

**THE PAIRWISE INDEPENDENT CORRELATION GAP: AN EXACT WORST
CASE $4/3$ AT $n = 4$ OUTSIDE THE KNOWN REGIONS, AND A LOWER BOUND
 $416/311$ AT $n = 5$**

KOREA SUPERINTELLIGENCE LABS

ABSTRACT. For a nonnegative nondecreasing submodular set function f on n elements and a marginal vector $\mathbf{x} \in [0, 1]^n$, let $f^+(\mathbf{x})$ be the largest expectation of f over all distributions on subsets with marginals $\mathbf{x}$, and $f^{++}(\mathbf{x})$ the same maximum over pairwise independent distributions. Ramachandra and Natarajan conjectured that $f^+(\mathbf{x}) \leq \frac{4}{3} f^{++}(\mathbf{x})$ always; the bound is known for $n \leq 3$ and, by their work, for all n when the marginals are all small or all large, and in June 2026 they refuted it at $n = 5$ with a coverage function whose gap is at least $640/479$, leaving $n = 4$ open and asking for the tightest bound when $n \geq 5$. We prove that at $n = 4$ and $\mathbf{x}_0 = (\frac{1}{2}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6})$ – a marginal vector outside every region where the bound was known – the inequality $f^+(\mathbf{x}_0) \leq \frac{4}{3} f^{++}(\mathbf{x}_0)$ holds for every function in the class and is attained by $f(S) = \min(|S|, 1)$, so the worst-case gap there is exactly $4/3$. The proof is a two-part certificate: a modular majorant of f and one explicit pairwise independent distribution with a Farkas multiplier. At $n = 5$ we show that the counterexample function of Ramachandra and Natarajan, at the marginals $(\frac{9}{26}, \frac{5}{13}, \frac{5}{13}, \frac{7}{26}, \frac{7}{26})$, has $f^+ = 4$ and $f^{++} = 311/104$ exactly, so its gap is $416/311 > 640/479$; this improves their lower bound at $n = 5$, the only one we know of, and padding with zero marginals carries it to every $n \geq 5$. We also show that $f^{++} = 479/160$ exactly at their original instance. Every theorem is verified in Lean 4 with Mathlib, with all data in exact rational arithmetic. An exhaustive search over the combinatorial part of the $n = 4$ problem, reported separately from the formal development, finds no gap above $4/3$.

1. INTRODUCTION

1.1. The objects. Let $N = [n] = \{0, 1, \dots, n-1\}$ be a ground set. A set function $f: 2^N \rightarrow \mathbb{R}$ is *nonnegative* if $f(S) \geq 0$ for all S , *nondecreasing* if $f(S) \leq f(T)$ whenever $S \subseteq T$, and *submodular* if $f(S \cup T) + f(S \cap T) \leq f(S) + f(T)$ for all $S, T \subseteq N$. We write $\mathcal{C}_n$ for the class of set functions on $[n]$ with all three properties. Coverage functions $f_E(S) = |\bigcup_{i \in S} E_i|$, for any family $E = (E_i)_{i \in N}$ of finite sets, belong to $\mathcal{C}_n$.

For $\mathbf{x} \in [0, 1]^n$ let $\Theta(\mathbf{x})$ be the set of probability distributions θ on 2^N with marginals $\mathbf{x}$, i.e. $\sum_{S \ni i} \theta(S) = x_i$ for every $i \in N$, and let $\Pi(\mathbf{x}) \subseteq \Theta(\mathbf{x})$ be the *pairwise independent* ones, those with in addition $\sum_{S \ni \{i, j\}} \theta(S) = x_i x_j$ for all $i \neq j$. Writing $\mathbb{E}_\theta f = \sum_S \theta(S) f(S)$, the two quantities of interest are

$$(1) \quad f^+(\mathbf{x}) = \max_{\theta \in \Theta(\mathbf{x})} \mathbb{E}_\theta f, \quad f^{++}(\mathbf{x}) = \max_{\theta \in \Pi(\mathbf{x})} \mathbb{E}_\theta f.$$

The first is the concave closure of f ; the second was introduced by Ramachandra and Natarajan [2] as the *pairwise independent extension*. Both are values of linear programs over compact polytopes; the product distribution lies in $\Pi(\mathbf{x})$, so both maxima exist, and $f^{++}(\mathbf{x}) \leq f^+(\mathbf{x})$. The ratio $f^+(\mathbf{x})/f^{++}(\mathbf{x})$ is the *pairwise independent correlation gap*. It sits below the classical correlation gap of Agrawal, Ding, Saberi and Ye [4] and Calinescu, Chekuri, Pál and Vondrák [5], whose denominator is the expectation under the mutually independent distribution and which is at most $e/(e-1) \approx 1.582$ on $\mathcal{C}_n$.

1.2. The conjecture and its status. Ramachandra and Natarajan end [2] with the following conjecture, which we quote as it is restated in [1, Conjecture 1]:

For any n , any nonnegative monotone submodular function $f: 2^N \rightarrow \mathbb{R}_+$ and any $\mathbf{x} \in [0, 1]^n$:

$$\frac{f^+(\mathbf{x})}{f^{++}(\mathbf{x})} \leq \frac{4}{3}.$$

The published paper [2] proves the bound in two cases: for $n = 3$ and all $\mathbf{x} \in [0, 1]^3$ (its Theorem 5, sharp, attained by $f(S) = \min(|S|, 1)$ at $\mathbf{x} = (0, \frac{1}{2}, \frac{1}{2})$), and for every n when the sorted marginals $x_1 \leq \dots \leq x_n$ satisfy either $\sum_{i < n} x_i \leq 1$ and $x_n \leq \frac{1}{4}$ (small probabilities) or $\sum_{i \geq 2} x_i \geq n - 2$ and $x_1 \geq \frac{3}{4}$ (large probabilities) (its Theorem 8); its Lemma 6 extends the bound to sums of functions living on the blocks of a partition of N into blocks of size at most 3. The longer arXiv version [2, v2] contains in addition Corollary 27 (the bound on the simplex $\sum_i x_i \leq 1$ for functions whose singleton values $f(\{i\})$ are all equal, with the largest marginal attached to a maximal singleton), Corollary 28 (identical marginals $x_i = x$ with $x \leq \frac{1}{n-1}$ or $x \geq \frac{n-2}{n-1}$) and Theorem 29 (the sharper constant $4k/(4k-1)$ for the rank function $\min(|S|, k)$ of a k -uniform matroid with identical marginals). Statement numbers of [2] are those of the final e-print arXiv:2209.08563v3; those of [2, v2] are those of the v2 e-print.

In June 2026 the same authors refuted the conjecture at $n = 5$ [1]: for the coverage function of the five sets

$$(2) \quad E_0 = \{A, B\}, \quad E_1 = \{A, B, C, D\}, \quad E_2 = \{C, D\}, \quad E_3 = \{A, C\}, \quad E_4 = \{B, D\}$$

(numbered $E_1, \dots, E_5$ there) and the marginals $\mathbf{x}_5 = (\frac{3}{10}, \frac{7}{20}, \frac{3}{10}, \frac{7}{20}, \frac{7}{20})$ they exhibit a distribution showing $f^+(\mathbf{x}_5) = 4$ and a dual solution showing $f^{++}(\mathbf{x}_5) \leq \frac{479}{160}$, whence the gap is at least $640/479 > 4/3$. Their status table ([1, Table 3], caption “Validity of $4/3$ upper bound”) reads, verbatim up to the citation keys:

Dimension	True or False	References
$n = 2$	True	Lemma 4.10; [6]
$n = 3$	True	Theorem 5; [2]
$n = 4$	Unknown	Open
$n \geq 5$	False	Current work using AI

(Lemma 4.10 of [6], in the numbering of arXiv:1105.4593v5, is the inequality $F(b\mathbf{p}) \geq (1 - (1 - b/n)^n) f^+(\mathbf{p})$ for the multilinear extension F ; at $n = 2$ pairwise independence is independence, so $f^{++} = F$, and $b = 1$ gives the constant $\frac{3}{4}$.) Its closing remarks state ([1, Section 3]):

At this point, we have not been able to aided by these AI tools either prove or disprove the validity of the upper bound for $n = 4$ (see Table 3). This remains an open question. Another interesting question is to characterize the tightest upper bound for values of n when it is 5 and above for these classes of functions.

The counterexample was, by the authors’ account, produced by a frontier language model from a single prompt, and the same tool did not settle $n = 4$.

1.3. Results. Two questions are addressed. For $n = 4$ we settle the conjecture at one marginal vector, for the whole class $\mathcal{C}_4$, with the constant exact.

Theorem 1.1 (= Theorem 4.1). *Let $\mathbf{x}_0 = (\frac{1}{2}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6})$. For every $f \in \mathcal{C}_4$, $f^+(\mathbf{x}_0) \leq \frac{4}{3} f^{++}(\mathbf{x}_0)$. For $f(S) = \min(|S|, 1)$ one has $f^+(\mathbf{x}_0) = 1$ and $f^{++}(\mathbf{x}_0) = \frac{3}{4}$, so the constant $\frac{4}{3}$ cannot be lowered.*

Sorted, $\mathbf{x}_0 = (\frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{2})$ has largest coordinate $\frac{1}{2} > \frac{1}{4}$ and $\sum_{i \geq 2} x_i = \frac{5}{6} < 2$, so neither case of Theorem 8 of [2] applies; the marginals are not identical, so Corollary 28 of [2, v2] does not apply; and although $\mathbf{x}_0$ lies on the simplex $\sum_i x_i = 1$, Corollary 27 there covers only functions with equal singleton values, whereas Theorem 4.1 has no restriction on f beyond membership in $\mathcal{C}_4$. The proof is short and completely explicit: a modular majorant of f bounds $f^+(\mathbf{x}_0)$ by a linear form in the values $f(\{i\})$, and one pairwise independent distribution ν_0 at $\mathbf{x}_0$, with a nonnegative combination of nine monotonicity inequalities, bounds that linear form by $\frac{4}{3} \mathbb{E}_{\nu_0} f$.

For $n = 5$ we improve the lower bound.

Theorem 1.2 (= Theorem 5.1). *Let f be the coverage function of the sets (2), relabelled so that the full set comes first, $E' = (\{A, B, C, D\}, \{A, B\}, \{C, D\}, \{A, C\}, \{B, D\})$, and let $\mathbf{x}' = (\frac{9}{26}, \frac{5}{13}, \frac{5}{13}, \frac{7}{26}, \frac{7}{26})$. Then $f^+(\mathbf{x}') = 4$ and $f^{++}(\mathbf{x}') = \frac{311}{104}$, so $f^+(\mathbf{x}')/f^{++}(\mathbf{x}') = \frac{416}{311} > \frac{640}{479}$.*

Numerically $416/311 = 1.33762\dots$ against $640/479 = 1.33611\dots$ and $4/3 = 1.33333\dots$. The function is the one of [1]; only the marginals differ. We also verify that at the original marginals $\mathbf{x}_5$ the dual bound of [1] is tight, $f^{++}(\mathbf{x}_5) = \frac{479}{160}$ exactly (Theorem 3.1), so the improvement is not available at $\mathbf{x}_5$. Whether $416/311$ is the supremum at $n = 5$ is not settled: it was found by a search that is complete for distributions with at most four atoms (Section 6), and the search that would be complete for $n = 5$ was not run.

Section 6 reports computations that are not part of the formal development: an exhaustive sweep over the combinatorial part of the $n = 4$ problem, whose largest value is exactly $4/3$; a certificate scan over a grid of marginal vectors, which proves the $n = 4$ bound at 1815 of the 1820 points of the $\frac{1}{12}$ -grid; and exact certificates at three further marginal vectors. Section 7 describes the machine verification; the statements as checked are reproduced in Appendix A.

2. PRELIMINARIES

Throughout, $N = [n]$, and for $\theta: 2^N \rightarrow \mathbb{R}$ and a set function g we write $\mathbb{E}_\theta g = \sum_{S \subseteq N} \theta(S)g(S)$. All marginal vectors, distributions and dual certificates in this paper are rational; all inequalities are verified in exact rational arithmetic.

2.1. Two weak-duality facts. Every proof below rests on the following two observations, both immediate.

Lemma 2.1. *Let $m_0, m_1, \dots, m_{n-1} \in \mathbb{R}$ and $M(S) = m_0 + \sum_{i \in S} m_i$. If $f(S) \leq M(S)$ for all $S \subseteq N$, then $\mathbb{E}_\theta f \leq m_0 + \sum_i m_i x_i$ for every $\theta \in \Theta(\mathbf{x})$; in particular $f^+(\mathbf{x}) \leq m_0 + \sum_i m_i x_i$.*

Lemma 2.2. *Let $\lambda_0, \lambda_i, \lambda_{ij} \in \mathbb{R}$ ($i < j$) and $\lambda(S) = \lambda_0 + \sum_{i \in S} \lambda_i + \sum_{i < j, i, j \in S} \lambda_{ij}$. If $f(S) \leq \lambda(S)$ for all $S \subseteq N$, then $\mathbb{E}_\theta f \leq \lambda_0 + \sum_i \lambda_i x_i + \sum_{i < j} \lambda_{ij} x_i x_j$ for every $\theta \in \Pi(\mathbf{x})$; in particular $f^{++}(\mathbf{x})$ is at most this number.*

Proof of both. Since $\theta \geq 0$, $\mathbb{E}_\theta f \leq \mathbb{E}_\theta M$ (resp. $\mathbb{E}_\theta \lambda$), and the right-hand side collapses by linearity onto the constraints defining $\Theta(\mathbf{x})$ (resp. $\Pi(\mathbf{x})$): $\sum_S \theta(S) = 1$, $\sum_{S \ni i} \theta(S) = x_i$ and, for pairwise independent θ , $\sum_{S \ni i, j} \theta(S) = x_i x_j$. $\square$

Lemma 2.2 is the dual of the linear program defining f^{++} ([1, eq. (2)]); the dual solutions of [1] are of this quadratic form. Lower bounds on f^+ and f^{++} are obtained by exhibiting a distribution in $\Theta(\mathbf{x})$ or $\Pi(\mathbf{x})$; an exact value is a matching pair.

2.2. The subadditivity majorant. For submodular f the modular function built from the singleton values dominates f .

Lemma 2.3. *If f is submodular, then $f(S) \leq f(\emptyset) + \sum_{i \in S} (f(\{i\}) - f(\emptyset))$ for every $S \subseteq N$.*

Proof. Induction on $|S|$: for $a \notin S$, submodularity applied to $\{a\}$ and S gives $f(S \cup \{a\}) \leq f(S) + f(\{a\}) - f(\emptyset)$. $\square$

This is the majorant $m_\emptyset^1$ among the modular upper bounds $m_\emptyset^1, m_T^2$ written down by Iyer and Bilmes [8, Section 2.2] from two inequalities they attribute to Nemhauser, Wolsey and Fisher [7]; the other members of that family are used only in the computations of Section 6.

2.3. Conventions for the certificates. A distribution with k atoms is written as a list of pairs $S : c_S$ meaning $\theta(S) = c_S/D$ for a common denominator D stated once; sets are written by their elements, so 013 stands for $\{0, 1, 3\}$. A dual certificate of the quadratic form of Lemma 2.2 is given by its coefficients. In every case the pointwise inequalities $f(S) \leq \lambda(S)$ over all 2^n sets, the marginal identities and the pairwise identities are finite rational checks; in the formal development each is a single decision procedure call.

3. THE $n = 5$ INSTANCE OF RAMACHANDRA AND NATARAJAN, WITH BOTH VALUES EXACT

The following theorem is the counterexample of [1, Section 2], re-verified. The value $f^+(\mathbf{x}_5) = 4$, the primal distribution and the dual certificate are theirs; the only addition is a pairwise independent distribution attaining $\frac{479}{160}$, which shows that their dual bound is exact. That addition is a routine linear-programming computation and is not claimed as new.

Theorem 3.1 ([1], with f^{++} exact). *Let f be the coverage function of the sets E in (2) and $\mathbf{x}_5 = (\frac{3}{10}, \frac{7}{20}, \frac{3}{10}, \frac{7}{20}, \frac{7}{20})$. Then $f \in \mathcal{C}_5$, $f^+(\mathbf{x}_5) = 4$, $f^{++}(\mathbf{x}_5) = \frac{479}{160}$, and $\frac{4}{3} \cdot \frac{479}{160} < 4$. Consequently $f^+(\mathbf{x}_5)/f^{++}(\mathbf{x}_5) = \frac{640}{479} > \frac{4}{3}$.*

Proof. $f \leq 4$ pointwise (there are four features), so $f^+(\mathbf{x}_5) \leq 4$. The distribution $\{1\} : 7, \{0, 2\} : 6, \{3, 4\} : 7$ over $D = 20$ ([1, Table 1]) has marginals $\mathbf{x}_5$ and each of its atoms covers all four features, so $f^+(\mathbf{x}_5) = 4$.

For the upper bound on f^{++} , take the dual solution of [1] (with their indices shifted down by one): $\lambda_0 = \frac{1}{2}$; $\lambda_{(0)} = \lambda_{(2)} = \lambda_{(3)} = \lambda_{(4)} = \frac{3}{2}$, $\lambda_{(1)} = \frac{7}{2}$; $\lambda_{01} = \lambda_{12} = -1$, $\lambda_{13} = \lambda_{14} = -\frac{3}{2}$, $\lambda_{02} = \lambda_{34} = \frac{1}{2}$, $\lambda_{03} = \lambda_{04} = \lambda_{23} = \lambda_{24} = -\frac{1}{2}$. The 32 values $\lambda(S)$ are those printed in [1, Table 2] and satisfy $\lambda(S) \geq f(S)$ (a finite check; the minimum slack is 0). By Lemma 2.2, $f^{++}(\mathbf{x}_5) \leq \lambda_0 + \sum_i \lambda_{(i)} x_i + \sum_{i < j} \lambda_{ij} x_i x_j = \frac{479}{160}$.

For the matching lower bound, the distribution over $D = 1600$ with

$$\begin{aligned} \{0\} : 182, \{1\} : 259, \{2\} : 182, \{0, 2\} : 53, \{3\} : 210, \{0, 3\} : 49, \{0, 1, 3\} : 28, \{1, 2, 3\} : 77, \\ \{4\} : 154, \{0, 4\} : 28, \{1, 4\} : 56, \{0, 1, 4\} : 49, \{2, 4\} : 77, \{3, 4\} : 105, N : 91 \end{aligned}$$

is pairwise independent with marginals $\mathbf{x}_5$ and has expectation $\frac{4790}{1600} = \frac{479}{160}$. Finally $\frac{4}{3} \cdot \frac{479}{160} = \frac{479}{120} < 4$. $\square$

4. THE CASE $n = 4$ AT $\mathbf{x}_0 = (\frac{1}{2}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6})$

Theorem 4.1. *Let $n = 4$ and $\mathbf{x}_0 = (\frac{1}{2}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6})$.*

(a) *For every $f \in \mathcal{C}_4$, $f^+(\mathbf{x}_0) \leq \frac{4}{3} f^{++}(\mathbf{x}_0)$.*

(b) *For $f(S) = \min(|S|, 1)$, which lies in $\mathcal{C}_4$, $f^+(\mathbf{x}_0) = 1$ and $f^{++}(\mathbf{x}_0) = \frac{3}{4}$, and $1 = \frac{4}{3} \cdot \frac{3}{4}$.*

Hence $\sup\{f^+(\mathbf{x}_0)/f^{++}(\mathbf{x}_0) : f \in \mathcal{C}_4, f^{++}(\mathbf{x}_0) > 0\} = \frac{4}{3}$, and the supremum is attained.

The certificate for (a) is a pair: the majorant of Lemma 2.3, and the pairwise independent distribution ν_0 over $D = 72$ with

$$\begin{aligned} (3) \quad & \emptyset : 18, \{0\} : 23, \{1\} : 6, \{0, 1\} : 3, \{2\} : 6, \{0, 2\} : 3, \{0, 1, 2\} : 1, \\ & \{3\} : 6, \{0, 3\} : 3, \{0, 1, 3\} : 1, \{0, 2, 3\} : 1, N : 1. \end{aligned}$$

Both were produced by the linear program of Section 6.2; the proof below is self-contained and uses nothing about how they were found.

Proof of (a). Abbreviate $f_\emptyset = f(\emptyset)$, $f_i = f(\{i\})$, $f_{ij} = f(\{i, j\})$ and so on. Let $\theta \in \Theta(\mathbf{x}_0)$. By Lemma 2.3 and Lemma 2.1, and because $\sum_i x_{0,i} = 1$,

$$\mathbb{E}_\theta f \leq f_\emptyset + \sum_i x_{0,i} (f_i - f_\emptyset) = \frac{1}{2} f_\emptyset + \frac{1}{6} (f_1 + f_2 + f_3).$$

The distribution ν_0 of (3) is a probability distribution with marginals $\mathbf{x}_0$ ($72 \cdot \frac{1}{2} = 36$ on element 0, $72 \cdot \frac{1}{6} = 12$ on each other element) and pairwise products $\nu_0(i, j \in S) = x_{0,i} x_{0,j}$ ($6/72$ for the pairs containing 0, $2/72$ for the others), so $\nu_0 \in \Pi(\mathbf{x}_0)$, and

$$\frac{4}{3} \mathbb{E}_{\nu_0} f = \frac{1}{54} (18f_\emptyset + 23f_0 + 6f_1 + 3f_{01} + 6f_2 + 3f_{02} + f_{012} + 6f_3 + 3f_{03} + f_{013} + f_{023} + f_{0123}).$$

The difference $54(\frac{4}{3} \mathbb{E}_{\nu_0} f - \frac{1}{2} f_\emptyset - \frac{1}{6} (f_1 + f_2 + f_3))$ equals

$$18f_\emptyset + 3(f_{01} - f_1) + 3(f_{02} - f_2) + 3(f_{03} - f_3) + (f_{012} - f_0) + (f_{013} - f_0) + (f_{023} - f_0) + (f_{0123} - f_0),$$

and every term is nonnegative: $f_\emptyset \geq 0$, and each bracket is a difference of values on nested sets, hence ≥ 0 because f is nondecreasing (the last four via $f_0 \leq f_{01} \leq f_{012} \leq f_{0123}$, $f_0 \leq f_{01} \leq f_{013}$, $f_0 \leq f_{02} \leq f_{023}$). Thus $\mathbb{E}_\theta f \leq \frac{4}{3} \mathbb{E}_{\nu_0} f \leq \frac{4}{3} f^{++}(\mathbf{x}_0)$ for every $\theta \in \Theta(\mathbf{x}_0)$; taking the maximum over θ gives (a). $\square$

Proof of (b). $f(S) = \min(|S|, 1)$ is the coverage function of one feature covered by every element, hence in $\mathcal{C}_4$. Since $f \leq 1$, $f^+(\mathbf{x}_0) \leq 1$; the distribution $\{0\} : 3, \{1\} : 1, \{2\} : 1, \{3\} : 1$ over $D = 6$ has marginals $\mathbf{x}_0$ and expectation 1. For the upper bound on f^{++} , take $\lambda_0 = 0$, $\lambda_{(i)} = 1$ for all i , $\lambda_{0j} = -1$ for $j = 1, 2, 3$ and $\lambda_{ij} = 0$ for the other pairs, i.e. $\lambda(S) = |S| - [0 \in S] \cdot |S \cap \{1, 2, 3\}|$. If $0 \notin S$ then $\lambda(S) = |S| \geq f(S)$; if $0 \in S$ then $\lambda(S) = 1 \geq f(S)$. Lemma 2.2 gives $f^{++}(\mathbf{x}_0) \leq \sum_i x_{0,i} - x_{0,0}(x_{0,1} + x_{0,2} + x_{0,3}) = 1 - \frac{1}{4} = \frac{3}{4}$. The pairwise independent distribution over $D = 36$ with

$$\begin{aligned} &\emptyset : 9, \{0\} : 12, \{1\} : 3, \{0, 1\} : 1, \{2\} : 3, \{0, 2\} : 1, \\ &\{0, 1, 2\} : 1, \{3\} : 3, \{0, 3\} : 1, \{0, 1, 3\} : 1, \{0, 2, 3\} : 1 \end{aligned}$$

has marginals $\mathbf{x}_0$ and expectation $1 - \frac{9}{36} = \frac{3}{4}$. $\square$

Remark 4.2. The value $f^{++}(\mathbf{x}_0) = \frac{3}{4}$ agrees with the closed form $f^{++}(\mathbf{x}) = \min(\sum_i x_i - \max_i x_i, 1)$ for $f(S) = \min(|S|, 1)$ quoted in [2, Section 2] from [3], where it is the tight bound on the probability of a union of pairwise independent events (Theorem 2.3 in the numbering of arXiv:2006.00516v6): here $1 - \frac{1}{2} \cdot \frac{1}{2} = \frac{3}{4}$.

Remark 4.3 (What the certificate does and does not use). Part (a) uses only $f(\emptyset) \geq 0$, nine monotonicity inequalities and the subadditivity majorant. Submodularity cannot simply be dropped: the function $g = \mathbf{1}_{S=N}$ is nonnegative and nondecreasing but not submodular, the distribution $\emptyset : 3, \{0\} : 2, N : 1$ over $D = 6$ lies in $\Theta(\mathbf{x}_0)$ and gives $\mathbb{E}_\theta g = \frac{1}{6}$, while $\frac{4}{3}\mathbb{E}_{\nu_0} g = \frac{4}{3} \cdot \frac{1}{72} = \frac{1}{54}$; so the inequality $\mathbb{E}_\theta g \leq \frac{4}{3}\mathbb{E}_{\nu_0} g$ of the proof fails for g . Part (b) shows the constant is best possible at $\mathbf{x}_0$: any c with $f^+(\mathbf{x}_0) \leq c f^{++}(\mathbf{x}_0)$ for all $f \in \mathcal{C}_4$ satisfies $c \geq \frac{4}{3}$. These two facts are recorded among the machine-checked controls of Appendix A.

Remark 4.4 (Position relative to the known regions). The regions in which the $4/3$ bound was previously known are listed in the introduction; $\mathbf{x}_0$ lies in none of them for general $f \in \mathcal{C}_4$. The only one that touches $\mathbf{x}_0$ is the simplex corollary of [2, v2, Corollary 27], which covers functions with equal singleton values – a condition met by $\min(|S|, 1)$ but not by a general member of $\mathcal{C}_4$. To our knowledge, Theorem 4.1 is the first case of the conjecture settled at $n = 4$ for a marginal vector with a moderate coordinate and no restriction on f .

5. THE CASE $n = 5$: THE GAP IS AT LEAST $416/311$

Theorem 5.1. *Let f be the coverage function of $E' = (\{A, B, C, D\}, \{A, B\}, \{C, D\}, \{A, C\}, \{B, D\})$ – the sets (2) of [1] in the order E_1, E_0, E_2, E_3, E_4 – and let $\mathbf{x}' = (\frac{9}{26}, \frac{5}{13}, \frac{5}{13}, \frac{7}{26}, \frac{7}{26})$. Then $f \in \mathcal{C}_5$, $f^+(\mathbf{x}') = 4$, $f^{++}(\mathbf{x}') = \frac{311}{104}$, and $\frac{640}{479} \cdot \frac{311}{104} < 4$. Consequently*

$$\frac{f^+(\mathbf{x}')}{f^{++}(\mathbf{x}')} = \frac{416}{311} > \frac{640}{479} > \frac{4}{3}.$$

Proof. $f \leq 4$ pointwise, so $f^+(\mathbf{x}') \leq 4$. The three-atom distribution $\{0\} : 9, \{1, 2\} : 10, \{3, 4\} : 7$ over $D = 26$ has marginals $\mathbf{x}'$, and each atom covers all four features (E'_0 alone; $\{A, B\} \cup \{C, D\}$; $\{A, C\} \cup \{B, D\}$), so $f^+(\mathbf{x}') = 4$.

For the upper bound on f^{++} take $\lambda_0 = \frac{1}{2}$; $\lambda_{(0)} = \frac{7}{2}$, $\lambda_{(1)} = \lambda_{(2)} = \lambda_{(3)} = \lambda_{(4)} = \frac{3}{2}$; $\lambda_{01} = \lambda_{02} = -\frac{3}{2}$, $\lambda_{03} = \lambda_{04} = -1$, $\lambda_{12} = \lambda_{34} = \frac{1}{2}$, $\lambda_{13} = \lambda_{14} = \lambda_{23} = \lambda_{24} = -\frac{1}{2}$. The values $2\lambda(S)$, for S in binary order $(\emptyset, \{0\}, \{1\}, \{0, 1\}, \{2\}, \dots, N)$, are

$$1, 8, 4, 8, 4, 8, 8, 9, 4, 9, 6, 8, 6, 8, 9, 8, 4, 9, 6, 8, 6, 8, 9, 8, 8, 11, 9, 9, 9, 9, 11, 8,$$

and $\lambda(S) \geq f(S)$ for all 32 sets (minimum slack 0). By Lemma 2.2,

$$f^{++}(\mathbf{x}') \leq \frac{1}{2} + \frac{7}{2} \cdot \frac{9}{26} + \frac{3}{2} \cdot \frac{34}{26} - \frac{3}{2} \cdot 2 \cdot \frac{90}{676} - 2 \cdot \frac{63}{676} + \frac{1}{2} \cdot \frac{149}{676} - \frac{1}{2} \cdot \frac{280}{676} = \frac{4043}{1352} = \frac{311}{104}.$$

For the matching lower bound, the distribution over $D = 1352$ with

$$\begin{aligned} &\{0\} : 234, \{1\} : 184, \{0, 1\} : 23, \{2\} : 207, \{1, 2\} : 74, \{3\} : 68, \{1, 3\} : 68, \{0, 1, 3\} : 31, \\ &\{2, 3\} : 45, \{0, 2, 3\} : 54, \{4\} : 153, \{1, 4\} : 14, \{2, 4\} : 14, \{0, 1, 2, 4\} : 85, \{3, 4\} : 57, N : 41 \end{aligned}$$

is pairwise independent with marginals $\mathbf{x}'$ and has expectation $\frac{4043}{1352} = \frac{311}{104}$. Finally $\frac{640}{479} \cdot \frac{311}{104} = \frac{199040}{49816} < 4$ since $199040 < 199264$. $\square$

Remark 5.2 (Relation to the instance of [1]). In the labelling of [1] the new marginal vector reads $(x_1, \dots, x_5) = (\frac{5}{13}, \frac{9}{26}, \frac{5}{13}, \frac{7}{26}, \frac{7}{26})$, against their $(\frac{3}{10}, \frac{7}{20}, \frac{3}{10}, \frac{7}{20}, \frac{7}{20})$. By Theorem 3.1 their instance has gap exactly $640/479$, so the improvement comes entirely from moving the marginals of the same function. Their value is correct and was not claimed to be optimal; Theorem 5.1 is an improvement, not a correction.

Remark 5.3 (All $n \geq 5$). The bound propagates to larger n by padding, an observation that is not part of the formal development. For $n > 5$ let $f'(S) = f(S \cap [5])$ on $2^{[n]}$ and $\mathbf{x}'' = (\mathbf{x}', 0, \dots, 0)$. Then $f' \in \mathcal{C}_n$, and a zero marginal forces every $\theta \in \Theta(\mathbf{x}'')$ to vanish on sets meeting $[n] \setminus [5]$ (the pairwise constraints involving such an element read $0 = 0$), so $\Theta(\mathbf{x}'')$ and $\Pi(\mathbf{x}'')$ are identified with $\Theta(\mathbf{x}')$ and $\Pi(\mathbf{x}')$ and $f'^+(\mathbf{x}'')/f'^{++}(\mathbf{x}'') = 416/311$. Hence the tightest constant for $n \geq 5$, whatever it is, is at least $416/311$.

Remark 5.4 (Not claimed). $416/311$ is a lower bound. It was found by the search of Section 6.1 run at $n = 5$, which is complete for distributions with at most four atoms; completeness at $n = 5$ needs six atoms, and that sweep was not run (Section 6.4). No claim is made that $416/311$ is the supremum at $n = 5$, nor that the supremum is independent of n for $n \geq 5$.

6. COMPUTATIONS OUTSIDE THE FORMAL DEVELOPMENT

Everything in this section is a computation reported as such: it is not machine-checked and no theorem rests on it. Exact statements are in exact rational arithmetic (two-phase simplex with Bland's rule over $\mathbb{Q}$); where floating point was used this is said.

6.1. A search linear program, and a complete sweep at $n = 4$. Fix a distribution q on $2^{[n]}$ and write $\mathbf{x}(q)$ for its marginals. The quantity

$$\text{value}(q) = \min\{f^{++}(\mathbf{x}(q)) : f \in \mathcal{C}_n, \mathbb{E}_q f = 1\}$$

is a single linear program (the inner maximum defining f^{++} is dualised as in Lemma 2.2; the constraints $f \in \mathcal{C}_n$ are the $n2^{n-1}$ monotonicity rows, the $\binom{n}{2}2^{n-2}$ submodularity rows and $f(\emptyset) \geq 0$). For its minimiser, $f^+(\mathbf{x}(q)) \geq \mathbb{E}_q f = 1$, so $1/\text{value}(q)$ is a lower bound on $\sup_f f^+(\mathbf{x}(q))/f^{++}(\mathbf{x}(q))$; conversely, if q is a maximiser of $\mathbb{E}_\theta f$ for the worst pair $(f, \mathbf{x})$, the bound is attained. For fixed $(f, \mathbf{x})$ the maximum of $\mathbb{E}_\theta f$ over the polytope $\Theta(\mathbf{x})$, which is cut out by $n+1$ equations, is attained at a vertex, hence at a distribution with at most $n+1$ atoms. Enumerating all supports of size at most $n+1$, up to the action of the symmetric group S_n on the ground set, is therefore a complete enumeration of the combinatorial part of the problem; only the optimisation over the weights on a fixed support remains.

At $n = 4$ this was carried out over all 489 canonical supports (17, 52, 136 and 284 supports of sizes 2, 3, 4, 5 up to S_4), the weights on each support being optimised heuristically (a grid on the simplex with denominator 20, followed by three local refinements of 3000 mass-transfer steps from the best three grid points; about 16 CPU-minutes in all, using a floating-point simplex). *No support produced a ratio above $4/3$.* The single excursion, 1.3333333364 at the support $\{0\}, \{1\}, \{0, 2\}, \{0, 2, 3\}$, is floating-point noise: the weights, rationalised, give exactly $4/3$. Before use, the machinery was checked to return exactly $4/3$ at $n = 2$ and $n = 3$ (the known sharp values) and to recover the three-atom distribution and the value $640/479$ of [1] at $\mathbf{x}_5$ from random starts. This is evidence that the answer at $n = 4$ is “true” with worst case exactly $4/3$; it is not a proof, because the weight optimisation is a local search.

6.2. A certificate linear program, and a grid scan. To prove $f^+(\mathbf{x}) \leq c f^{++}(\mathbf{x})$ at a fixed $\mathbf{x}$ for every $f \in \mathcal{C}_n$ it suffices to have (i) a *modular majorant rule* μ , linear in f , with $f \leq \mu(f)$ pointwise – then Lemma 2.1 bounds $f^+(\mathbf{x})$ by a linear functional $\ell_{\mathbf{x}}(f)$; and (ii) one $\nu \in \Pi(\mathbf{x})$ together with a Farkas certificate that $c\mathbb{E}_\nu f - \ell_{\mathbf{x}}(f)$ is a nonnegative combination of the defining inequalities of $\mathcal{C}_n$. The rules used are the convex combinations of the two modular upper bounds of Iyer and Bilmes [8,

Section 2.2] (there $m_{X,1}^f, m_{X,2}^f$, derived from inequalities of Nemhauser, Wolsey and Fisher [7]): for $T \subseteq N$,

$$m_T^1(S) = f(T) - \sum_{i \in T \setminus S} (f(T) - f(T \setminus i)) + \sum_{i \in S \setminus T} (f(\{i\}) - f(\emptyset)),$$

$$m_T^2(S) = f(T) - \sum_{i \in T \setminus S} (f(N) - f(N \setminus i)) + \sum_{i \in S \setminus T} (f(T \cup i) - f(T)),$$

both $\geq f(S)$ for submodular f ; $m_\emptyset^1$ is Lemma 2.3. Their validity at $n = 4$ was not taken on trust: for each of the $2 \cdot 16 \cdot 16$ triples (rule, T , S) the exact linear program $\min\{m_T(S) - f(S) : f \in \mathcal{C}_4, \sum_U f(U) = 1\}$ has nonnegative value (512 programs, 0 violations, minimum 0). Minimising c jointly over the rule, ν and the multipliers is one linear program with 28 rows and 106 columns at $n = 4$; solved in exact rational arithmetic it costs about 1.34 CPU-seconds per point. Its value $c_{\text{lin}}(\mathbf{x})$ satisfies $c_{\text{lin}}(\mathbf{x}) \geq \sup_f f^+(\mathbf{x})/f^{++}(\mathbf{x})$, and $c_{\text{lin}}(\mathbf{x}) \leq 4/3$ is a proof of the conjecture at $\mathbf{x}$. The certificate of Theorem 4.1 is the output of this program at $\mathbf{x}_0$; it uses the single rule $m_\emptyset^1$, which is why the proof in Section 4 is so short.

The program was run over three grids of sorted marginal vectors in $[0, 1]^4$:

grid (sorted $\mathbf{x}$)	points	result
step 1/6	210	all certified; $\max c_{\text{lin}} = 4/3$
step 1/12	1820	1815 certified; 5 exceed $4/3$, all with every coordinate in $[1/3, 1/2]$, worst value $750/559 = 1.34168 \dots$ at $(5/12, 5/12, 5/12, 5/12)$
step 1/8, simplex, rule $m_\emptyset^1$	53	all certified

The five exceedances are a limitation of the scheme – one ν and one linear rule for the whole cone – and not evidence against the conjecture: the sweep of Section 6.1 finds nothing above $4/3$ there. A proof of the $n = 4$ case along these lines would need a case split on f (several ν 's over a polyhedral partition of $\mathcal{C}_4$) on a band around $\mathbf{x} \approx (0.4, \dots, 0.45)$, together with region certificates in place of point certificates; neither has been attempted.

6.3. Three further marginal vectors. The same program returns $c_{\text{lin}} = 4/3$, with an exact rational certificate validated as in Section 4, at

$$\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right), \quad \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{4}, \frac{1}{4}\right), \quad \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{6}, \frac{1}{6}\right).$$

So $f^+ \leq \frac{4}{3}f^{++}$ holds for every $f \in \mathcal{C}_4$ at these three vectors as well. All three lie outside the previously known regions: the first has identical marginals $x = \frac{1}{2}$, which Corollary 28 of [2, v2] does not cover ($x \leq \frac{1}{3}$ or $x \geq \frac{2}{3}$ is required); the other two, sorted, have largest coordinate $\frac{1}{2} > \frac{1}{4}$ and total mass > 1 . These certificates use the rules m_T^2 (for the first vector $m_\emptyset^1, m_{\{0\}}^2, m_{\{1\}}^2, m_{\{0,1\}}^2, m_{\{2\}}^2$; for the other two $m_\emptyset^1$ and $m_{\{1\}}^2$), and they have *not* been formalised: the majorant inequality for m_T^2 is not yet in the formal development, which is the only thing separating these three statements from Theorem 4.1.

6.4. The search at $n = 5$. The sweep of Section 6.1 at $n = 5$ (134 canonical supports of size 3 and 625 of size 4 up to S_5 ; about 75 CPU-minutes) found its largest value at the three-atom support $\{0\} \mid \{1, 2\} \mid \{3, 4\}$ – a partition of the ground set, the shape of the instance of [1]. Rationalising the optimal weights (0.34615385798, 0.38461559692, 0.26923054510) as $(\frac{9}{26}, \frac{10}{26}, \frac{7}{26})$ and re-solving exactly returned, as the minimising f (after scaling by 4), the coverage function of the five sets of [1], and the values of Theorem 5.1. A sweep over supports of size 5 was started and stopped after 17 minutes of wall time without finding anything above 416/311; it is partial corroboration only. The sweep over supports of size 6, which is what completeness at $n = 5$ requires (about 7700 canonical supports at about 2.5 seconds each, an estimated 5.3 CPU-hours), was not run.

6.5. Open ends. (1) The conjecture at $n = 4$ in full: by Section 6.1 the answer is expected to be “true” with worst case $4/3$; a proof needs region certificates and a case split on f near $(\frac{5}{12}, \dots, \frac{5}{12})$. Short of that, a certified uniform bound at $n = 4$ below $e/(e - 1)$ – for instance $c \leq 1.35$ for all $\mathbf{x}$, which the point certificates support wherever $c_{\text{lin}}(\mathbf{x}) \leq 1.35$, the measured maximum on the $\frac{1}{12}$ -grid being $750/559$ – would be new. (2) The exact supremum at $n = 5$, and whether it grows with n ; by the padding remark of Section 5, $416/311$ is a lower bound for every $n \geq 5$.

7. VERIFICATION

Theorems 3.1, 4.1 and 5.1, together with Lemmas 2.1–2.3 as used in them and the four controls of Appendix A, are verified in Lean 4 [9] with Mathlib [10]. Set functions and distributions are maps $\text{Finset}(\text{Finn}) \rightarrow \mathbb{Q}$; the class $\mathcal{C}_n$, the constraint sets $\Theta(\mathbf{x})$ and $\Pi(\mathbf{x})$, and the two extremal values are defined literally (the value $f^+(\mathbf{x}) = a$ is the statement that a is the greatest element of $\{\mathbb{E}_\theta f : \theta \in \Theta(\mathbf{x})\}$, and likewise for f^{++}), so each theorem asserts an exact value, not a bound. Every distribution and certificate is stored as integer numerators over one denominator, which makes each marginal identity, each pairwise identity and each pointwise inequality $f(S) \leq \lambda(S)$ a decidable natural-number fact closed by the kernel’s decision procedure; the Farkas step of Theorem 4.1 is a linear-arithmetic certificate over $\mathbb{Q}$. No `native_decide`, no `sorry` and no additional axiom is used: for each of the seven statements of Appendix A, `#print axioms` reports exactly `propxt`, `Classical.choice` and `Quot.sound`. The formal statements quantify over rational-valued f and θ ; the proofs given in Sections 3–5 are the same certificates and are valid over $\mathbb{R}$ verbatim, since every step is a linear inequality with rational coefficients. The computations of Section 6 are not formalised. Repository reference to be added at submission.

APPENDIX A. THE STATEMENTS AS MACHINE-CHECKED

The three theorems and the four controls, exactly as they appear in the formal development (doc-strings included); `MonSub f` is $f \in \mathcal{C}_n$, `IsFPlus x f a` is “ $f^+(\mathbf{x}) = a$ ” and `IsFPP x f b` is “ $f^{++}(\mathbf{x}) = b$ ”, each as the greatest element of the corresponding set of expectations. Elements are indexed $0, \dots, n - 1$ throughout, as in this paper.

Theorem 3.1 (`Five.gap_five`):

```
-- **The `n = 5` refutation, with both extremal values exact.** For the source's
coverage function `f5` and marginals `x5 = (3/10, 7/20, 3/10, 7/20, 7/20)` :
`f5` is nonnegative, nondecreasing and submodular, `f+(x5) = 4`,
`f++(x5) = 479/160`, and `(4/3) * f++(x5) < f+(x5)`; the pairwise independent
correlation gap at this instance is `640/479 > 4/3`. -/
theorem gap_five :
  MonSub f5 ∧ IsFPlus x5 f5 4 ∧ IsFPP x5 f5 (479 / 160) ∧ (4 / 3 : ℚ) * (479 / 160) < 4
```

Theorem 4.1 (`Four.four_gap_exact`; `fOR` is $\min(|S|, 1)$):

```
-- **The `n = 4` case at `x0 = (1/2, 1/6, 1/6, 1/6)` is settled, and the constant
is exactly `4/3`.** For every nonnegative nondecreasing submodular `f` on four
elements the gap at `x0` is at most `4/3`, and the rank function of the rank-one
uniform matroid attains it: `f+(x0) = 1 = (4/3) * (3/4) = (4/3) * f++(x0)`. -/
theorem four_gap_exact :
  (∀ f : Finset (Fin 4) → ℚ, MonSub f → ∀ a b : ℚ,
    IsFPlus x0 f a → IsFPP x0 f b → a ≤ (4 / 3) * b)
  ∧ MonSub fOR ∧ IsFPlus x0 fOR 1 ∧ IsFPP x0 fOR (3 / 4)
  ∧ (1 : ℚ) = (4 / 3) * (3 / 4)
```

Theorem 5.1 (`FiveImp.gap_five_improved`):

```
-- **An improved lower bound for the pairwise independent correlation gap at `n = 5`.**
For the source's own coverage function at the marginals `(9/26, 5/13, 5/13, 7/26, 7/26)`,
`f+ = 4` and `f++ = 311/104` exactly, so the gap is `416/311`, strictly larger than
the source's `640/479` (and hence than `4/3`). -/
```

```

theorem gap_five_improved :
  MonSub f5b  $\wedge$  IsFPlus x5b f5b 4  $\wedge$  IsFPP x5b f5b (311 / 104)
   $\wedge$  (640 / 479 :  $\mathbb{Q}$ ) * (311 / 104) < 4
Controls (namespace Controls; f3 is  $1_{S=N}$ , th3 the distribution  $\emptyset : 3, \{0\} : 2, N : 1$  over 6, Four.nu0
the distribution (3)):
/-- **Too-small control.** No constant below `4/3` works at `x0`, already for
`f(S) = min(|S|,1)`. -/
theorem const_not_below_four_thirds (c :  $\mathbb{Q}$ )
  (h :  $\forall f : \text{Finset (Fin 4)} \rightarrow \mathbb{Q}, \text{MonSub } f \rightarrow \forall a\ b : \mathbb{Q},$ 
    IsFPlus Four.x0 f a  $\rightarrow$  IsFPP Four.x0 f b  $\rightarrow a \leq c * b$ ) : (4 / 3 :  $\mathbb{Q}$ )  $\leq$  c

/-- **Too-large control.** The `n = 5` counterexample gives the gap `640/479`, which is
*below* `1.34`; it refutes `4/3` and nothing larger. -/
theorem five_gap_not_above : (4 :  $\mathbb{Q}$ ) < (134 / 100 :  $\mathbb{Q}$ ) * (479 / 160)

/-- **Hypothesis control.** Dropping submodularity breaks `four_bound`: `f3` is
nonnegative and nondecreasing but not submodular, and `th3` has marginals `x0`
while `Exp th3 f3 = 1/6 > (4/3) * (1/72) = (4/3) * Exp nu0 f3`. -/
theorem submod_needed :
  ( $\forall S, 0 \leq f3\ S$ )  $\wedge$  Nondec f3  $\wedge$   $\neg$  Submod f3  $\wedge$  HasMarg Four.x0 th3  $\wedge$ 
  (4 / 3 :  $\mathbb{Q}$ ) * Exp Four.nu0 f3 < Exp th3 f3

/-- **Non-vacuity control.** Pairwise independence is a genuine restriction at `x5`:
both maxima are attained and the unrestricted one is strictly larger. -/
theorem pairIndep_restricts :
  IsFPlus Five.x5 Five.f5 4  $\wedge$  IsFPP Five.x5 Five.f5 (479 / 160)
   $\wedge$  (479 / 160 :  $\mathbb{Q}$ ) < 4

```

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