On the distribution of scrambled \((0, m, s)\)-nets over unanchored boxes

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Abstract We introduce a new quality measure to assess randomized low-discrepancy point sets of finite size \(n\). This new quality measure, which we call “pairwise sampling dependence index”, is based on the concept of negative dependence. A negative value for this index implies that the corresponding point set integrates the indicator function of any unanchored box with smaller variance than the Monte Carlo method. We show that scrambled \((0, m, s)\)-nets have a negative pairwise sampling dependence index. We also illustrate through an example that randomizing via a digital shift instead of scrambling may yield a positive pairwise sampling dependence index.

1 Introduction

The quality of point sets used within quasi-Monte Carlo (QMC) methods is often assessed using the notion of discrepancy. For a point set \(P_n = \{u_i : i = 1, \ldots, n\}\), its star-discrepancy is given by
\[
D^*_n(P_n) = \sup_{A \in \mathcal{A}_0} |J_n(A) - \text{Vol}(A)|
\]
where \(\mathcal{A}_0\) is the set of all boxes \(A \subseteq \{0, 1\}^s\) anchored at the origin, and \(J_n(A) = \sum_{i=1}^n u_i \text{1}_{A} / n\). The extreme discrepancy is instead given by
\[
D_n(P_n) = \sup_{A \in \mathcal{A}} |J_n(A) - \text{Vol}(A)|
\]
where \(\mathcal{A}\) is the set of all boxes in \([0, 1]^s\). Both quantities are typically interpreted as comparing the empirical distribution induced by \(P_n\) with the uniform distribution over \([0, 1]^s\) in terms of the probability they assign to a given set \(A\) of boxes. Using inclusion-exclusion arguments, one can derive the bound
\[
D_n(P_n) \leq 2^s D^*_n(P_n).
\]
Many asymptotic results for \(D^*_n(P_n)\) and \(D_n(P_n)\) have been derived for various low-discrepancy sequences \([1, 6]\). These sequences are understood to be such that
\( D_n^* (P_n) \in O((\log n)^r/n) \), and the above mentioned results often focus on studying the constant terms in the big-Oh notation and how it behaves as a function of \( s \).

In practice, when using QMC methods, one is often working in settings where \( n \) is not too large, and a primary goal is to make sure that the QMC approximation will result in a better approximation than the one that would be obtained by using plain Monte Carlo sampling. One is also typically interested in assessing the approximation error, something naturally embedded in Monte Carlo methods via variance estimates and the central limit theorem.

In this setting, the use of randomized QMC methods is very appealing, as it preserves the advantage of QMC induced by the use of low-discrepancy sequences, while at the same time allowing for error estimates through independent and identically distributed (iid) replications.

In this paper, we focus on the above settings, i.e., where one (1) works with \( n \) not too large; (2) uses randomized QMC, and (3) hopes to do better than Monte Carlo.

To this end, we propose to reinterpret the measures \( D_n^* (P_n) \) and \( D_n (P_n) \) and propose a new, related measure that is designed for our chosen setting, which we refer to as “pairwise sampling dependence index”. While this measure is meant to assess the uniformity of point sets much like the star and extreme discrepancies do, it also has another interpretation, which is that a point set with negative pairwise sampling dependence index estimates the expected value of the indicator function \( 1_A \) for any \( A \in \mathcal{A} \) with variance smaller than the Monte Carlo method. This new measure is defined in Section 2, Eqn. (1). In Section 3 we revisit the result from [10], which shows that scrambled \((0, m, s)\)-nets have a negative pairwise sampling dependence index over all anchored boxes. In Section 5 we show that this result extends to unanchored boxes in Theorem 4 which is the main result of this paper. Hence the extension to unanchored boxes does not cause the same deterioration of the bound for this uniformity measure as is the case when applying an inclusion-exclusion argument to go from the star to the extreme discrepancy.

The proof of this result is essentially a very difficult problem in linear programming, (something that is rather obscured by the fact that, since the number of variables depends on \( m \), we work in \( \ell^1(\mathbb{N}) \) and its dual \( \ell^\infty(\mathbb{N}) \) rather than a finite dimensional space). Indeed, we must demonstrate that (1) is always negative for scrambled \((0, m, s)\)-nets. We see in Theorem 2 that (1) is actually a linear equation whose variables are non-negative and are further constrained, in the one-dimensional case, according to Lemma 2. The constraints define a convex region whose extreme points, in the one-dimensional case, are found in Theorem 1 and given by (10) in the higher dimensional case. The remainder of the proof boils down to proving that (1) is non-negative at these extreme points. This requires the use of several technical lemmas (given in the appendix) proving sufficiently tight bounds on various combinatorial sums, which is precisely why we do not have to rely on an inclusion-exclusion argument to go from the anchored case to the unanchored one. We briefly discuss in Section 6 the advantage of scrambling over simpler randomization methods such as a digital shift. Ideas for future work are presented in Section 7.
2 Pairwise Sampling Dependence

We start by revisiting the definition of extreme discrepancy using a probabilistic approach, despite the fact that the point set $P_n$ may be deterministic. We do so by introducing a quality measure we call sampling discrepancy, given by $\mathcal{D}_n(P_n) := \sup_{A \in \mathcal{A}} |\mathcal{P}_n(A) - \text{Vol}(A)|$, where $\mathcal{P}_n(A)$ is the probability that a randomly chosen point in $P_n$ will fall in $A$. For a deterministic point set, this probability is given by $\mathcal{P}_n(A) = \frac{1}{n} |A|$, and so in this case $\mathcal{D}_n(P_n) = \mathcal{D}(P_n)$. This definition captures how the discrepancy is often described as a distance measure between the empirical distribution induced by the point set $P_n$ and the uniform distribution. Since the uniform distribution is viewed as a target distribution in this setting, we want this distance to be as small as possible.

In this paper we are interested in randomized QMC point sets $\tilde{P}_n$. We assume $\tilde{P}_n$ is a valid sampling scheme, meaning that $U_i \sim U(0, 1)^d$ for each $U_i \in \tilde{P}_n$, with possibly some dependence among the $U_i$’s. When we write $\tilde{P}_n$, we are thus not referring to a specific realization of the randomization process, which we instead denote by $\tilde{P}_n(\omega)$, where $\omega \in \Omega$, and $\Omega$ is the sampling space associated with our randomization process for $P_n$.

In that setting, we could compute $\mathcal{D}_n(\tilde{P}_n(\omega))$ and then perhaps compute the expected value of $\mathcal{D}_n(\tilde{P}_n(\omega))$ over all these realizations $\omega$, or the probability that it will be larger than some value, as done in [3], for example. If we instead interpret $\mathcal{P}_n(A)$ as the probability that a randomly chosen point $U_i$ from $\tilde{P}_n$ falls in $A$, then we would get $\mathcal{D}_n(\tilde{P}_n) = 0$, which is of little use.

To define an interesting alternative measure of uniformity for randomized QMC point sets, we introduce instead a “second-moment” version of the sampling discrepancy, in which we consider pairs of points rather than single points, and where the distribution against which we compare the point set is that induced by random sampling, where points are sampled independently from one another. When considering pairs of points, our goal is to examine the propensity for points to repel each other, which is a desirable feature if we want to achieve greater uniformity than random sampling. Note that this notion of “propensity to repel” is in line with the concept of negative dependence.

More precisely, we want to verify that the pairs of points from $\tilde{P}_n$ are less likely to fall within the same box $A$ than they would if they were independent. Note that here, as was the case with $\mathcal{D}_n(P_n)$, we are comparing the distribution induced by $\tilde{P}_n$ with another distribution. But rather than comparing to a target distribution to which we want to be as close as possible, we are comparing to a distribution upon which we want to improve, and thus are not trying to be close to that distribution.

The measure we propose to assess the quality of a point set via the behavior of its pairs is called pairwise sampling dependence index and is given by

$$E_n(\tilde{P}_n) := \sup_{A \in \mathcal{A}} H_n(A) - \text{Vol}^2(A),$$  \hspace{1cm} (1)

where $H_n(A) := P((U, V) \in A \times A)$, \hspace{1cm} (2)
with \( U \) and \( V \) being distinct points randomly chosen from \( \tilde{P}_n \). We say \( \tilde{P}_n \) has a **negative pairwise sampling dependence index** when \( \mathcal{E}_n(\tilde{P}_n) \leq 0 \). (This terminology is consistent with other measures of negative dependence; see, e.g., [10].)

Note that because we are not taking the supremum over all products of the form \( A \times B \) with \( A, B \in \mathcal{A} \) and instead only consider \( A \times A \), it is possible, if \( \tilde{P}_n \) is designed so that points tend to cluster away from each other, that the probability \( H_n(A) \) will never be larger than what it is under random sampling, as given by \( \text{Vol}^2(A) \). This is not the case with the measure \( \mathcal{D}_n(\tilde{P}_n) \), where having \( \mathcal{P}_n(A) < \text{Vol}(A) \) implies there will be some \( A' \) for which \( \mathcal{P}_n(A') > \text{Vol}(A') \). There the goal is to show there exist point sets \( P_n \) with \( |\mathcal{P}_n(A) - \text{Vol}(A)| \) very close to 0, and becoming closer to 0 as \( n \) goes to infinity. In our case, we instead want to show, for a given \( n \), that there exist sampling schemes \( \tilde{P}_n \) with \( \mathcal{E}_n(\tilde{P}_n) \leq 0 \).

So far we mentioned the work done in [2] and [10], but concepts of dependence based on measures different from [11] have recently been used in other works to analyze lattices [11], Latin hypercube sampling [4] and scrambled nets [2].

### 3 Revisiting Pairwise Sampling Dependence over Anchored Boxes

In what follows, we assume \( \tilde{P}_n \) is a scrambled \((0, m, s)\)-net in base \( b \geq s \), where \( n = b^m \), and \( P_n \) represents the underlying \((0, m, s)\)-net being scrambled. We assume the reader is familiar with the concept of digital nets and \((t, m, s)\)-nets, as presented in e.g., [1] [6]. Also, when referring to scrambled nets, we refer to the scrambling method studied in [10], which originates from [8].

In [10], it was shown that if we restrict \( \mathcal{E}_n(\tilde{P}_n) \) to anchored boxes—denote this version of \( \mathcal{E}_n \) by \( \mathcal{E}_{n,0}(\tilde{P}_n) \)—then \( \mathcal{E}_{n,0}(\tilde{P}_n) \leq 0 \). In fact, a stronger result is shown in [10], which is that for \((U, V)\) a pair of distinct points randomly chosen from \( \tilde{P}_n \),

\[
P((U, V) \in \{0, x\} \times \{0, y\}) \leq \text{Vol}((0, x) \times \{0, y\}), \quad \text{for any } x, y \in [0, 1]^s.
\]

For simplicity, in what follows we assume \( x = y \) and let \( A = \{0, x\} \).

Next, to define a key quantity we called the **volume vector** of a subset of \([0, 1]^2\), we first define the regions \( D_i^b := \{(x, y) \in [0, 1)^2 : \gamma_b(x, y) = i\} \), where \( \gamma_b(x, y) := (\gamma_b(x_1, y_1), \ldots, \gamma_b(x_s, y_s)) \) and \( \gamma_b(x, y) \geq 0 \) is the unique number \( i \geq 0 \) such that

\[
[b^i]x = [b^i]y \quad \text{but} \quad [b^{i+1}]x \neq [b^{i+1}]y.
\]

That is, \( \gamma_b(x, y) \) is the exact number of initial digits shared by \( x \) and \( y \) in their base \( b \) expansion. If \( x = y \) then we let \( \gamma_b(x, y) = \infty \). Also, \( \gamma_b(x, y) \) is well defined for any \( x, y \in [0, 1] \) even if \( x, y \) do not have a unique expansion in base \( b \).

Let \( \mathbb{N}_0 = \{0, 1, 2, \ldots\} \). We can now define, for \( A, B \subseteq [0, 1]^s \), the volume vector \( V(A \times B) \in \ell^1(\mathbb{N}_0) \), whose component \( V_i(A \times B) \) associated to \( i \in \mathbb{N}_0 \) is given by

\[
V_i(A \times B) := \int_{A \times B} 1_{D_i^b} \, du \, dv = \text{Vol}((A \times B) \cap D_i^b) \in [0, 1].
\]
A key step used in \cite{10} to prove that $H_n(A) \leq \text{Vol}(A \times A)$ is to find a conical combination of products of the form $1_k \times 1_k$, where $1_k = \prod_{j=1}^s [0, b^{-k_j}), k_j \in \mathbb{N}_0, j = 1, \ldots, s$, whose volume vector is the same as that of $A \times A$. More precisely, one can find coefficients $t_k \geq 0$ with $\sum_{k \geq 0} t_k = \text{Vol}(A \times A)$, such that

$$V_i(A \times A) = \sum_{k \geq 0} t_k b^{2k|i|} V_i(1_k \times 1_k) \quad \text{for all } i \in \mathbb{N}_0^s. \quad (4)$$

The coefficients $t_k$ are shown in \cite{10} to be given by $t_k = \prod_{j=1}^s t_{k_j}$, where

$$t_k = \begin{cases} \frac{b V_0(k+1,A \times A)}{b-1} & \text{if } k > 0 \\ 1 & \text{if } k = 0. \end{cases} \quad (5)$$

From here, rather than following the proof in \cite{10}, we exploit the fact that the joint pdf is a simple function, these sums always have finitely many non-zero terms. See \cite{10, Sec. 2.3} for more details.

**Lemma 1** Let $A = [0, \mathbf{x})$ with $\mathbf{x} \in [0, 1]^s$, and let $t_k$ be the coefficients for which \cite{4} holds. Then for a scrambled $(0, m, s)$–net $\hat{P}_n$

$$H_n(A) = \sum_{k \geq 0} t_k b^{2k|i|} H_n(1_k). \quad (6)$$

**Proof** As shown in \cite{10}, we use the (constant) value $\psi_i$ of the joint pdf of $\mathbf{U}, \mathbf{V}$ from $\hat{P}_n$ over $D_i$ to compute $H_n(A)$ as

$$H_n(A) = \sum_{i \geq 0} \psi_i \times V_i(A \times A) \quad (7)$$

and then use \cite{4} to get $H_n(A) = \sum_{i \geq 0} \psi_i \sum_{k \geq 0} t_k b^{2k|i|} V_i(1_k \times 1_k) = \sum_{k \geq 0} t_k b^{2k|i|} H_n(1_k)$ where the order of summation can be changed thanks to Tonelli’s theorem. □

Next, rather than computing $H_n(1_k)$ by writing it as an integral involving the joint pdf associated with $(\mathbf{U}, \mathbf{V})$ (as we just did in the proof of Lemma 1), we instead use a conditional probability argument that allows us to directly connect this probability to the counting numbers $m_{\ell}(k; P_n)$ used in \cite{10}, which for $P_n$ a digital net, represents the number of points $u_j \in P_n$ satisfying $\gamma_{\ell}(u_i, u_j) \geq k$ for a given $l \neq j$. (For an arbitrary $P_n$, this number depends on $\ell$ but for a $(0, m, s)$–net, it is invariant with $\ell$, hence we drop the dependence on $\ell$ in our notation. Also, since $m_{\ell}(k; P_n) = m_{\ell}(k; \hat{P}_n)$, we work with the deterministic point sets when using these counting numbers.) This is a key step, as it allows us to write $H_n(A)$ as a linear equation instead of an integral, thereby yielding a linear programming formulation for our main result, which is to show $H_n(A) \leq \text{Vol}(A \times A)$. Specifically, we write
\[ H_n(1_k) = P(V \in 1_k | U \in 1_k) P(U \in 1_k) = \frac{m_b(k; P_n)}{n - 1} b^{-|k|}. \tag{8} \]

If \( P_n \) is a \((0,m,s)-net\) in base \( b \), then \( m_b(k; P_n) = \max(b^{m-|k|} - 1, 0) \) \[10\]. These counting numbers are also closely connected to the key quantities \[10\].

\[ C_b(k; P_n) = \frac{b^{|k|} m_b(k; P_n)}{n - 1}. \]

Combining \[6\] and \[8\], we get that for \( P_n \) a scrambled \((0,m,s)-net\),

\[ H_n(A) = \sum_{k \geq 0} t_k b^{|k|} \frac{m_b(k; P_n)}{n - 1} = \sum_{k \geq 0} t_k C_b(k; P_n) \leq \sum_{k \geq 0} t_k = \text{Vol}(A \times A), \tag{9} \]

since \( C_b(k; P_n) \leq 1 \) when \( P_n \) is a \((0,m,s)-net\) \[10\].

### 4 Decomposing unanchored intervals

We now consider the case where \( A \) is an unanchored box of the form \( A = \prod_{j=1}^{s} (a_j, A_j) \), with \( 0 \leq a_j < A_j \leq 1, j = 1, \ldots, s \). In Section \[5\] we will prove in Theorem \[5\] that for a scrambled \((0,m,s)-net\), we still have \( H_n(A) \leq \text{Vol}(A \times A) \) in this case, which is the main result of this paper. The proof of this result is much more difficult than in the anchored case because when \( A \) is not anchored at the origin, we cannot always find a conical decomposition of products of elementary intervals as in \[4\] that has the same volume vector as \( A \times A \).

Before going further, we note that it is sufficient to focus on the decomposition of one-dimensional intervals \( A \) since a box is just a product of intervals. Hence for the rest of this section, we assume \( s = 1 \).

The reason why the decomposition \[4\] cannot be used for unanchored intervals is that it may produce coefficients \( t_k \) that are negative, which makes the inequality in \[5\] not necessarily true. In turn, this happens because the key property \( bV_i(A \times A) \geq V_{i-1}(A \times A) \) that holds for an anchored interval \( A \) and that is used to show that \( t_k \geq 0 \) in \[10\] is not always satisfied when \( A \) is an unanchored interval. In this case, the volume vector corresponding to \( A \times A \) may be such that \( V_0(A \times A) > 0, V_1(A \times A) = \ldots = V_{r-1}(A \times A) = 0, V_r(A \times A) > 0 \) for \( i \geq r \). Because of this, we can see from \[5\] that some \( t_k \) may be negative.

To get a decomposition with non-negative coefficients, we introduce a family of regions of the form \( Y \times Y \) where \( Y \) is not an elementary interval anchored at the origin. More precisely, for \( d, k \) non-negative integers, we define what we call an **elementary unanchored \((d,k)\)-interval**

\[ Y_k^{(d)} := \left[ \frac{1}{b^{d+1}} - \frac{1}{b^{2+k+d}}, \frac{1}{b^{d+1}} + \frac{1}{b^{2+k+d}} \right]. \]
As a first step, in the following lemma we establish some key properties for the volume vector corresponding to an unanchored interval $A$. It is the counterpart to the property that $b V_{i}(A \times A) \geq V_{i-1}(A \times A)$ for anchored boxes, and shows that the $V_{i}(A \times A)$’s do not decrease too quickly with $i$ in the unanchored case, which is essential to prove the decomposition given in Theorem [11]. The proof of this lemma is in the appendix. Note that this lemma applies to half-open intervals strictly contained in $[0, 1)$; the interval $[0, 1)$ can be handled using the decomposition from [10], which was described in the previous section.

**Lemma 2** Let $A \subset [0, 1)$ be a half-open interval and let $r \geq 1$ be the smallest integer such that we can write $A = [hb^{−r+1} + gb^{−r} − z, hb^{−r+1} + Gb^{−r} + Z]$ with $0 \leq h < b$, $1 \leq g \leq G \leq b − 1$ and $z, Z \in [0, b^{−r})$. Then $V(A \times A)$ is such that:

\[
\begin{align*}
&i) V_i(A \times A) = 0 \text{ for } i = 0, \ldots, r - 2; \\
&ii) b V_{i+1}(A \times A) \geq V_i(A \times A) \text{ for all } i \geq r; \\
&iii) V_{r-1}(A \times A) - \frac{b^{r-2}2}{b-1} V_r(A \times A) \leq \tilde{V}_r(A \times A), \text{ where } \tilde{V}_r(A \times A) = \sum_{i=r}^{\infty} V_i(A \times A).
\end{align*}
\]

The next result establishes that any unanchored interval $A$ in $[0, 1)$ has a volume vector $V(A \times A)$ that can be decomposed into a conical combination of volume vectors of elementary unanchored $(d, k)$-intervals $Y^{(d)}_k$ and elementary (anchored) $k$-intervals $1_k$. Its proof is in the appendix.

**Theorem 1** Let $A \subset [0, 1)$ be a half-open interval. For $A \neq [0, 1)$, let $r \geq 1$ be the smallest positive integer such that we can write $A = [hb^{−r+1} + gb^{−r} − z, hb^{−r+1} + Gb^{−r} + Z]$ with $0 \leq h < b$, $1 \leq g \leq G \leq b − 1$, and $z, Z \in [0, b^{−r})$. For $A = [0, 1)$, let $r = 1$. Then there exists non-negative coefficients $(\alpha_k)_{k \geq 0}$ and $(\tau_k)_{k \geq 0}$ such that $\text{Vol}(A \times A) = \sum_{k \geq 0} (\alpha_k + \tau_k)$ and

\[
V(A \times A) = \sum_{k=0}^{\infty} \alpha_k \frac{b^{2(k+r+1)}}{4} V(Y^{(r-1)}_k \times Y^{(r-1)}_k) + \sum_{k=0}^{\infty} \tau_k b^{2k} V(1_k \times 1_k).
\]

5 Pairwise sampling dependence of scrambled $(0, m, s)$—nets on unanchored boxes

This section contains our main result, which is that scrambled $(0, m, s)$—nets have a negative pairwise sampling dependence index. That is, for this construction, $H_n(A) \leq \text{Vol}(A \times A)$ for any unanchored box $A$. To prove this result, we must first provide a decomposition for $H_n(A)$ that makes use of elementary intervals and elementary unanchored $(d, k)$—intervals. To do so, we use the decomposition of an unanchored interval given in Theorem [11]. First, we introduce some notation to denote regions in $[0, 1)^{2s}$ that will be used repeatedly in this section, starting with those we get from the decomposition proved in Theorem [11].

\[
D(k, d, J) := \prod_{j \in J} Y^{(d_j)}_{k_j} \times Y^{(d_j)}_{k_j} \prod_{j \in J^c} 1_{k_j} \times 1_{k_j},
\]

(10)
where \( J \subseteq \{1, \ldots, s\} \). The interval \( Y_{k_j}^{(dj)} \) is decomposed further using

\[
Y_{k_j,1}^{(dj)} := \left( \frac{1}{b_d j+1} - \frac{1}{b_d^{k_j+1} + 1}, \frac{1}{b_d^{k_j+1} + 1} \right), \quad \text{and} \quad Y_{k_j,2}^{(dj)} := \left( \frac{1}{b_d^{k_j+1} + 1} + \frac{1}{b_d^{k_j+2} + 1} \right).
\]

We also make use of the following sub-regions, where \( I, K \subseteq J \):

\[
E(k, d, J, I) := \prod_{j \in I} \prod_{j \in J \cap K} 1_k j \times 1_k j
\]

\[
\mathcal{E}(k, d, J, I, K) := \prod_{j \in I \cap K} Y_{k_j,1}^{(dj)} \times Y_{k_j,2}^{(dj)} \prod_{j \in I \cap K} Y_{k_j,1}^{(dj)} \times Y_{k_j,2}^{(dj)} \prod_{j \in J \cap K} 1_k j \times 1_k j
\]

\[
F(k, d, J, I) := E(k, d, J, I) \times \prod_{j \in J \cap K} Y_{k_j,1}^{(dj)} \times Y_{k_j,2}^{(dj)}
\]

\[
F(k, d, J, I, K) := \mathcal{E}(k, d, J, I, K) \prod_{j \in J \cap K \cap I} Y_{k_j,1}^{(dj)} \times Y_{k_j,2}^{(dj)} \prod_{j \in J \cap K \cap I} Y_{k_j,1}^{(dj)} \times Y_{k_j,2}^{(dj)}.
\]

The region \( F(k, d, J, I) \) in which a pair of points \((U, V)\) lies will sometimes be written as the product of the two regions obtained by projecting it over the coordinates of \( U \) and then \( V \), using the notation \( F(k, d, J, I) = F_1(k, d, J, I) \times F_2(k, d, J, I) \). That is, \( F_1(k, d, J, I) := \prod_{j \in I} 1_k j + 1_j d_j + 1_j j \). \( P_j \) for \( j = 1, 2 \).

Next, we define the counting numbers \( m_b(k, d, c, J, I) \). The parameter \( c \geq 0 \) is used to specify the number of initial common digits over the subset \( I \).

**Definition 1** For \( P_n \) a digital net, let \( m_b(k, d, c, J, I) \) be the number of points \( u_r \), for a given point \( u_r \in P_n \), which are different from \( u_r \) and satisfy:

\[
\begin{align*}
\gamma_b(u_{i,j}, u_{\ell,j}) &\geq k_j + d_j + c \quad \text{if} \ j \in I; \\
\gamma_b(u_{i,j}, u_{\ell,j}) &\geq k_j \quad \text{if} \ j \in J^c; \\
\gamma_b(u_{i,j}, u_{\ell,j}) &= d_j \quad \text{if} \ j \in J \cap J^c.
\end{align*}
\]

The properties stated in the next lemma involve the above regions and will be useful to prove Theorems 2 and 3. Its proof is in the appendix.

**Lemma 3** Let \( |J| \) denote the sum \( \sum_{j \in J} k_j \) with also \( |k + 2| = \sum_{j \in J} (k_j + 2) = |k| + 2|J| \). Then:

1. \( \Vol(D(k, d, J)) = 2^{2|J|} b^{-2(|k| + |d| + 2|J|)} \).
2. \( \Vol(F_1(k, d, J, I) = b^{-(|k| + |d| + 2|J|)} \).
3. \( P(V \in F_2(k, d, J, I) | U \in F_1(k, d, J, I)) = \frac{m_b(k, d, 2, J, I, P_n)}{b^{2(|k| + |d| + 2|J|)}} \).
4. \( P((U, V) \in F(k, d, J, I, K)) = P((U, V) \in F(k, d, J, I)) \).

The next result provides us with a key decomposition for \( H_n(A) \).

**Theorem 2** Let \( A = \prod_{j=1}^s [a_j, a_j] \) be an anchored box, where \( 0 \leq a_j < A_j \leq 1, \) \( j = 1, \ldots, s \). For \( J \subseteq \{1, \ldots, s\} \) and \( k \in \mathbb{N}_0^s \), let \( \tilde{a}_{k,j} = \prod_{j \in J} a_{k_j} \prod_{j \in J^c} A_{k_j}^{(j)} \), where
where the $a_{k_j}^{(j)}$ and $r_{k_j}^{(j)}$ come from the decomposition given in Theorem 1 applied to the interval $[a_j, A_j)$, $j = 1, \ldots, s$. In particular, this means $\tilde{a}_{k, J} \geq 0$ and
\begin{equation}
\sum_{k \geq 0} \sum_{J \subseteq \{1, \ldots, s\}} \tilde{a}_{k, J} = \text{Vol}(A \times A).
\end{equation}

Let $(U, V)$ be a randomly chosen pair of points from a point set $P_n$. Then
\begin{equation}
H_n(A) = \sum_{k \geq 0} \sum_{J \subseteq \{1, \ldots, s\}} \frac{\tilde{a}_{k, J}}{\text{Vol}(D(k, d, J))} P((U, V) \in D(k, d, J)).
\end{equation}

**Proof** Using Theorem 1 we can write
\begin{align*}
V(A \times A) &= \prod_{j=1}^{s} \left( \sum_{k_j \geq 0} a_{k_j}^{(j)} b^{2(k_j+d_j+2)} \right) V(Y_{k_j}^{(d_j)} \times Y_{k_j}^{(d_j)}) + \sum_{k_j \geq 0} r_{k_j}^{(j)} b^{2k_j} V(1_{k_j} \times 1_{k_j}) \\
&= \sum_{k \geq 0} \sum_{J \subseteq \{1, \ldots, s\}} \left( \prod_{j \in J} a_{k_j}^{(j)} b^{2(k_j+d_j+2)} \prod_{j \not\in J} b^{2k_j} \right) V(D(k, d, J)) \\
&= \sum_{k \geq 0} \sum_{J \subseteq \{1, \ldots, s\}} \frac{\tilde{a}_{k, J}}{\text{Vol}(D(k, d, J))} V(D(k, d, J)),
\end{align*}

where the last equality follows from Part 1 of Lemma 3. Then, using the same kind of reasoning as in Lemma 1 we get
\begin{equation}
H_n(A) = \sum_{k \geq 0} \sum_{J \subseteq \{1, \ldots, s\}} \frac{\tilde{a}_{k, J}}{\text{Vol}(D(k, d, J))} P((U, V) \in D(k, d, J)).
\end{equation}

It is clear from Theorem 2 that in order to prove that $H_n(A) \leq \text{Vol}(A \times A)$, it is sufficient to prove that $P((U, V) \in D(k, d, J)) \leq \text{Vol}(D(k, d, J))$ for all $k, d, J$. That is, the regions $D(k, d, J)$ correspond to the extreme points in the linear programming formulation of our problem.

A key quantity to analyze this probability is the following weighted sum of counting numbers for $P_n$, where $J \subseteq \{1, \ldots, s\}$ and $I^* := I \cup J^*$:
\begin{equation}
\bar{m}_b(k, d, J; P_n) := \frac{1}{2^{|I^*|}} \sum_{I \subseteq J} b^{|k|+|d|+|J|+|I|} (b-1)^{|I|-|J|} \frac{m_b(k, d, 2, J, I; P_n)}{n-1}.
\end{equation}

**Theorem 3** Let $A$ be an unanchored box in $[0, 1]^s$. Let $H_n(A)$ and $\tilde{a}_{k, J}$ be defined as in Theorem 2. Let $P_n$ have counting numbers $m_b(k, d, 2, J, I; P_n)$ such that
\begin{equation}
\bar{m}_b(k, d, J; P_n) \leq 1,
\end{equation}

where \( \tilde{m}_b(k, d, J; P_n) \) is defined in (12). Then the scrambled point set \( P_n \) is such that

\[
H_n(A) \leq \sum_{k \geq 0} \sum_{J \subseteq \{1, \ldots, s\}} \tilde{a}_{k, J} = \text{Vol}(A \times A).
\]

**Proof** As mentioned earlier, based on Theorem\(^2\) it suffices to show that \( P((U, V) \in D(k, d, J)) \leq \text{Vol}(D(k, d, J)) \) for all 5-tuples \((m, s, k, d, J)\), where \( m \geq 1, s \geq 1, k \geq 0, d \geq 0, J \subseteq \{1, \ldots, s\} \). Indeed, if this holds, then from Theorem\(^2\) and using the fact that \( \tilde{a}_{k, J} \geq 0 \), we can derive the inequality

\[
H_n(A) = \sum_{k} \sum_{J} \tilde{a}_{k, J} \frac{P((U, V) \in D(k, d, J))}{\text{Vol}(D(k, d, J))} \leq \sum_{k} \sum_{J} \tilde{a}_{k, J} = \text{Vol}(A \times A),
\]

where the last equality is obtained from (11), also proved in Theorem\(^2\).

To analyze the probability \( P((U, V) \in D(k, d, J)) \), we use the decomposition of \( D(k, d, J) \) into the sub-regions \( F(k, d, J, I) \) outlined in Part 4 of Lemma\(^3\)

\[
\frac{P((U, V) \in D(k, d, J))}{\text{Vol}(D(k, d, J))} = \sum_{I \subseteq J} 2^{|I|} \frac{P((U, V) \in F(k, d, J, I))}{\text{Vol}(D(k, d, J))}
\]

\[
= \sum_{I \subseteq J} 2^{|I|} \frac{\text{Vol}(F_1(k, d, J, I))}{\text{Vol}(D(k, d, J))} \frac{m_b(k, d, 2, J, I; P_n)}{b^{k+1}|J|} \frac{(b-1)^{|I|}}{n-1}
\]

\[
= \sum_{I \subseteq J} 2^{|I|} \frac{b^{-|I|}m_b(k, d, 2, J, I; P_n)}{2^{|I|}b^{-2|I|}b^{k+1}|J|} \frac{(b-1)^{|I|}}{n-1} = \tilde{m}_b(k, d, J; P_n) \leq 1,
\]

where the first equality comes from Lemma\(^3\)(Part 4), the third from Lemma\(^3\)(Part 3), the fourth from Lemma\(^3\)(Parts 1, 2), and the last inequality follows from (13). \(\square\)

To get to our ultimate goal—which is captured in Theorem\(^4\) and is to prove that \( H_n(A) \leq \text{Vol}(A \times A) \) for an unanchored box \( A \) for a scrambled \((0, m, s)\)-net—thanks to Theorem\(^3\) all we need to do is to show that the condition (13) indeed holds for a \((0, m, s)\)-net. The rest of this section is devoted to this (cumbersome) task.

First we write \( \tilde{m}_b(k, d, J; P_n) = \sum_I \psi_m(k, d, J, I)/2^{|I|} \), where

\[
\psi_m(k, d, J, I) := b^{|I|}m_b(k, d, 2, J, I; P_n) \frac{(b-1)^{|I|}}{n-1}.
\]

The difficulty that arises when trying to bound the sum (12) by 1 is that some of the terms (14) can be larger than 1 for certain combinations of \( m, k, d \), and \( J \). Hence
we need to show that the smaller terms compensate for those larger than 1 so that overall, the average of these terms is indeed bounded by 1.

Now, we will not work directly with the counting numbers $m_p(k, d, 2, J; P_n)$ and will instead bound them, which in turn will yield a bound on $\psi_m(k, d, J, I)$ via (14). For the proof, we will break the problem in different cases, depending on the relative magnitude of $|k|, |d|_J$ and $|J|$, with resulting bounds shown in Propositions 1, 2 and 3.

The bounds on the $\psi_m(k, d, J, I)$ terms will make use of the following functions.

**Definition 2** Let $\ell, j, i$ be non-negative integers with $j > i$. We define

$$h_{j,i}(\ell) = \frac{b^{i+j-\ell}}{(b-1)^{j-i}} \binom{j-i-1}{\ell-2i}, \quad 2i + 1 < \ell < j + i, \quad 0 \leq i < j,$$  \hspace{1cm} (15)

and $g_{j,i}(\ell) = \begin{cases} 1 & \text{if } \ell \geq i + j \text{ or, if } \ell > 2i \text{ and } \ell \text{ is even} \\ 1 + h_{j,i}(\ell) & \text{if } 2i + 1 < \ell < j + i \text{ and } \ell \text{ is odd} \\ \left(\frac{b}{b-1}\right)^{j-i-1} & \text{if } \ell = 2i + 1 \\ 0 & \text{if } \ell \leq 2i. \end{cases}$  \hspace{1cm} (16)

In some cases, the following bound on $g_{i,j}(\ell)$ will be enough for our purpose. (Both Lemmas 4 and 5 are proved in the appendix.)

**Lemma 4** Let $j > i \geq 0$. Then

$$g_{i,j}(\ell) \leq \left(\frac{b}{b-1}\right)^{i+j-\ell} \text{ when } 2i < \ell < i + j.$$  

The next lemma gives a bound on $\psi_m(k, d, J, I)$ in the case of a $(0, m, s)$-net.

**Lemma 5** If $P_n$ is a $(0, m, s)$-net, then for $I \subset J$, $\psi_m(k, d, J, I)$ satisfies

$$\psi_m(k, d, J, I) \leq \frac{b^m}{b^m - 1} g_{|J| - |I|}(m - |k|_I - |d|_J).$$  \hspace{1cm} (17)

Moreover, when $2|I| < m - |k|_I - |d|_J < |J| + |I|$, then

$$\psi_m(k, d, J, I) \leq \frac{b^m}{b^m - 1} \left(\frac{b - 1}{b}\right)^{m - |k|_I - |d|_J - |I| - |J|}. \hspace{1cm} (18)$$

Having found a bound for $\psi_m(k, d, J, I)$ for the possible ranges of values for $m$, we can now return to the task of bounding the weighted sum $\tilde{m}_b(k, d, J; P_n)$. We start with the easiest case.

**Proposition 1** Let $P_n$ be a $(0, m, s)$-net. If $J \neq \emptyset$ and $m \geq |k| + |d|_J + 2|J|$ then $\tilde{m}_b(k, d, J; P_n) \leq 1$.

**Proof** In this case, $m - |k|_I - |d|_J \geq |I| + |J|$ for all $I$ (for a given $J$) and therefore
\[ \tilde{m}_b(k, d, J; P_n) = \frac{1}{2^{|J|}} \sum_{I \subseteq J} \psi_m(k, d, J, I) \leq \frac{1}{2^{|J|}} \frac{b^m}{b^m - 1} \sum_{I \subseteq J} 1 + \frac{1}{2^{|J|}} \psi_m(k, d, J, J), \]

where the inequality is derived from Lemma 5. Observing that \( m_b(k, d, 2, J; P_n) = m_b(\bar{k}; P_n) \), where \( \bar{k}_j := k_j \) if \( j \in J^c \) and \( \bar{k}_j := k_j + d_j + 2 \) if \( j \in J \), we get

\[ \psi_m(k, d, J, J) = b^{|k|+|d|+2|J|} \frac{m_b(\bar{k}; P_n)}{n - 1} = b^{m-|k|-|d|-2|J| - 1} \frac{b^{m-|k|-|d|-2|J| - 1}}{n - 1} \]

and therefore obtain

\[
\tilde{m}_b(k, d, J; P_n) \leq \frac{1}{2^{|J|}} \frac{b^m}{b^m - 1} \sum_{I \subseteq J} 1 + \frac{1}{2^{|J|}} b^{|k|+|d|+2|J|} \frac{b^{m-|k|-|d|-2|J| - 1}}{b^m - 1} = \frac{2^{|J|} - 1}{2^{|J|}} \frac{b^m}{b^m - 1} + \frac{1}{2^{|J|}} \frac{b^m - b^{|k|+|d|+2|J|}}{b^m - 1} = \frac{b^m}{b^m - 1} \left( \frac{2^{|J|} - b^{|k|+|d|+2|J|}}{2^{|J|} - 1} \right). \]

Therefore \( \tilde{m}_b(k, d, J; P_n) \leq 1 \) if \( b^m 2^{|J|} - b^{|k|+|d|+2|J|} \leq 2^{|J|} (b^m - 1) \), or equivalently, if \( 2^{|J|} \leq b^{|k|+|d|+2|J|} \), which is true since \( b \geq 2 \), and \( |k| + |d| + 2|J| > |J| \). \( \square \)

Next, we deal with the more difficult case \( m < |k| + |d| + 2|J| \), which implies that the bound given in Lemma 5 for \( \psi_m(k, d, J, I) \) is sometimes larger than 1. Note that from (19), we see that \( m_b(\bar{k}; P_n) = 0 \) and thus \( \psi_m(k, d, J, J) = 0 \) in this case.

To handle this case, we need to analyze the function

\[ G(m, s, J, k, d) = \sum_{I \subseteq J} g_{|J|, |I|} (m - |k|_I - |d|_I), \]

which we may at times write as

\[ G(m, s, J, k, d) = \sum_{l \subseteq J, m^* > l |I| + 1} 1 + \sum_{l \subseteq J, m^* = l |I| + 1} h_{|J|, |I|} (m^*) + \sum_{l \subseteq J, m^* = l |I| + 1} \left( \frac{b}{b - 1} \right)^{|I| - 0.5 m^*} \frac{b^{m^* - 1}}{b^{m^*} - 1} \]

where \( m^* := m - |k|_I - |d|_I \) and \( M(J) = \{ I \subseteq J : 2|I| + 1 < m^* < |J| + |I|, m^* \text{ odd} \} \).

To show \( m_b(k, d, J; P_n) = \sum_{l \subseteq J} \psi_m(k, d, J, I)/2^{|J|} \leq 1 \), from the bound (17) on \( \psi_m(k, d, J, I) \) we see it is sufficient to show

\[ G(m, s, J, k, d) \leq 2^{|J|} \frac{b^m}{b^m - 1} \]

since then

\[ \tilde{m}_b(k, d, J; P_n) \leq \frac{1}{2^{|J|}} \frac{b^m}{b^m - 1} G(m, s, J, k, d) \leq 1. \]

The following lemma will allow us to set \( d = 0 \) when bounding \( G(m, s, J, k, d) \).

**Lemma 6** If \( g_0 \geq 0 \) is a constant such that \( G(m, s, J, k, 0) \leq g_0 \) for all \( (m, s, J, k) \), then \( G(m, s, J, k, d) \leq g_0 \) for all \( (m, s, J, k, d) \).
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**Proof** If \(m < |d|_j\) then \(m^* < 2|I|\) for all \(I \subset J\) and therefore \(G(m, s, J, k, d) = 0\). If \(m \geq |d|_j\) then it is easy to see that \(G(m, s, J, k, d) = G(m - |d|_j, s, J, k, 0)\), because \((m, s, J, k, d)\) and \((m - |d|_j, s, J, k, 0)\) yield the same \(m^*\) for all \(I \subset J\), and \(G(m, s, J, k, d)\) only depend on \(m, k,\) and \(d\) through \(m^*\).

Based on this result, we set \(d = 0\) in what follows, and consider two different sub-cases. The respective bounds on \(G(m, s, J, k, 0)\) are given in Propositions \(\text{2}\) and \(\text{3}\) which also establish that the condition \(\text{13}\)—stating that \(\tilde{m}_b(k, d, J; P_n) \leq 1\)—holds for each sub-case. Before we state and prove these two propositions, we first state a technical lemma needed in the proof of Proposition \(\text{2}\) and proved in the appendix.

**Lemma 7** For \(b, s \geq 2\) and \(\tilde{s} = \lfloor \frac{s}{2} \rfloor - 1\). Then

\[
R(b, s) := \frac{1}{2s} \sum_{j=0}^{\tilde{s}} \binom{s}{j} \left( \frac{b}{b-1} \right)^{s-j} \leq 1.
\]

**Proposition 2** Let \(P_n\) be a \((0, m, s)\)-net. If \(J \neq \emptyset\) and \(m < |J|\) then \(G(m, s, J, k, 0) \leq (b-1)/b\) for all \(k\) and therefore \(\tilde{m}_b(k, 0, J; P_n) \leq 1\).

**Proof** The fact that \(m < |J|\) implies \(m - |k|_I < |J| + |I|\) for all \(I\). Also, if \(|J| \geq 0.5(|J| - 1)\) then \(m - |k|_I \leq 2|I|\) for all \(k\) and then \(g_{\frac{|J|}{|I|}}(m - |k|_I) = 0\). Thus

\[
G(m, s, J, k, 0) \leq \sum_{I: |J| < 0.5(|J| - 1)} \frac{1}{|J|} \left( \frac{b}{b-1} \right)^{|J|-1} (s - 1) \leq \sum_{i=0}^{\lfloor 0.5|J| - 1 \rfloor} \binom{s}{i} \left( \frac{b}{b-1} \right)^{|J|-i}.
\]

It turns out that in this case, the simpler but larger bound \(\text{18}\) can be used (since the only non-zero \(g_{\frac{|J|}{|I|}}(m - |k|_I)\) terms are those for which \(2|I| < m - |k|_I < |I| + |J|\), which means \(\text{18}\) can indeed be applied), so we have

\[
G(m, s, J, k, 0) \leq \sum_{I: |J| < 0.5(|J| - 1)} \left( \frac{b}{b-1} \right)^{m - |k|_I - |J|} \leq \sum_{i=0}^{\lfloor 0.5|J| - 1 \rfloor} \frac{b}{b-1} \left( \frac{b}{b-1} \right)^{|J| - i},
\]

where the second inequality comes from the fact that \(m - |k|_I > 2|I|\) implies \(|J| + |I| + |k|_I - m \leq |J| - |I| - 1\).

Using Lemma \(\text{7}\) with \(s = |J|\), we get that the sum in \(\text{20}\) is bounded by 1. Hence

\[
\tilde{m}_b(k, 0, J; P_n) \leq \frac{1}{2|J|} \frac{b^m - 1}{b^m - 1} < 1, \text{ for any } |J| \geq 2, m \geq 1.
\]

The last case we need to deal with is when \(m\) is such that \(|J| \leq m < |k| + 2|J|\). Let \(\mathcal{B}\) be the set of pairs \((m, k)\) satisfying this assumption.

To handle this case, we make use of the following two lemmas about \(G(m, s, k, J, 0)\). The first one shows that when \(k = d = 0\) the maximum is reached when \(m = 2|J| - 1\). The second one shows it is sufficient to bound \(G(m, s, J, k, 0)\) at \(k = 0\).
Lemma 8 If \( k = d = 0 \), then \( G(m, s, J, 0, 0) \leq G(2|J| - 1, s, J, 0, 0) = 2^{|J|} - 1 \) for all \( m \) such that \((m, 0) \in \mathcal{B}\).

Lemma 9 Consider a pair \((m, k)\) with possibly \( k \neq 0\). Then there exists an odd integer value \( \tilde{m} \) such that \( G(\tilde{m}, s, J, 0, 0) \geq G(m, s, J, k, 0)\).

Using these two lemmas (proved in the appendix), we get a bound on \( G(m, s, J, k, 0)\) for this last case, which in turn allows us to show that (13) also holds then.

Proposition 3 Let \( P_n \) be a \((0, m, s)\)-net. Assume \( m \) is such that \( |J| \leq m < |k| + 2|J|\). Then \( G(m, s, J, k, 0) \leq 2^{|J|} - 1 \) and therefore \( \tilde{m}_b(k, 0, J; P_n) \leq 1\).

Proof For a given \( s \) and \( J \), we need to find a bound for \( G(m, s, J, k, 0)\) over all pairs \((m, k) \in \mathcal{B}\), and do so by showing it is maximized when \( k = 0 \) and \( m = 2|J| - 1\).

First, from Lemma 9 we have that for a given \((m, k) \in \mathcal{B}\), we can find a pair in \( \mathcal{B} \) of the form \((\tilde{m}, 0)\) such that \( G(\tilde{m}, s, J, 0, 0) \geq G(m, s, J, k, 0)\). Hence we can set \( k = 0 \). Next, we use Lemma 8 which shows that for pairs in \( \mathcal{B} \) of the form \((m, 0)\), the function \( G(m, s, J, k, 0)\) is maximized when \( m = 2|J| - 1\).

Putting these two lemmas together, we get that for a given \( s \) and \( J \), \( G(m, s, J, k, 0) \leq G(\tilde{m}, s, J, 0, 0) \leq G(2|J| - 1, s, J, 0, 0) = 2^{|J|} - 1 \) for all \((m, k) \in \mathcal{B}\). Hence

\[
\tilde{m}_b(k, d, J; P_n) \leq \frac{1}{2|J|} \left( \frac{b^m}{b^m - 1} \right) (2^{|J|} - 1) = \frac{b^m - 1}{b^m - 1} \frac{2^{|J|} - 1}{2^{|J|}} \leq 1,
\]

which holds since \( 2^{|J|} \leq b^m \), as \( b \geq 2 \), and \( m \geq |J|\).

Having examined all possible cases, we can now state our main result.

Theorem 4 If \( \tilde{P}_n \) is a scrambled \((0, m, s)\)-net in base \( b \), then \( H_n(A) \leq \text{Vol}(A \times A) \) for any unanchored box \( A \in \mathcal{A}\), and thus its pairwise sampling dependence index satisfies \( \mathcal{E}_n(\tilde{P}_n) \leq 0\).

Proof Using Theorem 3, we need to show that \( \tilde{m}_b(k, d, J; P_n) \leq 1 \) for all \( k, d, J \) for a \((0, m, s)\)-net \( P_n \), i.e., that condition (13) holds for a \((0, m, s)\)-net. First, from Proposition 1 if \( J \neq \emptyset \) and \( m \geq |k| + |d| + 2|J|\) then

\[
\tilde{m}_b(k, d, J; P_n) \leq \frac{b^m}{b^m - 1} \left( \frac{2^{|J|} - b^{|J|} - 1}{2^{|J|} - 1} \right) \leq 1.
\]

Next, from Proposition 2 we have that if \( J \neq \emptyset \) and \( m < |J| \) then

\[
\tilde{m}_b(k, d, J; P_n) \leq \frac{b^m}{b^m - 1} \left( \frac{b - 1}{b} \right) \leq 1.
\]

Then, using Proposition 3 we get that if \( 0 < |J| < m < |k| + |d| + 2|J| \) then

\[
\tilde{m}_b(k, d, J; P_n) \leq \frac{b^m}{b^m - 1} \left( \frac{2^{|J|} - 1}{2^{|J|}} \right) \leq 1.
\]

Finally, if \( J = \emptyset \) then
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\[
\hat{m}_b(k,d,J;P_n) = \frac{P((U,V) \in D(k,d,J))}{\text{Vol}(D(k,d,J))} = \frac{1}{b^{-2|k|}b^{-|k|}} \frac{\max(b^{m-|k|} - 1, 0)}{b^m - 1} = C_b(k;P_n),
\]

which was shown to be smaller or equal to 1 in [10] for a \((0,m,s)\)-net. □

Using Theorem 4, we obtain the following result, which shows that a scrambled net integrates the indicator function \(1_A\) of any unanchored box \(A\) with variance no larger than the Monte Carlo estimator variance. To our knowledge, this was not previously known. What is well known is that since \(A\) is an axis-parallel box, then \(1_A\) has bounded variation in the sense of Hardy and Krause and therefore a scrambled net has variance in \(O(n^{-2} \log n)^3\) [9].

**Proposition 4** Let \(A\) be an unanchored box in \([0,1]^s\). Let \(\hat{\mu}_{n,A}\) be the estimator for \(\mu_A = E(1_A) = \text{Vol}(A)\) based on a scrambled \((0,m,s)\)-net in base \(b\) with \(n = b^m\). Then \(\text{Var}(\hat{\mu}_{n,A}) \leq \mu_A(1 - \mu_A)/n\).

**Proof** The result follows from the fact that \(\text{Var}(\hat{\mu}_{n,A}) = \mu_A(1 - \mu_A)/n + (H_n(A) - \mu_A^2)(n-1)/n\), and then applying Theorem 4 to show that \((H_n(A) - \mu_A^2) \leq 0\). □

6 The scrambling advantage

We now give an example showing the advantage of scrambling over a digital shift, which is a simpler randomization. It uses a point set \(P_n\) with \(C_b(k;P_n) \leq 1\) such that \(P((U,V) \in A \times A) > \text{Vol}(A \times A)\) for an anchored box \(A\), for \((U,V)\) a pair of distinct points randomly chosen from the digitally shifted point set \(P_n^{\text{dig}}\). So even the less restrictive condition \(E_{n,0}(\rho_n^{\text{dig}}) \leq 0\) is not met. On the other hand, since \(C_b(k;P_n) \leq 1\), Theorem 4.16 in [10] implies that \(P(U \in A, V \in A) \leq \text{Vol}^2(A)\) for \((U,V)\) randomly chosen from the scrambled point set \(\tilde{P}_n\).

**Example 1** Consider the two-dimensional point set \(P_n = \{(i/5,i/5), (i/5,(i + 1) \mod 5)/5), i = 0, \ldots, 4\}\). We first verify that \(C_b(k;P_n) \leq 1\): this clearly holds for \(k = \mathbf{0}\). For \(k \in \{(1,0),(0,1)\}\), we have \(C_b(k;P_n) = 5 \times 1/9\). And for \(k\) with \(|k| \geq 2\) we have \(C_b(k;P_n) = 0\). Now consider the box \(A = [0.1/10 \times 0.2/5]\). Let us compute \(P((U,V) \in A \times A)\), where \((U,V)\) is a pair of distinct points randomly chosen from \(\tilde{P}_n^{\text{dig}}\), where \(\tilde{P}_n^{\text{dig}} = P_n + v\), where the addition is done digitwise and \(v \sim U(0,1)^2\). Let \(v = (v_1,v_2)\) with \(v_j = 0.0v_{j,1}v_{j,2} \ldots, j = 1,2\). Then we see that among the \(5^2\) possibilities for \((v_{1,1},v_{2,1})\), one point from \(\tilde{P}_n^{\text{dig}}\) will be in the square \([0,1/5] \times [0,1/5]\) and one in the square \([0,1/5] \times [1/5,2/5]\) if and only if \(v_{1,1} = v_{2,1}\), which happens with probability 1/5. Given that this happens, then it should also be clear that both points in that pair will be in \(A\) if and only if \((0.0v_{1,2}v_{1,3} \ldots, 0.0v_{2,2}v_{2,3} \ldots) \in [0,1/10] \times [0,1/5]\), which happens with probability 1/2 since \(v \sim U(0,1)^2\). Putting this all together, we get
\[ P((U, V) \in A \times A) = \frac{1}{\frac{1}{45^2}} = \frac{1}{450}, \] where the fraction 1/45 corresponds to the probability of choosing the pair of points falling in the squares (0,0) and (0,1) among the 45 different (unordered) pairs. Since \( \text{Vol}(A) = 1/25 \), we have that
\[ P((U, V) \in A \times A) > (\text{Vol}(A))^2 = 1/625. \]

7 Future work

In this paper, we have introduced a measure of uniformity for randomized QMC point sets that compares them to random sampling. This pairwise sampling dependence index was shown to be no larger than 0 for scrambled \((0, m, s)\)-nets, thus extending from anchored boxes to unanchored boxes the main result from [10]. For future work, we plan to try to extend our proof to the first \(n\) points of a scrambled \((0, s)\)-sequence. We also plan to explore how this result can lead to new bounds for the variance of scrambled \((0, m, s)\)-nets in terms of the Monte Carlo variance for some functions.

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Appendix: Proofs and Technical Lemmas

We first prove results stated in the main part of the paper. These proofs make use of Lemmas 10 to 15, which are presented in the second part of the appendix.

Proof of Lemma 2. In what follows, we will use the notation $x_\ell$ to represent the $\ell$th digit in the base $b$ representation of $x \in [0,1)$, i.e., $x = \sum_{\ell \geq 1} x_\ell b^{-\ell}$, and the corresponding notation $x = 0.x_1x_2x_3 \ldots$

First, we decompose $A$ into three parts as $A_1 = [hb^{-r+1} + gb^{-r} - z, hb^{-r+1} + gb^{-r})$, $A_2 = [hb^{-r+1} + Gb^{-r}, hb^{-r+1} + Gb^{-r} + Z)$, $A_3 = [hb^{-r+1} + gb^{-r}, hb^{-r+1} + Gb^{-r})$. Hence we have

$$V_i(A \times A) = \sum_{\ell=1}^{3} V_i(A_\ell \times A_\ell) + 2(V_i(A_1 \times A_2) + V_i(A_1 \times A_3) + V_i(A_2 \times A_3)), \quad i \geq 0. \tag{21}$$

Since $A_1$ and $A_2$ are both completely contained in the respective intervals $[hb^{-r+1} + (g-1)b^{-r}, hb^{-r+1} + gb^{-r})$ and $[hb^{-r+1} + Gb^{-r}, hb^{-r+1} + (G+1)b^{-r})$, any $x$ in $A_1$ is of the form $0.h_1 \ldots h_{r-1}(g-1)x_{r+1}x_{r+2} \ldots$. Similarly, $y \in A_2$ is of the form $0.h_1 \ldots h_{r-1}(G)x_{r+1}x_{r+2} \ldots$. On the other hand, for $z \in A_3$ we have that $z_\ell = h_i$ for $i \leq r-1$, $z_r \in \{g, \ldots, G-1\}$, and $z_\ell \geq 0$ for $\ell > r$. From this we infer:

1. No pair of points from $A_1$ or $A_2$ have less than $r$ initial common digits, thus $V_i(A_1 \times A_\ell) = 0$ for $i = 0, \ldots, r-1$ and $\ell = 1, 2$.
2. No pair of points from $A_3$ have less than $r-1$ initial common digits, thus $V_i(A_3 \times A_\ell) = 0$ for $i = 0, \ldots, r-2$.
3. A pair of points from any two of the following subsets: $A_1$, $A_2$, $[hb^{-r+1} + \beta b^{-r}$, $hb^{-r+1} + (\beta + 1)b^{-r}) \subseteq A_3$, where $\beta = g, \ldots, G-1$ has exactly $r-1$ initial common digits, thus $V_{r-1}(A_j \times A_\ell) = \text{Vol}(A_j) \text{Vol}(A_\ell)$ for $j \neq \ell$, $V_{r-1}(A_3 \times A_3) = (G-g)(G-g-1)b^{-2r}$ and $V_i(A_j \times A_\ell) = 0$ for $i \geq r, j \neq \ell$.

Note that this implies that $\tilde{V}_r(A_i \times A_i) = \text{Vol}^2(A_i)$ for $i = 1, 2$, and (using item (3)) $\tilde{V}_r(A_3 \times A_3) = \text{Vol}^2(A_3) - V_{r-1}(A_3 \times A_3) = (G-g)b^{-2r}$.

The above statements also allow us to simplify (21) as follows:

$$V_{r-1}(A \times A) = V_{r-1}(A_3 \times A_3) + 2 \sum_{1 \leq \ell < \ell \leq 3} V_{r-1}(A_\ell \times A_\ell)$$

$$= V_{r-1}(A_3 \times A_3) + 2 \sum_{1 \leq \ell < \ell \leq 3} \text{Vol}(A_i) \text{Vol}(A_\ell) \tag{22}$$

$$V_i(A \times A) = \sum_{\ell=1}^{3} V_i(A_\ell \times A_\ell), \quad i \geq r. \tag{23}$$

To prove (ii), consider the mappings $\varphi_j : [0,1) \to [0,1), 1 \leq j \leq 3$ defined as:
\[
\phi_1(hb^{-r+1} + gb^{-r} - x) = 1 - x, \quad 0 \leq x < b^{-r} \\
\phi_2(hb^{-r+1} + Gb^{-r} + x) = x, \quad 0 \leq x < b^{-r} \\
\phi_3(hb^{-r+1} + gb^{-r} + x) = x, \quad 0 \leq x < (G-g)b^{-r}.
\]

All three are isometric mappings and such that \(\phi_1(A_1) = [1-z, 1), \phi_2(A_2) = [0, Z),\) and \(\phi_3(A_3) = [0, (G-g)b^{-r}).\) Also, since \(\phi_j\) simply amounts to changing the first \(r\) digits of a point in \(A_j\) (and applies the same change to all points in \(A_j\)), it implies

\[
\gamma_h(\phi_j(v_{j,\ell}), \phi_j(v_{j,h})) = \gamma_h(v_{j,\ell}, v_{j,h}), \quad j = 1, 2, 3,
\]

where \(v_{1,\ell} = hb^{-r+1} + gb^{-r} - x, v_{1,h} = hb^{-r+1} + gb^{-r} - y, v_{2,\ell} = hb^{-r+1} + Gb^{-r} + x, v_{2,h} = hb^{-r+1} + Gb^{-r} + y,\) and \(v_{3,\ell} = hb^{-r+1} + gb^{-r} + w, v_{3,h} = hb^{-r+1} + gb^{-r} + z.\)

Therefore

\[
\begin{align*}
V_i(A_1 \times A_1) &= V_i(\phi_1(A_1) \times \phi_1(A_1)) = V_i([1-z, 1] \times [1-z, 1]) = V_i([0, z], [0, z]) \\
V_i(A_2 \times A_2) &= V_i(\phi_2(A_2) \times \phi_2(A_2)) = V_i([0, Z] \times [0, Z]) \\
V_i(A_3 \times A_3) &= V_i(\phi_3(A_3) \times \phi_3(A_3)) = V_i([0, (G-g)b^{-r}] \times [0, (G-g)b^{-r}]).
\end{align*}
\]

These intervals, being anchored at the origin, satisfy the assumptions of Lemma 2.6 from [10], which implies \(bV_{i+1}(A_j \times A_j) - V_i(A_j \times A_j) \geq 0\) for \(j = 1, 2, 3\) and \(i \geq 0.\) Combining this with (24), property (ii) in the statement of Lemma 2 is established.

For (iii), let us first assume \(g = G,\) and thus \(A_1 = \emptyset.\) Then, using (22), we get \(V_{r-1}(A \times A) = 2\text{Vol}(A_1 \times A_2).\) Furthermore, \(V_r(A, A) = V_r(A_1 \times A_1) + V_r(A_2 \times A_2) = \text{Vol}^2(A_1) + \text{Vol}^2(A_2).\) Since \(2\text{Vol}(A_1 \times A_2) \leq \text{Vol}^2(A_1) + \text{Vol}^2(A_2),\) (iii) is proved.

Now assume \(g < G.\) In this case, we need to further refine \(A_1\) and \(A_2\) as:

\[
\begin{align*}
A_1 &= [hb^{-r+1} + gb^{-r} - db^{-(r+1)} - f, hb^{-r+1} + gb^{-r}) \\
A_2 &= [hb^{-r+1} + Gb^{-r}, hb^{-r+1} + Gb^{-r} + Db^{-(r+1)} + F),
\end{align*}
\]

where \(0 \leq d, D \leq b - 1, f, F \in [0, b^{-(r+1)}).\) Using (22) and (23), we then write

\[
\begin{align*}
V_{r-1}(A \times A) &= V_{r-1}(A_3 \times A_3) + 2 \sum_{1 \leq i < \ell \leq 3} \text{Vol}(A_i)\text{Vol}(A_\ell) \\
&= \frac{(G-g)(G-g-1)}{b^{2r}} + 2 \left(\left(\frac{d}{b^{r+1} + f}\right) \left(\frac{D}{b^{r+1} + F}\right) + \frac{G-g}{b^{r}} \left(\frac{d}{b^{r+1} + f}\right)
\right)
\end{align*}
\]

\[
\frac{G-g}{b^{r}} \left(\frac{D}{b^{r+1} + F}\right)
\]

\[
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\[
V_r(A \times A) = \sum_{t=1}^{3} V_r(A_t \times A_t) = V_r(A_1 \times A_1) + V_r(A_2 \times A_2) + \frac{G - g \, b - 1}{b^{2r}}
\]

\[
= \frac{(d-1)d}{b^{2(r+1)}} + \frac{2fd}{b^{r+1}} + \frac{(D-1)D}{b^{2(r+1)}} + \frac{2FD}{b^{r+1}} + \frac{G - g \, b - 1}{b^{2r}}
\]

\[
\bar{V}_r(A \times A) = \left( \frac{d}{b^{r+1}} + f \right)^2 + \left( \frac{D}{b^{r+1}} + F \right)^2 + \frac{G - g}{b^{2r}}.
\]

The last equality for \(V_r(A \times A)\) is obtained by observing that for \((x, y)\) to be in \(V_r(A_1 \times A_1)\), either (i) \(x = 0, h_1, \ldots, h_{r-1}(g-1)d_1\ldots \) and \(y = 0, h_1, \ldots, h_{r-1}(g-1)d_2\ldots \) with \(d_1 \neq d_2 \in \{0, \ldots, d-1\}\), or (ii) one of them is of the form \(z_1 + (0, h_1, \ldots, h_{r-1}(g-1)d)\) with \(z_1 \in [0, f)\) and the other is of the form \(0, h_1, \ldots, h_{r-1}(g-1)d_1\ldots \) with \(d_1 \in \{0, \ldots, d-1\}\). Case (i) contributes a volume of size \((d-1)db^{-2(r+1)}\) and case (ii) contributes \(2fd db^{-2(r+1)}\). A similar argument can be used to derive \(V_r(A_2 \times A_2)\).

Therefore \(V_{r-1}(A \times A) - \frac{b^{2r}}{b^{2r} + 1} V_r(A \times A) \leq \bar{V}_r(A \times A)\) holds if

\[
\frac{(G-g)(G-g-1)}{b^{2r}} + \frac{2}{b^{r+1}} \left( \frac{D}{b^{r+1}} + F \right)^2 + \frac{d}{b^{r+1}} + f \right)^2
\]

\[
\leq \left( \frac{d}{b^{r+1}} + f \right)^2 + \left( \frac{D}{b^{r+1}} + F \right)^2 + \frac{G - g}{b^{2r}}.
\]

Since

\[
2 \left( \frac{d}{b^{r+1}} + f \right) \left( \frac{D}{b^{r+1}} + F \right) \leq \left( \frac{d}{b^{r+1}} + f \right)^2 + \left( \frac{D}{b^{r+1}} + F \right)^2
\]

it means that to prove (24) it is sufficient to show that

\[
\frac{(G-g)(G-g-1)}{b^{2r}} - \frac{(b-2)}{b^{2r}} \frac{G-g}{b^{2r}} + \frac{2}{b^{r+1}} \left( \frac{d+D}{b^{r+1}} + f + F \right)
\]

\[
\leq \frac{G - g}{b^{2r}},
\]

or equivalently, that

\[
-b^2(G-g)(b-(G-g)) + 2b(G-g) \left( d + b^{r+1} + f + F \right)
\]

\[
- \frac{b(b-2)}{b-1} \left( - (d-1)d + 2fd + b^{r+1} + (D-1)D + 2FD \right) \leq 0.
\]

Note that \(G - g \leq b - 2\) by assumption. We proceed by considering three cases:

**Case 1:** \(G - g \leq b - 4\). This implies \(b - (G-g) \geq 4\) (and thus \(b \geq 4\)). Also, to handle this case we use the fact that \(0 \leq f b^{r+1}, Fb^{r+1} < 1\). By making appropriate substitutions for \(f\) and \(F\), we see that to prove (25) holds it is sufficient to show that
We will show this holds by finding the value $d$. We view the LHS as the sum of two quadratic polynomials, $p(d)$ and $p(D)$, and thus argue it is sufficient to show that

$$-4b^2(G-g) + 2b(G-g)(d + D + 2) - \frac{b(b-2)}{b-1}(d(d-1) + D(D-1)) \leq 0$$

which holds because $d + D + 2 \leq 2b$.

**Case 2:** $G-g = b-3$ First note that this implies $b \geq 3$. Next, we replace $G-g$ with $b-3$ in (23) and divide each term by $b$. For this case, we can use the bound $0 \leq f b^{r+1}, Fb^{r+1} < 1$ and by substituting appropriately, it means it is sufficient to show

$$-3b(b-3) + 2(b-3)(d + D + 2) - \frac{b-2}{b-1}(d(d-1) + D(D-1)) \leq 0.$$

We view the LHS as the sum of two quadratic polynomials, $p(d)$ and $p(D)$, and show that $p(d_{max}) \leq 0$. We have that

$$p'(d) = -2d \frac{b-2}{b-1} + 2(b-3) + \frac{b-2}{b-1}.$$ 

Therefore

$$d_{max} = \left( 2(b-3) + \frac{b-2}{b-1} \right) \frac{b-1}{2(b-2)} = \left( \frac{(b-3)(b-1)}{b-2} + \frac{1}{2} \right).$$

Hence $d_{max} \in (b-2.5, b-1.5)$. Thus it is sufficient to show $p(b-2) \leq 0$. Now,

$$p(b-2) = -\frac{(b-2)^3}{b-1} + (b-2) \left( 2(b-3) + \frac{b-2}{b-1} \right) - (b-3)(3b/2 - 2)$$

therefore

$$(b-1)p(b-2) = -(b-2)^3 + 2(b-1)(b-2)(b-3) + (b-2)^2 - \left( \frac{3b}{2} - 2 \right)(b-3)(b-1)$$

$$= (3-b)(b^2 - 3b + 4)/2 = (3-b)(b(b-3) + 4)/2 \leq 0$$

since $b \geq 3$.

**Case 3:** $G-g = b-2$

In this case (25) becomes

$$-2b^2(b-2) + 2b(b-2)(d + D + (f + F)b^{r+1}) - \frac{b(b-2)}{b-1} \left( d(d-1) + D(D-1) + 2b^{r+1}(fd + FD) \right) \leq 0$$

$$\Leftrightarrow -2b + 2(d + D + (f + F)b^{r+1}) - \frac{1}{b-1} \left( d(d-1) + D(D-1) + 2b^{r+1}(fd + FD) \right) \leq 0.$$
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As in the case \(G - g = b - 3\), we argue it is sufficient to show each of the quadratic polynomials in \(d\) and \(D\) on the LHS (which are the same) is bounded from above by 0. That is, we need to show

\[
q(d) := -\frac{d^2}{b - 1} + d \left( 2 + \frac{1}{b - 1} - \frac{2fb^{r+1}}{b - 1} \right) - (b - 2fb^{r+1}) \leq 0.
\]

Now

\[
q'(d) = -\frac{2d}{b - 1} + 2 + \frac{1}{b - 1} - \frac{2fb^{r+1}}{b - 1}
\]

and thus \(d_{\text{max}} = \left( 2 + \frac{1}{b - 1} - \frac{2fb^{r+1}}{b - 1} \right) \frac{b - 1}{2} = b - 0.5 - fb^{r+1}\), which implies \(d_{\text{max}} \in (b - 1.5, b - 0.5)\). Thus it is sufficient to show \(q(b - 1) \leq 0\). We have that

\[
q(b - 1) = -(b - 1) + (b - 1) \left( 2 + \frac{1}{b - 1} - \frac{2fb^{r+1}}{b - 1} \right) - (b - 2fb^{r+1})
\]

\[
= (b - 1) + 1 - 2fb^{r+1} - b + 2fb^{r+1} = 0
\]

as required.

\(\square\)

**Proof (of Theorem 1)** To simplify the notation, we define \(Z_k := b^{2k}V(1_k \times 1_k)\) and \((W_{k}^{(r-1)} := (b^{2(k+r+1)}/4)V(Y_k^{(r-1)} \times Y_k^{(r-1)})\) to be the (normalized) volume vectors of \(k\)-elementary intervals and elementary unanchored \((k, r - 1)\)-intervals, respectively. Since the coordinates of each of these vectors are positive and sum to one, \(V(A \times A) = \sum_{k \geq 0} (a_k + \tau_k)\) follows immediately from the last equality in the statement of the theorem.

Based on the definition of \(Y_k^{(r-1)}\), the vectors \(W_k^{(r-1)}\) satisfy, for \(i \geq 0, r \geq 1\),

\[
W_{i,k}^{(r-1)} = \begin{cases} 
1/2 & \text{if } i = r - 1 \\
(b - 1)/2b^{i-1}(k+r) & \text{if } i \geq k + r + 1 \\
0 & \text{otherwise},
\end{cases}
\]

while

\[
Z_{i,k} = \begin{cases} 
0 & \text{if } i < k \\
(b - 1)/b^{i-k+1} & \text{if } i \geq k.
\end{cases}
\]

Note that

\[
W_{r-1,k}^{(r-1)} = 1/2 \text{ for all } k \geq 0 \quad (26)
\]

\[
W_{i,k}^{(r-1)} = Z_{i,k+r+1}/2 \text{ for } i \geq k + r + 1. \quad (27)
\]

There are two cases to consider. First, if \(V_{r-1}(A \times A) \leq bV_r(A \times A)\), then based on Properties (i) and (ii) from Lemma 4 we can decompose \(V(A \times A)\) solely with the \(Z_k\)’s, i.e., we set \(a_k = 0\) for all \(k\) and
\[ \tau_k = \frac{b V_k(A \times A) - V_{k-1}(A \times A)}{b - 1} \quad k \geq r - 1 \]

and \( \tau_k = 0 \) if \( 0 \leq k \leq r - 2 \). Note that \( A = [0, 1] \) fits into this first case.

Second, if \( V_{r-1}(A \times A) \geq b V_r(A \times A) \), then we first decompose the vector \( \sum_{k=r}^{\infty} V_k(A \times A) e_k \), where \( e_k \) is a (canonical) vector of zeros with a 1 in position \( k \), (note that this agrees with the vector \( V(A \times A) \) everywhere except on index \( r - 1 \), where it has a 0 instead of \( 1 \)).

Second, if \( V_{r-1}(A \times A) \geq b V_r(A \times A) \), then we first decompose the vector \( \sum_{k=r}^{\infty} V_k(A \times A) e_k \), where \( e_k \) is a (canonical) vector of zeros with a 1 in position \( k \), (note that this agrees with the vector \( V(A \times A) \) everywhere except on index \( r - 1 \), where it has a 0 instead of \( 1 \)).

From Lemma 2 we know \( \bar{\tau}_k \geq 0 \) for \( k \geq r + 1 \). Note that \( b \bar{\tau}_r Z_{r-1} - \bar{\tau}_r Z_r = b V_r(A \times A) e_{r-1} \), i.e., \( b \bar{\tau}_r Z_{r-1} \) agrees with \( \bar{\tau}_r Z_r \) everywhere except on index \( r - 1 \). Therefore

\[ V(A \times A) - b \bar{\tau}_r Z_{r-1} - \sum_{k=r+1}^{\infty} \bar{\tau}_k Z_k = (V_{r-1}(A \times A) - b V_r(A \times A)) e_{r-1}. \]

Hence the \( \sum_{k=0}^{\infty} \alpha_k W_k^{(r-1)} \) part of the decomposition is only needed to decompose 
\[ V_{r-1}(A \times A) - b V_r(A \times A) \]. We claim there exists \( \bar{\alpha}_k \geq 0, k \geq r + 1 \) such that

\[ V_{r-1}(A \times A) - b V_r(A \times A) = \sum_{k=r+1}^{\infty} \bar{\alpha}_k / 2, \quad \text{(28)} \]

and such that \( \bar{\alpha}_k / 2 \leq \bar{\tau}_k \) for \( k \geq r + 1 \). This can be seen using Part (iii) of Lemma 2. Indeed, to ensure the existence of these \( \bar{\alpha}_k \)’s, we need to prove that

\[ V_{r-1}(A \times A) - b V_r(A \times A) \leq \sum_{k=r+1}^{\infty} \bar{\tau}_k. \quad \text{(29)} \]

Now,

\[ \sum_{k=r+1}^{\infty} \bar{\tau}_k = \sum_{k=r+1}^{\infty} \frac{b V_k(A \times A) - V_{k-1}(A \times A)}{b - 1} \]
\[ = \bar{V}_{r+1}(A \times A) - b V_r(A \times A) - V_r(A \times A) - V_r(A \times A) - \frac{V_r(A \times A)}{b - 1}. \]

Therefore, (29) holds if and only if

\[ V_{r-1}(A \times A) - b V_r(A \times A) \leq \bar{V}_r(A \times A) - V_r(A \times A) - \frac{V_r(A \times A)}{b - 1}. \]
which holds if and only if $V_{r-1}(A \times A) \leq V_r(A \times A) + \frac{b(b-2)}{b-1}V_r(A \times A)$, which is precisely what Part (iii) of Lemma 3 shows. Having proved the existence of non-negative coefficients $\tilde{a}_k$ satisfying (28), we can write $V_{r-1}(A \times A) - bV_r(A \times A) = \sum_{k=r+1}^{\infty} \tilde{a}_k W_{r-1,k-(r+1)}^{(r-1)}$ by using (26). Hence all that is left to do is to find the combination of $Z_k$’s that can cancel out $\sum_{k=r+1}^{\infty} \tilde{a}_k W_{i,k-(r+1)}^{(r-1)}$ for $i \geq r+1$ (we can ignore the case $i = r$ because $W_{r,k-(r+1)}^{(r-1)} = 0$ for all $k \geq r+1$). This is done by using (27), which implies that

$$\sum_{k=r+1}^{\infty} \tilde{a}_k W_{i,k-(r+1)}^{(r-1)} = \sum_{k=r+1}^{\infty} (\tilde{a}_k / 2) Z_{i,k}.$$ 

Hence the final decomposition is given by

$$V(A \times A) = \sum_{k=r+1}^{\infty} \tilde{a}_k W_{k-(r+1)}^{(r-1)} + b\tilde{r} Z_{r-1} + \sum_{k=r+1}^{\infty} (\tilde{r}_k - \tilde{a}_k / 2) Z_k,$$

with $a_k = \tilde{a}_{k+(r+1)}$, $k \geq 0$, $\tau_k = \tilde{r}_k - \tilde{a}_k / 2$, $k \geq r+1$, $\tau_{r-1} = b\tilde{r}_r$ and $\tau_k = 0$ for $0 \leq k \leq r-2$, $k = r$. □

**Proof of Lemma 3** (1) From the definition of $D(k,d,J)$, we have that

$$\text{Vol}(D(k,d,J)) = b^{-2|k|\epsilon} 2^{|J|} b^{-2(|k+d+2|\epsilon)} = 2^{|J|} b^{-2(|k+d+2|\epsilon)}.$$ 

(2) Similarly, from the definition of $F_1(k,d,J,I)$ we get

$$\text{Vol}(F_1(k,d,J,I)) = b^{-|k|\epsilon} b^{-(|k+d+2|\epsilon)} = b^{-(|k+d+2|\epsilon)}.$$ 

(3) This conditional probability is given by $\eta/n - 1$, where $\eta$ is the number of points $u_i$ with $\ell \neq i$ that are in $F_2$ if $u_i \in F_1$. Hence for $j \in I$ we must have $\gamma_p(u_{i,j}, u_{\ell,j}) \geq k_j + d_j + 2$; for $j \in I^c$ we must have $\gamma_p(u_{i,j}, u_{\ell,j}) \geq k_j$. For $j \in J \cap I^c$, the requirement that $u_{i,j} \in F_1$ means $u_{\ell,j}$ must satisfy:

(a) it must have the same first $d_j$ digits as $u_{i,j}$;
(b) its $(d_j + 1)$th digit must be 1 (while the $(d_j + 1)$th digit of $u_{i,j}$ is 0);
(c) the digits $u_{\ell,j,r}$ for $d_j + 2 \leq r d_j + k_j + 2$ must be 0

If we only had to satisfy requirement (a), then we would have $\eta = m_b(k,d,2,J,I)$. However, the requirements (b) and (c) imply

$$\eta = m_b(k,d,2,J,I) \prod_{j \in J \cap I^c} \frac{1}{b-1} \frac{1}{b^{k_j+1}},$$

where the term $1/(b-1)$ handles restriction (b) while the term $b^{-k_j-1}$ handles restriction (c). Therefore
\( P(V \in F_2(k, d, J, I) | U \in F_1(k, d, J, I)) = \frac{m_p(k, d, 2, J, I)}{n-1} \left( \frac{1}{b-1} \right)^{|J|-|I|} \frac{1}{b^{k-1}r^{|J|-|I|}} \)

\[ = \frac{m_p(k, d, 2, J, I)}{n-1} \left( \frac{1}{b-1} \right)^{|J|-|I|} \]

(4) The decomposition \( \cup_{K, I \subseteq J} F(k, d, J, I, K) \) is obtained by expanding each \( Y_{k_j}^{(d_j)} \) as \( Y_{k_{j,1}}^{(d_{j,1})} \cup Y_{k_{j,2}}^{(d_{j,2})} \). Then, we need to prove that for \( K_1, K_2 \subseteq J \),

\[ P(U, V) \in F(k, d, J, I, K_1) = P(U, V) \in F(k, d, J, I, K_2). \quad (30) \]

Noting that the equality (30) can be generalized to \( P( (U, V) \in \mathcal{R}) = \sum_{i \geq 0} \psi_i V_i(\mathcal{R}) \), it is clear that to prove (30), it is sufficient to show that the volume vectors corresponding to \( F(k, d, J, I, K_1) \) and \( F(k, d, J, I, K_2) \) are equal. To do so, since each entry \( V_i(\mathcal{R}) = \prod_{j=1}^{s} V_{k_j}(\mathcal{R}_j) \) (where for \( \mathcal{R} = \mathcal{R}_1 \times \mathcal{R}_2 \) we write \( \mathcal{R}_j = \mathcal{R}_{k_j \times \mathcal{R}_{k_j}} \)), it is sufficient to show that for fixed \( k \) and \( d \), \( V_{11} := V(Y_{k_1}^{(d_1)} \times Y_{k_1}^{(d_1)}) = V(Y_{k_2}^{(d_1)} \times Y_{k_2}^{(d_1)}) =: V_{22} \) and \( V_{12} := V(Y_{k_2}^{(d_2)} \times Y_{k_2}^{(d_2)}) = V(Y_{k_2}^{(d_2)} \times Y_{k_2}^{(d_2)}) =: V_{21} \). But this follows from an argument similar to the one used in the proof of Lemma 4.14 in [10], which we adapt for our setup. First we introduce the set \( \mathcal{F} = \{ ab^{-k} : a \in \mathbb{Z}, k \in \mathbb{N} \} \subseteq \mathbb{R} \) which has Lebesgue measure 0. Then, we argue that for \( x, y \in (0, b^{-k+1}) \cap \mathcal{F}^c \), we have

\[
\gamma_b \left( \frac{1}{b^d+1} - x, \frac{1}{b^d+1} - y \right) = \gamma_b \left( \frac{1}{b^d+1} + x, \frac{1}{b^d+1} + y \right) \\
\gamma_b \left( \frac{1}{b^d+1} - x, \frac{1}{b^d+1} + y \right) = \gamma_b \left( \frac{1}{b^d+1} + x, \frac{1}{b^d+1} - y \right).
\]

Therefore, for \( (x, y) \in Y_{k_1}^{(d_1)} \times Y_{k_1}^{(d_1)} \), \( D_l \) is, up to a set of measure 0, invariant under the transformation \( (x, y) \mapsto \left( \frac{2}{b^{d+1}} - x, \frac{2}{b^{d+1}} - y \right) \). This transformation maps \( Y_{k_1}^{(d_1)} \times Y_{k_1}^{(d_1)} \) to \( Y_{k_2}^{(d_2)} \times Y_{k_2}^{(d_2)} \) (and vice-versa) and \( Y_{k_2}^{(d_2)} \times Y_{k_2}^{(d_2)} \) to \( Y_{k_2}^{(d_2)} \times Y_{k_2}^{(d_2)} \) (and vice-versa). Therefore \( V_{11} = V_{22} \) and \( V_{12} = V_{21} \), as required. \( \square \)

**Proof of Lemma 4** First, if \( \ell = 2i + 1 \), then

\[
g_{i,j}(\ell) = \left( \frac{b}{b-1} \right)^{i-j-1} \leq \left( \frac{b}{b-1} \right)^{i+j-\ell}
\]

and

\[
\left( \frac{b}{b-1} \right)^{i+j-\ell} = \left( \frac{b}{b-1} \right)^{i+1-j}
\]

so in this case we actually have an equality, i.e.,

\[
g_{i,j}(\ell) = \left( \frac{b}{b-1} \right)^{i+j-\ell}.
\]
If $2i < \ell < i + j$ and $\ell$ is even, then
\[
\left( \frac{b}{b-1} \right)^{i+j-\ell} \geq 1 = g_{j,i}(\ell)
\]
since $\ell < i + j$. If $2i < \ell < i + j$ and $\ell$ is odd, then we must show that
\[
1 + \frac{b^{j+i-\ell}}{(b-1)j-i} \left( \frac{j-i-1}{\ell-2i} \right) \leq \left( \frac{b}{b-1} \right)^{i+j-\ell}.
\]  
(31)

Now let $k = \ell - 2i$ and $r = j - i$. This means $k$ is odd and $k > 1$, and also $k < r \leq j \leq s$ which means $r \geq 4$. Using this notation, (31) is equivalent to
\[
b^k \left( \frac{b-1}{b} \right)^r + \binom{r-1}{k} \leq (b-1)^k
\]
and thus to
\[
\left( \frac{b-1}{b} \right)^r = \sum_{j=0}^{r-k} \binom{r}{j} \left( \frac{-1}{b} \right)^j
\]
(32)
and $(\ell)/b^j$ is decreasing with $j$, therefore
\[
\left( \frac{b-1}{b} \right)^r \leq 1 - \frac{r-k}{b} + \frac{(r-k)(r-k-1)}{2b^2},
\]
because the condition that $k > 1$ and $k$ is odd implies $k \geq 3$. Therefore a sufficient condition for the second inequality in (32) to hold is if we have
\[
1 - \frac{r-k}{b} + \frac{(r-k)(r-k-1)}{2b^2} + \frac{(r-k)(r-2)\ldots(r-k)}{(b-1)(b-1)\ldots(b-1)k!} \leq 1
\]
which holds iff
\[
\frac{(r-k)(r-k-1)}{2b^2} + \frac{(r-1)(r-2)\ldots(r-k)}{(b-1)(b-1)\ldots(b-1)k!} \leq \frac{r-k}{b}
\]
which holds iff
\[
\frac{r-k-1}{2b} + \frac{(r-1)(r-2)\ldots(r-k+1)}{(b-1)(b-1)\ldots(b-1)k!} \leq \frac{1}{b}
\]
(33)
Now,
\[
\frac{r-k-1}{2b} < \frac{1}{2} \iff r-k-1 < b,
\]
and the latter inequality holds since $b \geq s \geq r$ and $k \geq 3$. Also,
\[
\frac{r-k+1}{2(b-1)} \leq \frac{1}{2} \iff r-k+1 \leq b-1 \iff r+2-k \leq b
\]
and the latter inequality holds since $k \geq 3$ and $b \geq s \geq r$. Therefore, for $k \geq 3$ the LHS of (33) is bounded (strictly) from above by
Hence if
\[
\frac{1}{2} + \frac{1}{2} \frac{(r-1)(r-2) \ldots (r-k+2)}{(b-1)(b-1) \ldots (b-1)} \frac{b}{b-1} \frac{1}{k(k-1) \ldots 3} < 1
\]
because
\[
\frac{(r-1)(r-2) \ldots (r-k+2)}{(b-1)(b-1) \ldots (b-1)} \leq 1
\]
since \( b \geq s \geq r \) and
\[
\frac{b}{b-1} \frac{1}{k(k-1) \ldots 3} \leq \frac{4}{3} \frac{1}{3} < 1
\]
since \( b/(b-1) \) decreases with \( b \), and the condition \( 1 < k < r \leq s \) with \( k \geq 3 \) means we can assume \( b \geq s \geq r \geq 4 \). This proves that (32) holds.

**Proof of Lemma**

(i) Using Lemma 12 with \( c = 2 \) (which implies \( c|I| + |I^c| = |J| + |I| \)), we first consider the case where \( m - |k|_r - |d|_J \geq |I| + |J| \). In this case
\[
m(k, d, 2, J, I) = (b-1)^{|J||-|I|} b^{m-|k|_r-|d|_J-|I|} (b-1)^{|J|-|J|} = \frac{b^m}{b^m - 1}.
\]
Hence if \( m - |k|_r - |d|_J \geq |I| + |J| \), then
\[
\psi_m(k, d, J, I) = \frac{b^m}{b^m - 1} \left( b^{m-|k|_r-|d|_J-2|I|} \left( \frac{b-1}{b} \right)^{|J|-|I|} + \left( m - |k|_r - |d|_J - 2|I| \right) \right).
\]
Hence in that case
\[
\psi_m(k, d, J, I) \leq \frac{1}{b^m - 1} \left( b^{m-|k|_r+|d|_J+|I|} (b-1)^{|J|-|J|} \left( b^{m-|k|_r-|d|_J-2|I|} \left( \frac{b-1}{b} \right)^{|J|-|I|} \right) + \left( m - |k|_r - |d|_J - 2|I| \right) \right)
\]
\[
= \frac{1}{b^m - 1} \left( b^{m+|k|_r+|d|_J+|I|} (b-1)^{|J|-|J|} \left( m - |k|_r - |d|_J - 2|I| \right) \right)
\]
\[
= \frac{b^m}{b^m - 1} \left( 1 + \frac{b^{|k|_r+|d|_J+|I|}}{(b-1)^{|J|-|J|}} \left( m - |k|_r - |d|_J - 2|I| \right) \right).
\]
A similar calculation shows that if \( m - |k|_r - |d|_J \) is even then
\[
\psi_m(k, d, J, I) \leq \frac{b^m}{b^m - 1}.
\]
If \( m \neq |k|_r - |d|_J - 2|I| = 1 \), then from Lemma 12 we know that \( m(k, d, 2, J, I) = (b - 1) \), and thus

\[
\psi_m(k, d, J, I) = \frac{1}{b^m - 1} b^{k|I|_r + |d|_J + |J| + |I|} (b - 1)^{|U| - |J|} (b - 1)
\]

\[
= \frac{b^m}{b^m - 1} b^{|J| - |I| - 1} (b - 1)^{1 + |I| - |J|} = \frac{b^m}{b^m - 1} \left( \frac{b}{b - 1} \right)^{|J| - |I| - 1}.
\]

Combining these three cases, we get that for \( 2|I| < m - |k|_r - |d|_J < |J| + |I| \),

\[
\psi_m(k, d, J, I) = \frac{b^m}{b^m - 1} g_{|J|, |I|}(m - |k|_r - |d|_J)
\]

with

\[
g_{|J|, |I|}(m - |k|_r - |d|_J) = \begin{cases} 
1 + h_{|J|, |I|}(m - |k|_r - |d|_J) & \text{if } m - |k|_r - |d|_J > 2|I| + 1 \\
\left( \frac{b}{b - 1} \right)^{|J| - |I| - 1} & \text{if } m - |k|_r - |d|_J = 2|I| + 1 \\
1 & \text{if } m - |k|_r - |d|_J \text{ is odd}
\end{cases}
\]

where

\[
h_{j,i}(\ell) = \frac{b^{j+i-\ell}}{(b - 1)^{j+i}} \left( j - i - 1 \right) \frac{\ell}{\ell^2 - 2i}.
\]

(iii) When \( m - |k|_r - |d|_J \leq 2|I| \), then \( m(k, d, 2, J, I) = 0 \) and therefore we can set \( g_{|J|, |I|}(m - |k|_r - |d|_J) = 0 \).

**Proof (of Lemma 7)** First we observe that

\[
R(b, s) = \left( \frac{b}{2(b - 1)} \right)^s P_{\tilde{s}, s}((b - 1)/b),
\]

where \( P_{m,n}(z) \) is the polynomial defined in Lemma 10 and recall that \( \tilde{s} = [s/2] - 1 \). In the notation of (12), \( z = (b - 1)/b, z/(z + 1) = (b - 1)/(2b - 1) \), and \( 1 + z = (2b - 1)/b \). Therefore

\[
R(b, s) = \left( \frac{b}{2(b - 1)} \right)^s \left( \frac{2b - 1}{b} \right)^s P_{\tilde{s}, s} \left( X > \frac{b - 1}{2b - 1} \right),
\]

where \( X \) is a Beta rv with parameters \( \tilde{s} + 1, s - \tilde{s} \). Now, it is known that a beta distribution with parameters \( a, c \) such that \( 1 < a < c \) has a median no larger than \( a/(a + c) \). Therefore, if we can show that

\[
\frac{\tilde{s} + 1}{s + 1} \leq \frac{b - 1}{2b - 1},
\]

then it means \( P_r(X > (b - 1)/(2b - 1)) \leq 1/2 \). Now,
On the other hand,
\[
\frac{b - 1}{2b - 1} = \frac{1}{2} - \frac{1}{2(2b - 1)} \geq \frac{1}{2} - \frac{1}{2(2s - 1)}.
\]

Since \(2(2s - 1) \geq 2(s + 1)\) for \(s \geq 2\), we have that
\[
\frac{s_1 + 1}{s + 1} \leq \frac{s}{2(s + 1)} = \frac{1}{2} - \frac{1}{2(2s - 1)}.
\]

as required. So the last step is to show that
\[
\frac{1}{2} \left( \frac{b}{2(b - 1)} \right)^{s} \left( \frac{2b - 1}{b} \right)^{s} \leq 1.
\]

The inequality (35) is equivalent to
\[
\left( \frac{2b - 1}{2b - 2} \right)^{s} \leq 2 \text{ to } s \ln \frac{2b - 1}{2b - 2} \leq \ln 2, \text{ and finally to } s \ln(1 + \frac{1}{2(b - 1)}) \leq \ln 2.
\]

Now, \(\ln(1 + \frac{1}{2(b - 1)}) \leq \ln(1 + \frac{1}{2(s - 1)}) \leq \frac{1}{2(s - 1)}\), hence it is sufficient to show that
\[
\frac{1}{2(s - 1)} \leq \ln 2 / s \Leftrightarrow \frac{s}{s - 1} \leq 2 \ln 2 = 1.3862...
\]

which holds for any \(s \geq 4\). For \(s = 2\), we have that \(R(b, 2) = 0.25(b/(b - 1))^2\) and since \(b \geq 4\) we have that \(b/(b - 1) \leq 2,\) which implies \(0.25(b/(b - 1))^2 \leq 1\) for all \(b \geq 2\). When \(s = 3\), then \(R(b, 3) = 0.125(b/(b - 1))^3 \leq 1\). \(\square\)

Proof (of Lemma 8) We have that \((m, 0) \in B\) is equivalent to assuming \(|J| \leq m < 2|J|\). We will deal with the case \(m = 2|J| - 1\) separately, and will first assume \(|J| \leq m \leq 2|J| - 3\) and \(m\) is odd.

(i) Case where \(|J| \leq m \leq 2|J| - 3\) and \(m\) is odd:

In this case, \(m' = m > 2|J|\) if and only if \(|J| < 0.5m\), i.e., \(|J| \leq 0.5(m - 1)\). Also, \(m' = m < |J| + |J|\) if and only if \(|J| > m - |J|\). So \(G(m, s, J, 0, 0)\) is of the form
\[
G(m, s, J, 0, 0) = \sum_{j=0}^{0.5(m-3)} \binom{|J|}{j} \frac{0.5(m-3)}{j} h_j(m) + \binom{|J|}{0.5(m-1)} \left( \frac{b}{b - 1} \right)^{|J|} - 0.5(m-1)-1
\]
\[
= \sum_{j=0}^{0.5(m-3)} \binom{|J|}{j} \frac{0.5(m-3)}{j} h_j(m) + \sum_{j=m-|J|+1}^{0.5(m-3)} \binom{|J|}{j} \left( \frac{b}{b - 1} \right)^{|J| - |J| - j - 1} \left( \frac{b(b - 1)}{m - 2j} \right)^{|J|} - 0.5(m-1)-1
\]
\[
+ \binom{|J|}{0.5(m-1)} \left( \frac{b}{b - 1} \right)^{|J| - 0.5(m-1)-1}.
\]

(36)
Using Lemma \((\ref{lem14})\) with \(s = |J|\), we know that \((\ref{eq36})\) is increasing with \(m\), so \(G(m, s, J, 0, 0) \leq G(2|J| - 3, s, J, 0, 0)\) for all \(m \leq 2|J| - 3\) such that \((m, 0) \in \mathcal{B}\). Furthermore, we have that

\[
G(2|J| - 3, s, J, 0, 0) = \sum_{j=0}^{[J]-3} \binom{|J|}{j} + \binom{|J|}{1} \frac{b}{b - 1} \\
= 2^{|J| - 1} - |J| + \frac{|J|||J|-1|}{2} \left( \frac{b}{b - 1} - 1 \right) \\
= 2^{|J| - 1} - |J| + \frac{|J|||J|-1|}{2(b - 1)} \leq 2^{|J| - 1} - \frac{|J|}{2},
\]

where the last inequality is obtained by observing that \(|J| \leq s \leq b\).

(ii) Case where \(m = 2|J| - 1\).

In this case, \(m \geq |I| + |J|\) for all \(I\) such that \(|I| \leq |J| - 2\). Also, for subsets \(I\) such that \(|I| = |J| - 1\), we cannot have \(2|J| < m < |I| + |J|\) since in that case \(|I| + |J| - 2| = |J| - |I| = 1\). Therefore, there is no \(I\) such that \(2|I| < m < |I| + |J|\), and thus

\[
G(2|J| - 1, s, J, 0, 0) = \sum_{j=0}^{[J]-1} \binom{|J|}{j} = 2^{|J| - 1} - 2^{|J| - 1} \geq G(2|J| - 3, s, J, 0, 0). \tag{37}
\]

(iii) If \(m\) is even with \(|J| \leq m < 2|J|\), then \(G(m, s, J, 0, 0) \leq \sum_{j=0}^{[J]-1} \binom{|J|}{j} = 2^{|J| - 1}\). \(\square\)

**Proof (of Lemma \((\ref{lem9})\))** We let \(j = |J|\) and write

\[
G(m, k) = \sum_{I: |I| \leq j-1} g_{j, |I|}(m - |k|_{I^*}).
\]

That is, \(G(m, k) = G(m, s, J, k, 0)\), i.e., we drop the dependence on \(s\), \(J\) and \(d\).

First, we define \(\iota\) as the size of the largest (strict) subset \(I\) of \(J\) that contributes a non-zero value to \(G(m, k)\). That is,

\[
\iota := \max \{|I| : I \subset J, m - |k|_{I^*} \geq 2|I| + 1\}.
\]

Note that \(0 \leq \iota \leq j - 1\). Also, it is useful at this point to mention that our optimal solution \((\tilde{m}, 0)\) will be such that \(\tilde{m} = 2\iota + 1\).

We then define \(\mathcal{G}_{m,k} := \{I : 0 \leq |I| \leq \iota\}\). Using this notation we can write

\[
G(m, k) = \sum_{I: |I| \in \mathcal{G}_{m,k}} g_{j, |I|}(m - |k|_{I^*}). \tag{38}
\]

This holds because if \(I \notin \mathcal{G}_{m,k}\), then \(m - |k|_{I^*} \leq 2|I|\) and thus \(g_{j, |I|}(m - |k|_{I^*}) = 0\).
Next we introduce a definition:

**Definition:** For a given $J$ and $I \subset J$, we say that $(m, k)$ is dominated by $(m', 0)$ at $I$ if $g_{j, |I|}(m - |k|_r) \leq g_{j, |I|}(m')$.

Our strategy will be as follows: consider the set $M = \{1, 3, \ldots, 2l + 1\}$. We claim that for each $I \in G_{m, k}$, there exists $(m', 0)$ with $m' \in M$ such that $(m, k)$ is dominated by $(m', 0)$ at $I$. In turn, this will allow us to bound each term $g_{j, |I|}(m - |k|_r)$ in (38) by a term of the form $g_{j, |I|}(m')$. We then only need to keep track, for each $m'$, of how many times $g_{j, |I|}(m')$ has been used in this way—something we will do by introducing counting numbers denoted by $\eta(\cdot)$. This strategy is a key intermediate step to get to our end result, which is to show that $G(m, k) \leq G(\tilde{m}, 0)$.

To prove the existence of this $m'$, we define a mapping $L_{m,k} : G_{m,k} \to M$ that will, for a given $m$ and $k$, assign to each subset $I \in G_{m,k}$ the largest integer $m' \in M$ such that $(m, k)$ is dominated by $(m', 0)$ at $I$. The reason why we choose the largest $m' \in M$ is that this provides us with the tightest bound on $g_{j, |I|}(m - |k|_r)$, as should be clear from the behavior of the function $g_{j, i}(\ell)$, as described in Lemma 13.

The mapping $L_{m,k}(I)$ is defined as follows:

$$L_{m,k}(I) = \begin{cases} 2\ell + 1 & \text{if } m - |k|_r \geq 2\ell + 1 \\ 2\ell + 1 & \text{if } 2\ell + 1 \leq m - |k|_r \leq 2\ell + 2 \text{ where } 0 \leq \ell < i \\ 1 & \text{if } m - |k|_r \leq 0. \end{cases}$$

**Claim:** For each $I \in G_{m,k}$, $(L_{m,k}(I), 0)$ dominates $(m, k)$ at $I$.

**Proof:** We need to show that $g_{j, |I|}(m - |k|_r) \leq g_{j, |I|}(L_{m,k}(I))$. We proceed by examining the three possible cases for $L_{m,k}(I)$ based on its definition.

(i) Assume $m - |k|_r \geq 2\ell + 1$ and therefore $L_{m,k}(I) = 2\ell + 1$. By definition of $\ell$ we have $2\ell + 1 > 2i$, and therefore $L_{m,k}(I) = 2\ell + 1$. By definition of $\ell$, we now have $2\ell + 1 < m - |k|_r \leq 2\ell + 2$ for some $0 \leq \ell < i$. In this case, $L_{m,k}(I) = 2\ell + 1$ and $m - |k|_r$ is either equal to $2\ell + 1$ or to $2\ell + 2$. If $m - |k|_r = 2\ell + 1$ then clearly $g_{j, |I|}(L_{m,k}(I)) \geq g_{j, |I|}(m - |k|_r)$ since in fact these two quantities are equal. If $m - |k|_r = 2\ell + 2$ then since $L_{m,k}(I) = 2\ell + 1 \geq 1$ is odd we can use Part 1 of Lemma 13 to conclude that $g_{j, |I|}(L_{m,k}(I)) \geq g_{j, |I|}(m - |k|_r)$. (ii) If $m - |k|_r \leq 0$, then $m - |k|_r \leq 2\ell$ since $L_{m,k}(I)$ implies $0 \leq |I| \leq i$, and therefore $g_{j, |I|}(m - |k|_r) = 0 \leq g_{j, |I|}(1)$. \(\Box\)

Now, recall that shortly after stating (38), when we explained our strategy to replace the terms $g_{j, |I|}(m - |k|_r)$ by $g_{j, |I|}(m')$ in (38), we also said we would need counting numbers $\eta(\cdot)$ to tell us how many times, for each $m'$, the term $g_{j, |I|}(m')$ has been used in this way. These counting numbers are essential to apply the optimization result involving weighted sums that is given in Lemma 13, which is the key to get our final result. They are defined as follows, for $0 \leq i, \ell \leq i$:

$$\eta(\ell, i, k) := \{ |I| \in G_{m,k} : |I| = i, L_{m,k}(I) = 2(\ell - i) + 1 \}.$$

Note that $\sum_{i=0}^{\ell} \eta(\ell, i, k) = \binom{\ell}{i}$. Also we can think of $p(\ell, i, k) = \eta(\ell, i, k)/\binom{\ell}{i}$ as the probability that a randomly chosen subset $I$ of $i$ elements from $J$ is such that $|k|_r \in R_{\ell}$, where
On the distribution of scrambled \((0, m, s)\)-nets over unanchored boxes

\[
\mathcal{R}_\ell := \begin{cases} 
\{0, 1, \ldots, m - (2\ell + 1)\} & \text{if } \ell = 0 \\
\{m - (2\ell + 1) + 2\ell - 1, m - (2\ell + 1) + 2\ell\} & \text{if } 1 \leq \ell < \ell \\
\{m - 2, m - 1, \ldots\} & \text{if } \ell = \ell.
\end{cases}
\] (39)

To get the final result, we write:

\[
G(m, k) = \sum_{i=0}^{\ell} g_j,\ell | (m - |k|, \ell) \leq \sum_{i=0}^{\ell} \sum_{i=0}^{\ell} \eta(\ell, i, k) g_j,\ell (2(\ell - \ell) + 1)
\]

\[
= \sum_{i=0}^{\ell} \sum_{i=0}^{\ell} p(\ell, i, k) (j_i) g_j,\ell (2(\ell - \ell) + 1)
\]

\[
= \sum_{i=0}^{\ell} (j_i) g_j,\ell (2(\ell + 1) = G(m, 0),
\]

where \(\tilde{m} = 2\ell + 1\). In the above, the first inequality is obtained by replacing \(g_j,\ell | (m - |k|, \ell)\) by \(g_j,\ell (2(\ell - \ell) + 1)\) for each of the \(\eta(\ell, i, k)\) pairs \((m, k)\) dominated by \(2(\ell - \ell) + 1, 0\) at \(i\), where \(|l| = i\); the third equality holds because if \(\ell > \ell - i\), then \(2(\ell - \ell) + 1 < 2(\ell - (\ell - i)) + 1 = 2i + 1\) and therefore \(g_j,\ell (2(\ell - \ell) + 1) = 0\). Similarly, \(\ell \leq \ell - i\) implies \(2(\ell - \ell) + 1 \geq 2i + 1\) and so \(g_j,\ell (2(\ell - \ell) + 1) > 0\) in this case. The last inequality comes from applying Lemma \[15\] whose conditions hold because:

1. \((j_i) g_j,\ell (2(\ell - \ell) + 1)\) corresponds to \(x_{\ell, i+1} \times i\) in Lemma \[15\]
2. Lemma \[16\] together with \(37\) shows the decreasing row-sums condition is satisfied, i.e., \(G(2(\ell - \ell) + 1, 0) = \sum_i x_{\ell, i+1} \times i\) is decreasing with \(\ell\);
3. The increasing-within-column assumption of Lemma \[15\] is satisfied because the sum \(41\) only includes positive values of \(g_j,\ell (2(\ell - \ell) + 1)\) (as shown above), which in turn allows us to invoke Part 2 of Lemma \[15\]
4. \(p(\ell, i, k)\) corresponds to \(x_{\ell, i+1} \times i\) in Lemma \[15\]
5. To see that the \(p(\ell, i, k)\)'s obey the decreasing-cumulative-sums condition \(52\) in Lemma \[15\] we argue that our probabilistic interpretation of the \(p(\ell, i, k)\) based on the sets defined in \(39\) should make it clear that for \(i = 0, \ldots, \ell - 1\) and \(0 \leq r \leq \ell,
\[
\sum_{\ell=0}^{r} p(\ell, i, k) \geq \sum_{\ell=0}^{r} p(\ell, i + 1, k).
\]

Therefore \(G(m, k) \leq G(\tilde{m}, 0)\), as required.
Technical lemmas

The following result [7, Lemma2] is used to prove intermediate inequalities needed in our analysis.

**Lemma 10** Let \( P_{m,n}(z) \) be the polynomial defined by

\[
P_{m,n}(z) = \sum_{j=0}^{m} \binom{n}{j} z^j, \quad 0 < m < n - 1.
\]

Then for \( z \neq -1 \)

\[
\frac{P_{m,n}(z)}{(1 + z)^n \binom{n}{m}} = \int_{z/(z+1)}^1 u^m (1-u)^{n-m-1} du.
\]

We also need the following identity for integers \( c > a \geq 0 \), which may be found in [5, (5.16)]

\[
\sum_{j=0}^{a} \binom{c}{j} (-1)^j = \binom{c - 1}{a} (-1)^a.
\]

We now state and prove a number of technical lemmas that were used within the above proofs. The first two lemmas are used to prove Lemma 5, and the next three are used for Lemmas 8 and 9.

**Lemma 11** For \( b \geq s \geq 2 \) and \( 0 \leq k < s \), let

\[
Q(b, k, s) := \sum_{j=0}^{k} (-1)^j \binom{s}{j} (b^{k-j} - 1).
\]

Then

\[
Q(b, k, s) \leq \begin{cases} 
  b^k \left( \frac{b-1}{b} \right)^s & \text{if } k \text{ is even} \\
  b^k \left( \frac{b-1}{b} \right)^s + \binom{s-1}{k} & \text{if } k > 1 \text{ is odd}, \\
  (b - 1) & \text{if } k = 1.
\end{cases}
\]

**Proof** The statement holds trivially for \( k = 0 \). For \( k > 0 \) we apply Lemma 10 and (43) to obtain

\[
Q(b, k, s) = b^k P_{k,s}(-1/b) - \binom{s-1}{k} (-1)^k
\]

\[
= b^k \left( \frac{b-1}{b} \right)^s \int_{-1/(b-1)}^1 u^k (1-u)^{s-k-1} c_{k,s} du - \binom{s-1}{k} (-1)^k
\]

\[
= b^k \left( \frac{b-1}{b} \right)^s \left( \int_{-1/(b-1)}^0 u^k (1-u)^{s-k-1} c_{k,s} du + 1 \right) - \binom{s-1}{k} (-1)^k
\]
where \( c_{k,s} \) is the constant that makes the integrand a beta pdf with parameters 
\( (k+1, s-k) \), i.e., \( c_{k,s} = s \left( \frac{s-1}{k} \right) \).

Now, if \( k \) is odd then \( \int_{1/(b-1)}^{0} u^k (1-u)^{s-k-1} c_{k,s} du \leq 0 \) and thus we get
\[
Q(b, k, s) \leq b^k \left( \frac{b-1}{b} \right)^s \left( \frac{s-1}{k} \right).
\]

Note also that when \( k = 1, Q(b, k, s) = b-1 \) (which is not necessarily bounded
from above by \( b^k \left( \frac{b-1}{b} \right)^s + \left( \frac{s-1}{k} \right) = b((b-1)/b)^s + s-1 \). It is for this reason we
treat the case \( k = 1 \) separately). If \( k \) is even, then
\[
\int_{1/(b-1)}^{0} u^k (1-u)^{s-k-1} c_{k,s} du \leq c_{k,s} \frac{1}{b-1} \left( \frac{1}{b-1} \right)^k \left( 1 + \frac{1}{b-1} \right)^{s-k-1} \leq c_{k,s} \left( \frac{b^s}{b-1} \right).
\]

Therefore when \( k \) is even
\[
Q(b, k, s) = b^k \left( \frac{b-1}{b} \right)^s \left( 1 + c_{k,s} \frac{b^s-1}{b-1} \right) \leq b^k \left( \frac{b-1}{b} \right)^s \left( \frac{s-1}{k} \right)
\]

since \( s \leq b \).

\[
\begin{align*}
\text{Lemma 12} & \quad \text{Consider a } (0, m, s, s)-\text{net in base } b. \text{ Let } \emptyset \neq J \subset \{1, \ldots, s\}, \text{ and } I \subseteq J, \\
& \quad \text{with } I^* = I \cup I^c. \text{ Then the following bounds hold:} \\
(i) & \quad \text{if } m \geq |k|_I^* + d_J + c|I| + |I^c|, \text{ then } \\
& \quad m_b(k, d, c, J, I; P_n) = b^{m-|k|_I^* - d_J - c|I|} \left( b - 1 \right)^{|I^c|}; \\
(ii) & \quad \text{if } m < |k|_I^* + d_J + c|I| + 1 < m < |k|_I^* + d_J + c|I| + |I^c| \text{ then } \\
& \quad m_b(k, d, c, J, I; P_n) \leq b^{m-|k|_I^* - d_J} \left( b - 1 \right)^{|I^c|} + \left( m - |k|_I^* - d_J - c|I| \right) 1_{x \text{ odd}}; \\
& \quad \text{where } 1_x = \begin{cases} 1 & \text{if } x \text{ is odd} \\ 0 & \text{otherwise.} \end{cases} \\
(iii) & \quad \text{if } m = |k|_I^* + d_J + c|I| + 1 \text{ then } \\
& \quad m_b(k, d, c, J, I; P_n) = (b - 1). \\
(iv) & \quad \text{if } m \leq |k|_I^* + d_J + c|I| \text{ then } m_b(k, d, c, J, I; P_n) = 0.
\end{align*}
\]

\textbf{Proof} Using the quantities \( n_b(k) \) defined in [10], their relation to \( m_b(k; P_n) \) and
the value of the latter for a \((0, m, s)-\text{net}, we write
\[ m_b(k, d, c, J; P_n) = \sum_{i_j \geq j, j \in J^c} n_b(i_j : d_{I^c}) \]
\[ = \sum_{e \in \{0, 1\}^{|I^c|}} (-1)^{|e|} m_b((k_{I^c} : (k + d + 2)^{J^c} : (d + e)_{I^c}); P_n) \]
\[ = \sum_{j=0}^{|I^c|} (-1)^j \binom{|I^c|}{j} \max(b^{m-|k|_{I^c}-|d|_{J^c}|-c| - j - 1, 0) \, (45) \]

where \((i_j : d_{I^c})\) represents the vector with \(j\)th component given by \(i_j\) if \(j \in I\) and by \(d_j\) if \(j \notin I\). If \(m - |k|_{I^c} - |d|_{J^c} - c| \geq 0\) then the above sum is given by

\[ m_b(k, d, c, J; P_n) = b^{m-|k|_{I^c}-|d|_{J^c}|-c|} \sum_{j=0}^{|I^c|} (-1)^j \binom{|I^c|}{j} b^{|I^c|-j} \]
\[ = b^{m-|k|_{I^c}-|d|_{J^c}-c|} (b - 1)^{|I^c|}. \]

If \(m - |k|_{I^c} - |d|_{J^c} - c| \leq 0\) then the max inside the sum \((45)\) always yields 0. When \(1 < m - |k|_{I^c} - |d|_{J^c} - c| \leq |I^c|\), then \((45)\) is given by

\[ m_b(k, d, c, J; P_n) \leq \sum_{j=0}^{m-|k|_{I^c}-|d|_{J^c}-c|} (-1)^j \binom{|I^c|}{j} (b^{m-|k|_{I^c}-|d|_{J^c}-c|} + (m - |k|_{I^c} - |d|_{J^c} - c|) b^{m-|k|_{I^c}-|d|_{J^c}-c|}) \]
\[ \leq b^{m-|k|_{I^c}-|d|_{J^c}} (b - 1)^{|I^c|} (m - |k|_{I^c} - |d|_{J^c} - c| - 1) \]

where the last inequality is obtained by applying Lemma \((11)\) with \(s = |I^c|\) and \(k = m - |k|_{I^c} - |d|_{J^c} - c|\). Finally, when \(m = |k|_{I^c} + |d|_{J^c} + c| + 1\), then \((45)\) is given by

\[ \sum_{j=0}^{1} (-1)^j \binom{|I^c|}{j} (b^{1-j} - 1) = b - 1. \]

**Lemma 13** The function \(g_{j,i}(\ell)\) defined in \((16)\) with \(0 \leq i < j \) and \(j \geq 1\) satisfies the following properties.

1. For a given \(i\), if \(\ell \geq 1\) is odd then \(g_{j,i}(\ell) \geq g_{j,i}(\ell + 1)\).
2. For a given \(i\), if \(\ell > 2i\) is odd then \(g_{j,i}(\ell) \geq g_{j,i}(\ell + r)\) for all \(r \geq 0\).

**Proof** For (1): if \(\ell \geq j + i\) then \(g_{j,i}(\ell) = g_{j,i}(\ell + 1) = 1\); if \(2i < \ell < j + i\), then \(g_{j,i}(\ell) > 1\) while \(g_{j,i}(\ell + 1) = 1\); if \(\ell \leq 2i\) then \(g_{j,i}(\ell) = 0\) and since \(\ell\) is odd, it means \(\ell \leq 2i - 1\), and thus \(\ell + 1 \leq 2i\), implying that \(g_{j,i}(\ell + 1) = 0\). For (2): if \(\ell \geq j + i\) then \(g_{j,i}(\ell + r) = 1\) for all \(r \geq 0\); if \(2i + 1 < \ell < j + i\), then the function \(g_{j,i}(\ell)\) is increasing as \(\ell\) decreases over odd values strictly between \(j + i\) and \(2i + 1\); this is because when \(\ell\) decreases by 2, \(h_{j,i}(\ell)\) increases by a factor of at
least \(2b^2/(j-i-1)(j-i-2)\), which is at least 1 since \(j \leq s \leq b\). Finally, we need to show that \(g_{i,j}(2i+1) = (b/(b-1))^{j-i-1} \geq g_{i,j}(2i+3)\), i.e., that
\[
\left(\frac{b}{b-1}\right)^{j-i-1} \geq 1 + \frac{b^{j-i-(2i+3)}}{(b-1)^{j-i}} \left(\frac{j-i-1}{2i+3-2j}\right) = 1 + \left(\frac{b}{b-1}\right)^{j-i} \frac{1}{b^2}\left(\frac{j-i-1}{3}\right).
\]
Using the bound \((b-1)/b)^j \leq (b-j-1)/(b-1)\) shown in the proof of Lemma 14 we have that the above holds if
\[
\frac{b-1}{b} \geq \frac{(j-i-1)(j-i-2)(j-i-3)}{6b^3} + \frac{b-(j-i)-1}{b-1}
\]
\[
\Leftrightarrow (b-1)^2 - b(b-j+i-1) \geq \frac{(j-i-1)(j-i-2)(j-i-3)}{6b^3}
\]
\[
\Leftrightarrow 6b^2(1+b(j-i-1)) \geq (b-1)(j-i-1)(j-i-2)(j-i-3),
\]
which is clearly true since \(j \leq s \leq b\) and \(i \geq 0\) and therefore \(6b^3(j-i-1) \geq (b-1)(j-i-1)(j-i-2)(j-i-3)\).

**Lemma 14** Let \(s \geq 3\) and \(b \geq s\). Let \(m\) be odd with \(1 \leq m \leq 2s-3\), and consider the function
\[
G(m,s) = \sum_{j=0}^{0.5m-3} \left(\begin{array}{c} s \\ j \end{array}\right) + \sum_{j=\max(0,m-s+1)}^{0.5m-3} \left(\begin{array}{c} s \\ j \end{array}\right) h_{s,j}(m) + \left(\begin{array}{c} s \\ m \end{array}\right) \left(\frac{b}{b-1}\right)^{s-0.5m-1},
\]
where \(h_{s,j}(m)\) is as defined in (15), i.e.,
\[
h_{s,j}(m) = \left(\frac{s-j-1}{m-2j}\right) \left(\frac{b^{s-j-m}}{(b-1)^{s-m}}\right).
\]
Then \(G(m,s) \geq G(m-2,s)\) for \(m \geq 3\) odd. That is, \(G(m,s)\) is decreasing over the odd integers from \(2s-3\) down to 3.

**Proof** First, we compute
\[
\left(\frac{b}{b-1}\right)^{s-0.5m-1} - h_{s,0.5m-1}(m)
\]
\[
= \left(\frac{b}{b-1}\right)^{s-0.5m-1} - \left(\frac{s-0.5m-1-1}{1}\right) \frac{b^{0.5m-1+s-m}}{(b-1)^{s-0.5m-1}}
\]
\[
= \left(\frac{b}{b-1}\right)^{s-0.5m-1} \frac{b-1-(s-0.5m-1)}{b}
\]
\[
= \left(\frac{b}{b-1}\right)^{s-0.5m-1} \frac{b-(s-0.5m-1)}{b}.
\]
Using this, we can write
\[ G(m, s) = \sum_{j=0}^{0.5(m-3)} \binom{s}{j} + \sum_{j=\max(0, m-s+1)}^{0.5(m-1)} \binom{s}{j} h_{s,j}(m) + \binom{s}{0.5(m-1)} \left( \frac{b}{b-1} \right)^{s-0.5(m-1)} \frac{0.5(m-1)+b-s}{b}. \] (46)

Next, we show that for \( 2 \leq j \leq 0.5(m-1) \):

\[ \left( \binom{s}{j} h_{s,j}(m) \right) \geq \left( \binom{s}{j-2} h_{s,j-2}(m-2) \right). \] (47)

\[
\binom{s}{j} h_{s,j}(m) \geq \binom{s}{j-2} h_{s,j-2}(m-2) \\
\geq \binom{s}{j} \frac{b^{s+j-m}}{(b-1)^{s-j}} - \binom{s}{j-2} \frac{(s-j+1)(s-j)}{(b-1)^{s-j+2}} \\
= \binom{s}{j} \frac{b^{s+j-m}}{(b-1)^{s-j}} - \binom{s}{j-2} \frac{(s-j+1)(s-j)}{(b-1)^{s-j+2}} \\
= \binom{s}{j} \frac{b^{s+j-m}}{(b-1)^{s-j}} \left( 1 - \frac{j(j-1)}{(s-j+2)(s-j+1)(m-2j+2)(m-2j+1)} \right) \\
\]

Hence to prove (47), we need to show that

\[ 1 \geq \frac{j(j-1)}{(s-j+2)(s-j+1)(m-2j+2)(m-2j+1)} \]

which holds because

\[
\frac{j(j-1)}{(s-j+2)(s-j+1)(m-2j+2)(m-2j+1)} \leq \frac{j(j-1)}{6} \leq \frac{1}{6} \leq 1, \\
\]

since \( j \leq 0.5(m-1) \leq s-2 \) and \( b \geq s \).

Using (46), \( G(m, s) \geq G(m-2, s) \) can be shown to hold if
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\[
0.5(m-3) \sum_{j=0}^{s} \binom{s}{j} + 0.5(m-1) \sum_{j=\max(0,m-s+1)}^{s} \binom{s}{j} h_{x,j}(m) \\
+ \left( \frac{s}{0.5(m-1)} \right) \left( \frac{b}{b-1} \right)^{s-0.5(m-1)} \frac{0.5(m-1) + b - s}{b} \\
\geq \sum_{j=0}^{0.5(m-5)} \binom{s}{j} h_{x,j}(m - 2) \\
+ \left( \frac{s}{0.5(m-3)} \right) \left( \frac{b}{b-1} \right)^{s-0.5(m-3)} \frac{0.5(m-3) + b - s}{b}.
\]

(48)

In turn, using (47), we know that:

\[
0.5(m-1) \sum_{j=\max(0,m-s+1)}^{s} \binom{s}{j} h_{x,j}(m) \geq \sum_{j=\max(0,m-2-s+1)}^{0.5(m-5)} \binom{s}{j} h_{x,j}(m - 2)
\]

and therefore to show (48) it is sufficient to show that

\[
\left( \frac{s}{0.5(m-3)} \right) + \left( \frac{s}{0.5(m-1)} \right) \left( \frac{b}{b-1} \right)^{s-0.5(m-1)} \frac{0.5(m-1) + b - s}{b} \\
\geq \left( \frac{s}{0.5(m-3)} \right) h_{x,0.5(m-3)}(m - 2) \\
+ \left( \frac{s}{0.5(m-3)} \right) \left( \frac{b}{b-1} \right)^{s-0.5(m-3)} \frac{0.5(m-3) + b - s}{b}.
\]

(49)

where

\[
h_{x,0.5(m-3)}(m - 2) = \left( \frac{s - 0.5(m-3) - 1}{m - 2 - (m-3)} \right) \frac{b^{s+0.5(m-3)-(m-2)}}{(b-1)^{s-0.5(m-3)}} \\
= \left( s - 0.5(m-1) \right) \left( \frac{b}{b-1} \right)^{s-0.5(m-1)} \frac{1}{b-1}.
\]

The following inequality will be helpful in this proof:

**Claim** For \(b \geq 2\) and \(j \geq 1\), we have that

\[
\left( \frac{b}{b-1} \right)^{j} \leq \frac{b - 1}{b - (j + 1)}.
\]

(50)

**Proof** The inequality is equivalent to having

\[(b - 1)^{j+1} \geq b^{j}(b - (j + 1)).\]
Applying the mean value theorem to \( f(x) = x^{j+1} \) and noticing \( f'(x) \) is monotone increasing for \( x \geq 0 \), we get that
\[ f(b) - f(b - 1) = f'(\xi) \leq f'(b) \]
for some \( \xi \in (b - 1, b) \) and thus \( (b - 1)^{j+1} \geq b^{j+1} - (j + 1)b^j \). 
\[ \square \]

Going back to our goal of proving (49), it is sufficient to show that
\[
1 + \left( \frac{b}{b - 1} \right)^{s-0.5(m-1)} \left( \frac{s - 0.5(m-3)}{0.5(m-1)} + \frac{0.5(m-1) + b - s}{b} \right)
\gtrless \left( \frac{s - 0.5(m-1)}{b - 1} + \frac{0.5(m-3) + b - s}{b} \right)
\gtrless \left( \frac{s - 0.5(m-1)}{b - 1} + \frac{0.5(m-3) + b - s}{b} \right).
\]

(51)

Using (50) to simplify the LHS of (51), we see that (51) holds if
\[
\frac{b - (s - 0.5(m-1) - 1)}{b - 1} + \frac{s - 0.5(m-3) + 0.5(m-1) + b - s}{0.5(m-1)} \gtrless \frac{s - 0.5(m-1)}{b - 1} + \frac{0.5(m-3) + b - s}{b - 1}
\gtrless \frac{s - 0.5(m-1)}{b - 1} + \frac{0.5(m-3) + b - s}{b - 1}
\gtrless \frac{s - 0.5(m-3) + 0.5(m-1) + b - s}{b}
\gtrless \frac{s - 0.5(m-1)}{s - 0.5(m-3) + 0.5(m-1) + b - s}
\]

which holds because \( s - 0.5(m-3) \leq s \leq b \) and \( \frac{b-1}{b} \geq \frac{b-1}{b-x} \) if \( x \geq 0 \). 
\[ \square \]

**Definition 3** We denote by \( \mathcal{A}_w \) the set of \( w \times \ell \) weight matrices \( A \) with entries \( a_{i,j} \geq 0 \) that satisfy the following two conditions: 1) \( \sum_{i=1}^w a_{i,j} = 1 \) for all \( j = 1, \ldots, \ell \); 2) the weights \( a_{i,j} \) obey a decreasing-cumulative-sums condition as follows: for \( 1 \leq i \leq w, 1 \leq j \leq \ell \), let
\[
A_{i,j} = \sum_{k=1}^i a_{k,j}.
\]

Then \( A_{i,j} \geq A_{i,j+1} \) for each \( i = 1, \ldots, w \) and \( j = 1, \ldots, \ell - 1 \) (when \( i = w \) we have \( A_{w,j} = 1 \) for all \( j \)). This means the weights on the first row are decreasing from left to right; the partial sums of the two first rows are decreasing from left to right, etc.

**Lemma 15** Let \( X \) be a \( w \times \ell \) matrix with \( \ell \geq w \) and entries \( x_{i,j} \geq 0 \) and of the form
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\[
X = \begin{bmatrix}
x_{1,1} & \cdots & x_{1,\ell-w+1} & \cdots & x_{1,\ell-1} & x_{1,\ell} \\
x_{2,1} & \cdots & x_{2,\ell-w+1} & \cdots & x_{2,\ell-1} & 0 \\
\vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\
x_{w-1,1} & \cdots & x_{w-1,\ell-w+1} & x_{w-1,\ell-w+2} & \cdots & 0 \\
x_{w,1} & \cdots & x_{w,\ell-w+1} & 0 & \cdots & 0
\end{bmatrix}
\]

that is \(x_{i,j} > 0\) if and only if \(i + j \leq \ell + 1\), for \(1 \leq i \leq w, 1 \leq j \leq \ell\). We assume \(X\) satisfies the following two conditions: first,

\[
\sum_{j=1}^{\ell} x_{1,j} \geq \sum_{j=1}^{\ell-1} x_{2,j} \geq \ldots \geq \sum_{j=1}^{\ell-w+1} x_{w,j}
\]

(we refer to this as the decreasing-row-sums condition) and second,

\[
x_{1,j} \leq x_{2,j} \leq \ldots \leq x_{\min(w,\ell-i+1),j}, \quad j = 1, \ldots, \ell
\]

(we refer to this as the increasing-within-column condition).

Let \(A\) be a weight matrix in \(A_w\) and let

\[
\|A \circ X\|_1 = \sum_{j=1}^{\ell} \alpha_{1,j}x_{1,j} + \sum_{j=1}^{\ell-1} \alpha_{2,j}x_{2,j} + \ldots + \sum_{j=1}^{\ell-w+1} \alpha_{w,j}x_{w,j}.
\]

Then for any \(A \in A_w\)

\[
\|A \circ X\|_1 \leq \sum_{j=1}^{\ell} x_{1,j}.
\]

That is, the weight matrix \(A \in A_w\) that maximize the LHS of (54) is the one with \(1\)'s on the first row and \(0\)'s elsewhere.

**Proof** First, note that \(A \in A_w\) implies that cumulative sums from the last row up are increasing, i.e., for \(R_{i,j} = \sum_{k=i}^{w} \alpha_{k,j}\), we have \(R_{i,j} \leq R_{i,j+1}\) for \(j = 1, \ldots, \ell - 1\).

We proceed by induction on \(w \geq 2\).

If \(w = 2\), then it suffices to show that for \(A \in A_2\), we have that

\[
\sum_{j=1}^{\ell} \alpha_{1,j}x_{1,j} + \sum_{j=1}^{\ell-1} (1 - \alpha_{1,j})x_{2,j} \leq \sum_{i=1}^{\ell} x_{1,j} \Rightarrow \sum_{j=1}^{\ell-1} (1 - \alpha_{1,j})x_{2,j} \leq \sum_{j=1}^{\ell} (1 - \alpha_{1,j})x_{1,j},
\]

or, equivalently, that

\[
\sum_{j=1}^{\ell-1} (1 - \alpha_{1,j})(x_{2,j} - x_{1,j}) \leq (1 - \alpha_{1,\ell})x_{1,\ell}.
\]

Now, we know that
\[ \sum_{j=1}^{\ell} x_{1,j} \geq \sum_{j=1}^{\ell-1} x_{2,j} \iff \sum_{j=1}^{\ell-1} (x_{2,j} - x_{1,j}) \leq x_{1,\ell} \]

with \( x_{2,j} - x_{1,j} \geq 0 \). Therefore

\[ \sum_{j=1}^{\ell-1} (1 - \alpha_{1,j})(x_{2,j} - x_{1,j}) \leq (1 - \alpha_{1,\ell}) \sum_{j=1}^{\ell-1} (x_{2,j} - x_{1,j}) \leq (1 - \alpha_{1,\ell}) x_{1,\ell}, \]

where the first inequality holds because the \( \alpha_{1,j} \)'s are decreasing.

Now assume the statement holds for \( w - 1 \geq 2 \). First we create a new weight matrix \( \bar{A} \) by merging the two last rows into the second-to-last one and setting the last one to zero, i.e., we define \( \bar{A}_{w-1,j} \) as

\[
\begin{align*}
\bar{a}_{w-1,j} &= \alpha_{w-1,j} + \alpha_{w,j} & j &= 1, \ldots, \ell \\
\bar{a}_{w,j} &= 0 & j &= 1, \ldots, \ell \\
\bar{a}_{i,j} &= \alpha_{i,j}, i = 1, \ldots, w - 2, j = 1, \ldots, \ell.
\end{align*}
\]

With this change, we claim that \( \bar{A} \in \mathcal{A}_w \). Indeed:

1. \( \bar{a}_{i,j} \geq 0 \)
2. \( \sum_{i=1}^{w-2} \bar{a}_{i,j} = \sum_{i=1}^{w-2} \alpha_{i,j} + (\alpha_{w-1,j} + \alpha_{w,j}) + 0 = 1. \)
3. \( \bar{A}_{i,j} = A_{i,j} \) for \( i = 1, \ldots, w - 2 \) and \( \bar{A}_{w-1,j} = A_{w,j} = 1 \) for \( j = 1, \ldots, \ell \).

Next, we show that

\[ \| \bar{A} \circ X \|_1 \geq \| A \circ X \|_1. \quad (55) \]

Since \( a_{i,j} = \bar{a}_{i,j} \) for \( i < w - 1 \), then (55) holds if and only if

\[
\begin{align*}
\sum_{j=1}^{\ell-w+2} (\alpha_{w-1,j} + \alpha_{w,j}) x_{w-1,j} &\geq \sum_{j=1}^{\ell-w+2} \alpha_{w-1,j} x_{w-1,j} + \sum_{j=1}^{\ell-w+1} \alpha_{w,j} x_{w,j} \\
\iff \sum_{j=1}^{\ell-w+1} \alpha_{w,j} x_{w-1,j} + \alpha_{w,\ell-w+2} x_{w-1,\ell-w+2} &\geq \sum_{j=1}^{\ell-w+1} \alpha_{w,j} x_{w,j} \\
\iff \sum_{j=1}^{\ell-w+1} \alpha_{w,j} (x_{w,j} - x_{w-1,j}) &\leq \alpha_{w,\ell-w+2} x_{w-1,\ell-w+2}.
\end{align*}
\]

By the decreasing-row-sum assumption on the \( x_{i,j} \)'s we know that

\[ 0 \leq \sum_{j=1}^{\ell-w+1} (x_{w,j} - x_{w-1,j}) \leq x_{w-1,\ell-w+2} \]

and by assumption that \( A \in \mathcal{A}_w \) we have that \( \alpha_{w,1} \leq \alpha_{w,2} \leq \ldots \leq \alpha_{w,\ell} \). Therefore
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\[
\sum_{j=1}^{\ell-w+1} \alpha_{w,j} (x_{w,j} - x_{w-1,j}) \leq \alpha_{w,\ell-w+1} \sum_{j=1}^{\ell-w+1} (x_{w,j} - x_{w-1,j})
\]

\[
\leq \alpha_{w,\ell-w+1} x_{w-1,\ell-w+2} \leq \alpha_{w,\ell-w+2} x_{w-1,\ell-w+2},
\]

as required to show that (55) holds.

Next, to use the induction hypothesis, we observe that \( \tilde{\alpha}_{w,j} = 0 \) implies we can essentially ignore the \( x_{w,j} \)'s. More formally, let \( \tilde{A}_{w-1} \) be the matrix formed by the first \( w-1 \) rows of \( \tilde{A} \) and similarly for \( A_{w-1} \). Then \( \tilde{A}_{w-1} \in A_{w-1} \), since

1. \( \tilde{\alpha}_{i,j} \geq 0 \) for \( i = 1, \ldots, w-1, j = 1, \ldots, \ell \)
2. \( \sum_{i=1}^{w-1} \tilde{\alpha}_{i,j} = \sum_{i=1}^{w} \alpha_{i,j} = 1 \) for \( j = 1, \ldots, \ell \)
3. \( \tilde{\alpha}_{i,j} \geq \tilde{\alpha}_{i,j+1} \) as verified earlier (and note that \( \tilde{\alpha}_{w-1,1} \leq \ldots \leq \tilde{\alpha}_{w-1,\ell} \) by assumption that \( A \in A_{w} \) and since \( \tilde{\alpha}_{w-1,1} = R_{w-1,1} \)).

By applying the induction hypothesis, we obtain

\[
\| \tilde{A}_{w-1} \circ X_{w-1} \|_1 \leq \sum_{j=1}^{\ell} x_{1,j}
\]

and since \( \| A \circ X \|_1 \leq \| \tilde{A} \circ X \|_1 = \| \tilde{A}_{w-1} \circ X_{w-1} \|_1 \), this proves the result. \( \square \)