tfrac{1}{2}(x_{j^\star}+x_{k^\star})-x_{i^\star}\tfrac{1}{2}(x_{j^\star}+x_{k^\star})]-3 \quad [\text{ since } \sum_{i=1}^{3}x_i\leq 2 \text{ in } R_{52}]\\&\geq 0 \quad \text{[using } I_2 \text{ since } x_{i^\star}+\tfrac{1}{2}(x_{j^\star}+x_{k^\star})>1 \text{ in } R_{52} \text{ by setting } \alpha=x_{i^\star},\beta=\tfrac{1}{2}(x_{j^\star}+x_{k^\star})]\end{aligned}$$

This completes the proof for all $f\in\mathcal{F}_3^1$ and marginal probability vectors $\boldsymbol{x}\in[0,1]^3$. The proof for $f\in\mathcal{F}_3^2,\mathcal{F}_3^3$ follows by symmetry.

A.8. Proof of Corollary 21

Proof For each $i\in[m]$, $f_i^+(\boldsymbol{x}_i)=\max_{\theta_i\in\Theta_i}\mathbb{E}_{\theta_i}[f_i(S)]$ where Θ_i is the set of joint distributions of the random inputs with given marginal probability vector $\boldsymbol{x}_i$. To compute $f^+(\boldsymbol{x})$, we need to evaluate $\max_{\theta\in\Theta}\mathbb{E}_\theta[\sum_{i=1}^m f_i(S)]$ where Θ is the set of joint distributions of the entire random input with the given marginal probability vector $\boldsymbol{x}=(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_m)$. Note that since Θ is specified by the marginals of the partitioned distributions, the maximum values can be computed individually for each f_i and summed up. Hence:

$$f^+(\boldsymbol{x})=\sum_{i=1}^{m}\max_{\theta\in\Theta_i}\mathbb{E}_\theta[f_i(S)]=\sum_{i=1}^{m}f_i^+(\boldsymbol{x}_i).$$

Similarly, for the upper pairwise independent extension, we have $f^{++}(\boldsymbol{x}) = \sum_{i=1}^{m} f_i^{++}(\boldsymbol{x}_i)$. Furthermore, $f_i^{+}(\boldsymbol{x}_i)/f_i^{++}(\boldsymbol{x}_i) \leq 4/3$ for all $\boldsymbol{x}_i \in [0,1]^{n_i}$ and $n_i \leq 3$ from Lemma 12 and Theorem 19. Together this gives:

$$\frac{f^{+}(\boldsymbol{x})}{f^{++}(\boldsymbol{x})} = \frac{\sum_{i=1}^{m} f_i^{+}(\boldsymbol{x}_i)}{\sum_{i=1}^{m} f_i^{++}(\boldsymbol{x}_i)} \leq \frac{4}{3}.$$

■

A.9. Proofs of Corollaries 27 and 28

Proof The proof for Corollary 27 part (i) follows from (6) as follows:

$$\begin{aligned}
\delta &= \sum_{i=1}^{n-1} x_i(1-4x_n)f(i) + x_n f(n) \\
&= \sum_{i=1}^{n-1} x_i f(i) + x_n f(n) - 4x_n \sum_{i=1}^{n-1} x_i f(i) \\
&= \sum_{i=1}^{n-1} x_i f(i) + x_n f(n) - 4\frac{x_n f(n)}{f(n)} \sum_{i=1}^{n-1} x_i f(i) \\
&\geq 0
\end{aligned}$$

where the last equation follows by using a generalization of I_1 as follows:

$$(I_3) \qquad \alpha + \beta - 4\frac{\alpha\beta}{\gamma} \geq 0, \qquad \forall \alpha, \beta \in [0,1], \alpha + \beta \leq \gamma \leq 1 \qquad \text{[where } \gamma > 0 \text{ is a constant]}$$

and by setting $\alpha = \sum_{i=1}^{n-1} x_i f(i)$, $\beta = x_n f(n)$, $\gamma = f(n)$ which satisfies I_3 since $\alpha + \beta = \sum_{i=1}^{n} x_i f(i) \leq f(n) \sum_{i=1}^{n} x_i \leq f(n)$ by the conditions of case (i). For part (ii), the proof follows by:

$$\begin{aligned}
\delta &= \sum_{i=1}^{n-1} x_i f(i) + x_n f(n) - 4x_n \sum_{i=1}^{n-1} x_i f(i) \\
&= f_u \left(\sum_{i=1}^{n-1} x_i + x_n - 4x_n \sum_{i=1}^{n-1} x_i f(i) \right) \\
&\geq 0 \text{ [using } I_1 \text{ since } \textstyle\sum_{i=1}^{n} x_i \leq 1 \text{ and by setting } \alpha = \sum_{i=1}^{n-1} x_i, \beta = x_n].
\end{aligned}$$

Proof of Corollary 28: With identical probabilities $x_i = x$ for $i \in [n]$, the conditions in Theorem 24 reduce to $x \leq \min(1/4, 1/(n-1))$ and $x \geq \max(3/4, (n-2)/(n-1))$. We will next show that the $x \leq 1/4$ and $x \geq 3/4$ conditions are redundant. For $n \geq 5$, the result follows directly since $x \leq \min(1/4, 1/(n-1)) = 1/(n-1)$ and $x \geq \max(3/4, (n-2)/(n-1)) = (n-2)/(n-1)$. For $n = 2, 3$, the earlier results in Sections 3.4 and 3.7 subsume the identical marginal case and thus we only need to prove the result for $n = 4$ with $1/4 < x \leq 1/3$

Table 9: Feasible pairwise independent distributions for $n = 4$ wih $x \leq 1/3$ (left) and $x \geq 2/3$ (right)

S	$\theta(S)$	S	$\theta(S)$
$\emptyset$	$(1-3x)(1-x)$	$\emptyset$	$(1-x)^2$
$\{1\}$	$x(1-x)$	$[4] \setminus \{1\}$	$x(1-x)$
$\{2\}$	$x(1-x)$	$[4] \setminus \{2\}$	$x(1-x)$
$\{3\}$	$x(1-x)$	$[4] \setminus \{3\}$	$x(1-x)$
$\{4\}$	$x(1-x)$	$[4] \setminus \{4\}$	$x(1-x)$
$[4]$	x^2	$[4]$	$x(3x-2)$

and $2/3 \leq x < 3/4$. We can use the pairwise independent distributions from Table 7 to compute $\underline{f}^{++}(\boldsymbol{x})$ for $n = 4$. The difference here is that due to the identical nature of the marginal probabilities, it is easy to explicitly specify the distributions as shown in Table 9. We first prove the result for $x \in (1/4, 1/3]$. The (left) distribution in Table 9 gives the lower bound $\underline{f}^{++}(\boldsymbol{x}) = ax(1-x) + x^2$ where $a = \sum_{i=1}^{4} f(i)$. Next, to compute $\overline{f}^{+}(\boldsymbol{x})$, we consider the dual feasible solution $\lambda_0 = 0, \lambda_i = 1$ for $i \in [4]$. Along with the dual solution $\lambda_0 = 1, \lambda_i = 0$ for $i \in [4]$, we get an upper bound $\overline{f}^{+}(\boldsymbol{x}) = \min(ax, 1)$ and it is sufficient to verify the inequality

$$4\underline{f}^{++}(\boldsymbol{x}) - 3\overline{f}^{+}(\boldsymbol{x}) = 4ax(1-x) + 4x^2 - 3\min(ax, 1), \quad \forall x \in (1/4, 1/3]$$

$$\begin{aligned} &\text{When } ax \leq 1, \quad 4ax(1-x) + 4x^2 - 3ax = ax(1-4x) + 4x^2 \geq 1 - 4x + 4x^2 = (1-2x)^2 \geq 0 \\ &\text{When } ax > 1, \quad 4ax(1-x) + 4x^2 - 3 \geq 4(1-x) + 4x^2 - 3 = (1-2x)^2 \geq 0 \end{aligned}$$

where we used the fact that $1 - 4x < 0$ for the first inequality. When $x \in [2/3, 3/4)$. the (right) distribution in Table 9 gives the lower bound $\underline{f}^{++}(\boldsymbol{x}) = bx(1-x) + x(3x-2)$ where $b = \sum_{i=1}^{4} f([4] \setminus \{i\}) \geq 3$ (by submodularity). Next, we consider the dual feasible solution $\lambda_0 = \sum_{i=1}^{4} f([4] \setminus \{i\}) - 3$ and $\lambda_i = 1 - f([4] \setminus \{i\})$ for all $i \in [4]$ which gives $\overline{f}^{+}(\boldsymbol{x}) = (b-3) + (4-b)x$ and it is sufficient to verify the inequality

$$4\underline{f}^{++}(\boldsymbol{x}) - 3\overline{f}^{+}(\boldsymbol{x}) = 4[bx(1-x) + x(3x-2)] - 3[(b-3) + (4-b)x] \quad \forall x \in [2/3, 3/4).$$

$$\begin{aligned} &\text{When } b(1-x) \leq 3, \quad 4\underline{f}^{++}(\boldsymbol{x}) - 3\overline{f}^{+}(\boldsymbol{x}) = [b(1-x) - 3](4x-3) + 4x(3x-2) \geq 4x(3x-2) \geq 0 \\ &\qquad [\text{since} \quad 4x - 3 < 0 \text{ and } x \geq 2/3] \\ &\text{When } b(1-x) > 3, \quad 4\underline{f}^{++}(\boldsymbol{x}) - 3\overline{f}^{+}(\boldsymbol{x}) \geq 4[3x + x(3x-2)] - 3 \geq 4[3.(2/3) + 0] - 3 = 5 \\ &\qquad [\text{since} \quad (b-3) + (4-b)x \leq b - 3 + 4 - b = 1 \text{ and } x \geq 2/3] \end{aligned}$$

and the proof is completed. ■

References

S. Agrawal, Y. Ding, A. Saberi, and Y. Ye. Price of correlations in stochastic optimization. *Operations Research*, 1(60):150–162, 2012.

B. Assarf, E. Gawrilow, K. Herr, M. Joswig, B. Lorenz, A. Paffenholz, and T. Rehn. Computing convex hulls and counting integer points with `polymake`. *Mathematical Programming Computation*, 9(1):1–38, 2017.

F. Bach. Learning with submodular functions: A convex optimization perspective. *Foundations and Trends in Machine Learning*, 6(2-3):145–373, 2013.

S.N. Bernstein. *Theory of Probability.* Moscow-Leningrad, 1946.

D. Bertsimas, K. Natarajan, and C-P. Teo. Probabilistic combinatorial optimization: Moments, semidefinite programming, and asymptotic bounds. *SIAM Journal on Optimization*, 15(1):185–209, 2004.

J. Borcea, P. Branden, and T. M. Liggett. Negative dependence and the geometry of polynomials. *Journal of the American Mathematical Society*, 22(2):521–567, 2009.

G. Calinescu, C. Chekuri, M. Pál, and J. Vondrák. Maximizing a monotone submodular function subject to a matroid constraint. *Proceedings of the 12th IPCO Conference*, pages 182–196, 2007.

G. Calinescu, C. Chekuri, M. Pál, and J. Vondrák. Maximizing a monotone submodular function subject to a matroid constraint. *SIAM Journal on Computing*, 40(6):1740–1766, 2011.

S. Chawla, J. D. Hartline, D. L. Malec, and B. Sivan. Multi-parameter mechanism design and sequential posted pricing. In *Proceedings of the forty-second ACM symposium on Theory of computing*, pages 311–320, 2010.

C. Chekuri and V. Livanos. On submodular prophet inequalities and correlation gap. In *Proceedings of SAGT 2021*, 2021.

C. Chekuri, J. Vondrak, and R. Zenklusen. Submodular function maximization via the multilinear relaxation and contention resolution schemes. *SIAM Journal on Computing*, 43(6):1831–1879, 2014.

L. Chen, W. Ma, K. Natarajan, D. Simchi-Levi, and Z. Yan. Distributionally robust linear and discrete optimization with marginals. *Operations Research*, 70(3):1822–834, 2022.

Y. Derriennic and A. Kłopotowski. On Bernstein's example of three pairwise independent random variables. *Sankhyā: The Indian Journal of Statistics, Series A*, pages 318–330, 2000.

S. Dughmi. Submodular functions: Extensions, distributions, and algorithms. a survey, 2009.

M. Feldman, O. Svensson, and R. Zenklusen. Online contention resolution schemes with application to bayesian selection problems. *SIAM Journal on Computing*, 50(2):255–300, 2021.

S. Geisser and N. Mantel. Pairwise independence of jointly dependent variables. *The Annals of Mathematical Statistics*, 33(1):290–291, 1962.

H. Joe. *Multivariate Models and Multivariate Dependence Concepts.* CRC Press, 1997.

M. R. Karimi, M. Lucic, H. Hassani, and A. Krause. Stochastic submodular maximization: The case of coverage functions. In *31st Conference on Neural Information Processing Systems*, pages 6856–6866, 2017.

H. Karloff and Y. Mansour. On construction of k-wise independent random variables. In *Proceedings of the 26th Annual ACM Symposium on Theory of Computing*, pages 564–573, 1994.

K. Kashiwabara. Extremality of submodular functions. *Theoretical Computer Science*, 235: 239–256, 2000.

D. Koller and N. Meggido. Construcing small sample spaces satisfying given constraints. *SIAM Journal on Discrete Mathematics*, 7(2):260–274, 1994.

A. Krause and S. Jegelka. Submodularity in machine learning: New directions. *ICML Tutorial*, 2013.

M. Luby and A. Wigderson. Pairwise independence and derandomization. *Foundations and Trends in Theoretical Computer Science*, 1(4):239–201, 2005.

H-Y. Mak, Y. Rong, and J. Zhang. Appointment scheduling with limited distributional information. *Management Science*, 61:316–334, 2015.

I. Meilijson and A. Nádas. Convex majorization with an application to the length of critical paths. *Journal of Applied Probability*, 16(3):671–677, 1979.

K. Natarajan. *Optimization with Marginals and Moments.* Dynamic Ideas LLC, Belmont, Massachusetts, 2021.

R. Pemantle. Towards a theory of negative dependence. *Journal of Mathematical Physics*, 41:1371–1390, 2000.

A. Ramachandra. *Towards tightness with pairwise independence, extremal dependence and robust satisficing using linear and conic duality.* PhD thesis, National University of Singapore, scholar bank (10635/204937), 2021.

A. Ramachandra and K. Natarajan. Tight probability bounds with pairwise independence. *SIAM Journal on Discrete Mathematics*, 37(2):516–555, 2023.

J. Rosenmuller and H. G. Weidner. Extreme convex set functions with finite carrier: General theory. *Discrete Mathematics*, 10:384–382, 1974.

A. Rubinstein and S. Singla. Combinatorial prophet inequalities. In *Proceedings of 28th Annual ACM-SIAM Symposium on Discrete Algorithms*, pages 1671–1687, 2017.

E. Schneidman, M. J. Berry, R., and W. Bialek. Weak pairwise correlations imply strongly correlated network states in a neural population. *Nature*, (440):1007–1012, 2006.

L. S. Shapley. Core of convex games. *International Journal of Game Theory*, 1:11–26, 1971.

M. Staib, B. Wilder, and S. Jegelka. Distributionally robust submodular maximization. In *Proceedings of the 22nd International Conference on Artificial Intelligence and Statistics*, 2019.

D. M. Topkis. *Supermodularity and Complementarity*. Princeton University Press, Princeton, New Jersey, 1998.

A. Wigderson. The amazing power of pairwise independence (abstract). In *Proceedings of the Twenty-Sixth Annual ACM Symposium on Theory of Computing, Montréal, Québec, Canada*, pages 645–647, 1994.

Q. Yan. Mechanism design via correlation gap. In *Proceedings of the 22th ACM-SIAM SODA*, pages 710–719, 2011.