

Low-discrepancy sequences: Atanassov's methods revisited

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Abstract

We revisit Atanassov's methods for Halton sequences, (t, s) -sequences, and (t, \mathbf{e}, s) -sequences by providing a unifying framework enlightening the power and the efficiency of these methods for the study of low-discrepancy sequences. In this context, we obtain new improved explicit bounds for the star-discrepancy of these sequences, showing in most cases a better behavior than preceding ones in the non-asymptotic regime. Theoretical comparisons of discrepancy bounds in the non-asymptotic regime are much more difficult to achieve than in the asymptotic regime, where results exist to compare the leading constants c_s . Hence in this paper we mostly proceed via numerical comparisons to compare bounds. But in the case of (t, s) -sequences in base 2, we are able to compare two discrepancy bounds and prove that one is demonstrably better than the other for any $N \geq 2^s$. The proof is far from trivial as the two bounds are based on different combinatorial arguments.

Keywords: Discrepancy bounds, low-discrepancy sequences.

1. Introduction

Low-discrepancy sequences have been shown to be useful for various tasks in integration and approximation, providing estimates with a smaller error than those based on sequences of random points. The term discrepancy refers to the distance between the distribution induced by the points in the sequence and the uniform distribution. Low-discrepancy sequences are often assessed via *bounds* on this discrepancy measure. Several breakthroughs in the study of these bounds were achieved over the last decade or so by using an approach originally developed by Atanassov in [1]. This approach is the

main focus of this paper, whose purpose is two-fold. First, we present a general description of this approach, which allows us to review in a unifying way the bounds that have been obtained via this approach for different types of low-discrepancy sequences. Second, we establish new discrepancy bounds by using tighter combinatorial arguments to handle the leading term of these bounds, as well as tighter bounds on their complementary terms. We also establish comparisons between these new bounds and previously obtained ones. The rest of this section is devoted to the presentation of a few basic definitions and some terminology, as well as an outline of the rest of the paper.

Let us begin with the notion of discrepancy that will be used throughout the paper. For short, we only consider the so-called *star-discrepancy*, which corresponds to the worst-case error in the domain of complexity of multivariate problems. Let $X = (X_n)_{n \geq 1}$ be an infinite sequence in $I^s = [0, 1]^s$, with $s \geq 2$, and let J be an interval of I^s . The *discrepancy function* of X at rank N , on J is the difference $E(J; N; X) = A(J; N; X) - NV(J)$, where $A(J; N; X) = \#\{n; 1 \leq n \leq N, X_n \in J\}$ and $V(J)$ is the volume of J . Then, the *star-discrepancy* D^* (at rank N) is defined by $D^*(N, X) = \sup_{J \in \mathcal{J}^*} |E(J; X; N)|$, where \mathcal{J}^* is the set of intervals $J = \prod_{j=1}^s [0, z_j)$ with $z_j \in [0, 1]$. Note that several authors have a $1/N$ factor when defining the above quantities. We notice too that for our purpose here, one-dimensional sequences, for which more precise results exist (see among others [9, Section 2] and the survey [7]), are not relevant. Further, the condition $s \geq 2$ will be useful later.

A sequence satisfying $D^*(N, X) = O((\log N)^s)$ is considered to be a *low-discrepancy sequence* (LDS), or more precisely, in order to see the leading constant, if:

$$D^*(N, X) \leq c_s (\log N)^s + O((\log N)^{s-1}). \quad (1)$$

Here, we are mainly interested in the behavior of LDS in the finite regime and hence we are looking for best possible bounds with exact formulas rather than (1).

We now briefly recall the definitions of the LDS we are going to study:

- Halton sequences have coordinates given by van der Corput sequences in pairwise coprime bases, these sequences $(x_n)_{n \geq 1}$ being obtained by means of the famous radical inverse function that consists in reversing the b -adic expansion of n . That is, in base $b \geq 2$, x_n is given by $x_n = \sum_{r=0}^{\infty} a_r(n) b^{-r-1}$, where the $a_r(n)$ are such that $n - 1 = \sum_{r=0}^{\infty} a_r(n) b^r$ for $n \geq 1$. Here, let us

mention again the survey [7] dedicated to the memory of van der Corput on the occasion of his 125th birthday.

– Let $b \geq 2$ and $0 \leq t \leq m$ be integers. Then a (t, m, s) -net in base b is a point set in I^s with b^m points such that any (elementary) interval $\prod_{i=1}^s [a_i b^{-d_i}, (a_i + 1) b^{-d_i}]$ in base b (with $0 \leq a_i < b^{d_i}$ for $1 \leq i \leq s$) with volume b^{t-m} contains exactly b^t points of the set. Now, a sequence $(X_n)_{n \geq 1}$ in I^s is a (t, s) -sequence in base b if the subset $\{[X_n]_{b,m}; kb^m < n \leq (k+1)b^m\}$ is a (t, m, s) -net in base b for all integers $k \geq 0$ and $m \geq t$, where $[X]_{b,m}$ means an m -truncation is applied to each coordinate. Van der Corput sequences are the backbone for the construction of concrete (t, s) -sequences, as well as for (t, \mathbf{e}, s) -sequences which we now define.

– The notion of (t, \mathbf{e}, s) -sequences, where $\mathbf{e} = (e_1, \dots, e_s)$ with positive integers e_i , was recently introduced by Tezuka [17]: A (t, m, \mathbf{e}, s) -net in base b is a point set in I^s with b^m points such that any elementary interval $\prod_{i=1}^s [a_i b^{-d_i}, (a_i + 1) b^{-d_i}]$ with $0 \leq a_i < b^{d_i}$ and $e_i | d_i$ for $1 \leq i \leq s$, and with volume b^{t-m} , contains exactly b^t points of the set. Then the definition of a (t, \mathbf{e}, s) -sequence in base b is the same as for a (t, s) -sequence with (t, m, \mathbf{e}, s) -nets in place of usual (t, m, s) -nets.

What we call Atanassov's methods (At.Ms) is a new approach introduced by Atanassov [1] about 10 years ago to compute upper bounds for LDS. In fact, this approach recovers two kinds of meanings: first, when it is applied to arbitrary Halton sequences (including scrambled versions with permutations), in which case one speaks of the first Atanassov's method (first At.M.); and second, when a further refinement allows much tighter bounds for a special class of permutations in scrambled Halton sequences, in which case one speaks of the second Atanassov's method (second At.M.) (see [5] for a general updated survey on both methods). Until now, only the first At.M. has received further *extensions* to other families of LDS.

The first *extension* of the first At.M. concerns arbitrary (t, s) -sequences and was set out in [12]. This extension was further significantly improved in [9] in the case of even bases, hence getting what was then the best constant c_s for even b .

The second *extension* of the first At.M., due to Tezuka [17], concerns (t, \mathbf{e}, s) -sequences. Applied to generalized Niederreiter sequences with quality parameter t , his new bound improves the leading constant c_s by a factor of about $\prod_{i=1}^s e_i^{-1}$. It is worth noting that these results were all obtained with close extensions of Atanassov's ideas for Halton sequences to a single base

(including the special treatment required for even bases in [9]).

Following our investigations of the extension of At.M. for (t, s) -sequences in [9], we have found an original *variant* of this extension, which led to new bounds for (t, s) -sequences in [10]. This *variant* for (t, s) -sequences has no equivalent for Halton sequences and (t, \mathbf{e}, s) -sequences, which can only be dealt with using the argument on diophantine geometry used by Atanassov in his fundamental Lemma 3.3. But the ideas involved in this variant have led to a key lemma in a proof of a new bound for (t, \mathbf{e}, s) -sequences in the same paper [10].

The rest of the paper is organized as follows. In Section 2, we present in a unifying way the different discrepancy bounds that have been obtained using the first At.M., including the variant mentioned previously. In addition, we introduce a tighter bound for the complementary term in these bounds. In Sections 3, 4, and 5, we revisit our variant of the first At.M. for (t, s) -sequences, (t, \mathbf{e}, s) -sequences, and Halton sequences, respectively, hence getting new bounds for the discrepancy of these sequences. Numerical experiments, based on a new approach for the comparison of various explicit bounds due to P. Kritzer on a ingenious suggestion of H. Woźniakowski, are presented in Section 6 and show the behavior of old and new bounds in the non-asymptotic regime. These experiments confirm that the new bounds are often smaller than previously obtained ones. Nevertheless, we have been able to prove at the end of Section 3 that for (t, s) -sequences in base 2, the bound obtained from our original variant is demonstrably better than the newly obtained one for any dimension s and all $N \geq 2^s$.

2. Review of results for Halton, (t, s) - and (t, \mathbf{e}, s) -sequences

In short, if b_1, \dots, b_s are integers with $b_i \geq 2$ for all i , we can say that Halton sequences are obtained with pairwise coprime bases (and for which an adapted definition of the quality parameter t would be set to 0, see [5, p. 111]), (t, s) -sequences in base b are obtained with $b_i = b$ for all i , and (t, \mathbf{e}, s) -sequences in base b are obtained with $b_i = b^{e_i}$ for all i . With this correspondence, we can easily state in a condensed way the different steps of the first At.M., its extensions and its variant. We postpone the statement of the theorems until the next sections – where they will be useful for comparisons with our new results, and later, as they relate to Section 6 – and focus on the method in itself.

It is essentially based on three ingredients: A well-known property that permits to bound the discrepancy function on an elementary interval, a decomposition of intervals by means of signed splittings using signed numeration systems, and a fundamental lemma, coming from diophantine geometry, applied to bound the sums resulting from the above decomposition. These three ingredients were respectively introduced in [16, p. 9], in [3] and [4], and in [1] (see [5, p. 111–112] for more details on each of these items). They read as follows:

Lemma 1. *Let J be an interval of the form $J = \prod_{i=1}^s [c_i b_i^{-d_i}, c'_i b_i^{-d_i})$ with integers c_i, c'_i satisfying $0 \leq c_i < c'_i \leq b_i^{d_i}$. Then for every $N \geq 1$*

$$|A(J; N; X) - NV(J)| \leq b^t (c'_1 - c_1) \cdots (c'_s - c_s).$$

Further if $N < b^t b_1^{d_1} \cdots b_s^{d_s}$ then $A(J; N; X) \leq b^t (c'_1 - c_1) \cdots (c'_s - c_s)$.

Lemma 1 applies to the three families of sequences, see [1, Lemma 3.1] (with t set to 0), [9, Lemma 2] and [17, Lemma 1].

Definition 1. Let be given an interval $J \subseteq I^s$, then a *signed splitting* of J is any collection of intervals J_1, \dots, J_n and respective signs $\epsilon_1, \dots, \epsilon_n$ equal to ± 1 , such that for any (finitely) additive function ν on the intervals in I^s , $\nu(J) = \sum_{i=1}^n \epsilon_i \nu(J_i)$.

Lemma 2. *Let $J = \prod_{i=1}^s [0, z^{(i)})$ be an interval in I^s and, for each $1 \leq i \leq s$, let $n_i \geq 0$ be given integers. Set $z_0^{(i)} = 0$, $z_{n_i+1}^{(i)} = z^{(i)}$ and, if $n_i \geq 1$, let $z_j^{(i)} \in [0, 1]$ be arbitrary given numbers for $1 \leq j \leq n_i$. Then the collection of intervals $\prod_{i=1}^s [\min(z_{j_i}^{(i)}, z_{j_i+1}^{(i)}), \max(z_{j_i}^{(i)}, z_{j_i+1}^{(i)})]$, with signs $\epsilon(j_1, \dots, j_s) = \prod_{i=1}^s \text{sgn}(z_{j_i+1}^{(i)} - z_{j_i}^{(i)})$, for $0 \leq j_i \leq n_i$, is a signed splitting of the interval J .*

Lemma 2 is independent of bases and thus it applies to the three families of sequences, see [1, Lemma 3.5], [9, Lemma 4] and [17, Lemma 3].

Lemma 3. *Let $N \geq 1, k \geq 1$ and b_1, \dots, b_s ($b_i \geq 2$) be integers. For integers $j \geq 0, 1 \leq i \leq k$, let some numbers $c_j^{(i)} \geq 0$ be given, satisfying $c_0^{(i)} \leq 1$ and $c_j^{(i)} \leq c_i$ for $j \geq 1$, for some fixed numbers c_i ($1 \leq i \leq k$). Then*

$$\sum_{\{\mathbf{j}=(j_1, \dots, j_k); b_1^{j_1} \cdots b_k^{j_k} \leq N\}} \prod_{i=1}^k c_{j_i}^{(i)} \leq \frac{1}{k!} \prod_{i=1}^k \left(c_i \frac{\log N}{\log b_i} + k \right). \quad (2)$$

Lemma 3 applies to the three families of sequences, see [1, Lemma 3.3], [9, Lemma 3] (where the fixed numbers $c_i = c$) and [17, Lemma 2] (there the given real α stands for $\log N / \log b - t$). Lemma 3 results from the following *essential* argument from diophantine geometry, saying that:

$$\text{for all integers } k \geq 1, \# \{ \mathbf{j}; b_1^{j_1} \dots b_k^{j_k} \leq N \} \leq \frac{1}{k!} \prod_{i=1}^k \frac{\log N}{\log b_i}. \quad (3)$$

Note that in (3), we assume $j_i > 0$ for $i = 1, \dots, k$ while in Lemma 3 $j_i \geq 0$ for $i = 1, \dots, k$.

Now we are in a position to present in one main result the four theorems [1, Theorem 2.1], [9, Theorems 2, 3] and [17, Theorem 2] (being agreed that for simplicity the truncation is omitted in the case of (t, s) - and (t, \mathbf{e}, s) -sequences). A complete proof is then given for this unifying scheme to obtain discrepancy bounds.

Theorem 1. (i) *For any Halton sequence X with pairwise co-prime bases b_i and $N \geq 1$, we have (AtHa04)*

$$D^*(N, X) \leq \frac{1}{s!} \prod_{i=1}^s \left(\frac{(b_i - 1) \log N}{2 \log b_i} + s \right) + \sum_{k=0}^{s-1} \frac{b_{k+1}}{k!} \prod_{i=1}^k \left(\left\lfloor \frac{b_i}{2} \right\rfloor \frac{\log N}{\log b_i} + k \right) + u,$$

with $u = \frac{b_r}{2(s-1)!} \prod_{1 \leq j \leq s, j \neq r} \left(\frac{(b_j - 1) \log N}{2 \log b_j} + s - 1 \right)$ if there is an even base b_r , and is 0 otherwise.

(ii) *For any (t, s) -sequence X in any base b and for any $N \geq 1$, we have (FL12-gen)*

$$D^*(N, X) \leq \frac{b^t}{s!} \left(\left\lfloor \frac{b}{2} \right\rfloor \frac{\log N}{\log b} + s \right)^s + b^t \sum_{k=0}^{s-1} \frac{b}{k!} \left(\left\lfloor \frac{b}{2} \right\rfloor \frac{\log N}{\log b} + k \right)^k.$$

(iii) *For any (t, s) -sequence X in an even base b and any $N \geq b^s$, we have (FL12-even)*

$$D^*(N, X) \leq \frac{b^t}{s!} \left(\frac{b-1}{2} \frac{\log N}{\log b} + s \right)^s + s b^t \left(\frac{b}{2} \right)^s \left(\frac{\log N}{\log b} \right)^{s-1} + b^t \sum_{k=0}^{s-1} \frac{b}{k!} \left(\frac{b}{2} \frac{\log N}{\log b} + k \right)^k.$$

(iv) For any (t, \mathbf{e}, s) -sequence X in base b and $N > b^t$, we have (Tez13)

$$D^*(N, X) \leq \frac{b^t}{s!} \prod_{i=1}^s \left(\frac{\lfloor b^{e_i}/2 \rfloor}{e_i} \left(\frac{\log N}{\log b} - t \right) + s \right) + \sum_{k=0}^{s-1} \frac{b^{t+e_{k+1}}}{k!} \prod_{i=1}^k \left(\frac{\lfloor b^{e_i}/2 \rfloor}{e_i} \left(\frac{\log N}{\log b} - t \right) + k \right).$$

Before proceeding to the proof, note that for (ii) and (iii), the stated bounds hold trivially for $N \leq b^t$ since it is larger than the obvious bound of N in that case.

Proof. Pick any $(z^{(1)}, \dots, z^{(s)}) \in [0, 1]^s$ and expand each $z^{(i)}$ as $\sum_{j=0}^{\infty} a_j^{(i)} b_i^{-j}$ according to signed numeration systems (where the digits $a_{j_i}^{(i)}$ are bounded by $(b_i - 1)/2$, $b_i/2$ and $(b_i - 2)/2$ in the respective cases where b_i is odd, b_i is even and j is even, and b_i is even and j is odd).

Let $n_i := \lfloor \log N / \log b_i \rfloor$, define $z_0^{(i)} = 0$ and $z_{n_i+2}^{(i)} = z^{(i)}$, and consider the numbers $z_k^{(i)} = \sum_{j=0}^{k-1} a_j^{(i)} b_i^{-j}$ for $k = 1, \dots, n_i + 1$. Applying Lemma 2 with $(z_j^{(i)})_{j=1}^{n_i+2}$, $J = \prod_{i=1}^s [0, z^{(i)})$ is expanded in the signed splitting:

$$I(\mathbf{j}) = \prod_{i=1}^s [\min(z_{j_i}^{(i)}, z_{j_i+1}^{(i)}), \max(z_{j_i}^{(i)}, z_{j_i+1}^{(i)})], \quad 0 \leq j_i \leq n_i + 1,$$

with signs $\epsilon(\mathbf{j}) = \prod_{i=1}^s \text{sgn}(z_{j_i+1}^{(i)} - z_{j_i}^{(i)})$, where $\mathbf{j} = (j_1, \dots, j_s)$.

Since V and $A(\cdot; N; X)$ are both additive, the discrepancy function is expanded as

$$A(J; N; X) - NV(J) = \sum_{j_1=0}^{n_1+1} \cdots \sum_{j_s=0}^{n_s+1} \epsilon(\mathbf{j}) (A(I(\mathbf{j}); \mathcal{P}_N) - NV(I(\mathbf{j}))) =: \Sigma_1 + \Sigma_2, \quad (4)$$

where we rearrange the terms so that in Σ_1 we put the terms \mathbf{j} such that $b_1^{j_1} \cdots b_s^{j_s} \leq N$ and in Σ_2 the rest.

It is easy to deal with Σ_1 in the case where all b_i are odd: from Lemma 1 and since $z_{k+1}^{(i)} - z_k^{(i)} = a_k^{(i)} b_i^{-k}$, for any $\mathbf{j} \in \Sigma_1$ we have that

$$|A(I(\mathbf{j}); N; X) - NV(I(\mathbf{j}))| \leq b^t \prod_{i=1}^s |z_{j_i+1}^{(i)} - z_{j_i}^{(i)}| b^{j_i} = b^t \prod_{i=1}^s |a_{j_i}^{(i)}|. \quad (5)$$

Hence, applying Lemma 3 with $k = s$, $c_j^{(i)} = |a_j^{(i)}|$ and $c_i = \lfloor b_i/2 \rfloor$, we obtain

$$|\Sigma_1| \leq \sum_{\{\mathbf{j}; b_1^{j_1} \dots b_s^{j_s} \leq N\}} |A(I(\mathbf{j}); N; X) - NV(I(\mathbf{j}))| \leq \frac{b^t}{s!} \prod_{i=1}^s \left(\frac{(b_i - 1) \log N}{2 \log b_i} + s \right), \quad (6)$$

which is the leading part of the bounds of the four theorems. Notice that (Tez13) in (iv) differs from (6) by terms $\log N / \log b$ instead of $\log N / \log b - t$. This point is addressed in Section 4.2 where the reader will find a detailed discussion and a further slight improvement of (Tez13).

In the case where one b_i is even, getting $(b_i - 1)/2$ instead of $b_i/2$ in the leading part of [1, Theorem 2.1], and [9, Theorem 3] requires a trick developed by Atanassov in his proof [1, pp. 22–23], which implies a further complementary term (denoted u in [1, Theorem 2.1]). This refinement is not considered in [17, Theorem 2].

The terms gathered in Σ_2 give the second part of the four bounds in Theorem 1. The idea of Atanassov is to divide the set of s -tuples (j_1, \dots, j_s) in Σ_2 into s disjoint sets B_0, \dots, B_{s-1} included in larger ones for which Lemma 3 applies and gives the desired upper bound. His proof can be transcribed as well in the present scheme and gives

$$|\Sigma_2| \leq b^t \sum_{k=0}^{s-1} \frac{b_{k+1}}{k!} \prod_{i=1}^k \left(\left\lfloor \frac{b_i}{2} \right\rfloor \frac{\log N}{\log b_i} + k \right). \quad (7)$$

□

The bound (7) on Σ_2 can be slightly improved by treating the cases b even and b odd separately in the first At.M. (for Halton sequences) and its extensions to (t, s) - and (t, \mathbf{e}, s) -sequences. A result describing this improved bound for Σ_2 will be given at the beginning of the next section, with a proof for both this new bound and for (7) given in the appendix.

The scheme used above to obtain the bounds in Theorem 1 runs for the original At.M. and its extensions to (t, s) -sequences and (t, \mathbf{e}, s) -sequences, all using the original diophantine geometry argument. While we tried to overcome an inaccuracy in our proof of [9, Theorem 3], we found a different way to deal with it that allowed us to improve further both [9, Theorems 2 and 3] and that also appeared suitable for (t, \mathbf{e}, s) -sequences. We call this

approach a *variant of Atanassov's method*. Before we recall the result that this variant leads to along with its proof, we first overview its main idea, which is based on the following two steps.

The first step consists in a more precise *combinatorial argument* in place of (3) (not applicable to Halton sequences and (t, \mathbf{e}, s) -sequences) to bound the discrepancy function of (t, s) -sequences (see [10, Lemma 4]):

Lemma 4. *Given two integers $k \geq 1$ and $n \geq 0$, the number of nonnegative integers solutions of the inequality $0 \leq j_1 + \dots + j_k \leq n$ is equal to $\binom{n+k}{k}$.*

Thanks to this property and using a careful worst-case configuration analysis in the case of an even base, with the quantities $c_j^{(i)}$ and $c_i = c$ of Lemma 3, we get

$$\sum_{\{\mathbf{j}; b^{j_1} \dots b^{j_k} \leq N\}} \prod_{i=1}^k c_{j_i}^{(i)} \leq \frac{c^k}{k!} \prod_{l=1}^k \left(\frac{\log N}{\log b} + l \right), \quad (8)$$

which was established in [10, Eq.(9)].

The second step, still based on our combinatorial argument together with a careful analysis of the distribution of even and odd j_i in k -tuples $\mathbf{j} = (j_1, \dots, j_k)$, consists in a variant of Inequality (8) useful to deal with even bases ([10, Lemma 5]):

$$\sum_{\{\mathbf{j}; b^{j_1} \dots b^{j_k} \leq N\}} \prod_{i=1}^k c_{j_i}^{(i)} \leq \frac{1}{k!} \left(\frac{c + c'}{2} \right)^k \prod_{l=1}^k \left(\frac{\log N}{\log b} + 2l \right), \quad (9)$$

in which the numbers $c_j^{(i)} \geq 0$ satisfy $c_{2h+1}^{(i)} \leq c$ and $c_{2h}^{(i)} \leq c'$ for $h \geq 0$ (where $c, c' \geq 0$ are some fixed numbers).

Altogether, using Inequalities (8) and (9) in place of Lemma 3, the proof of Theorem 1 valid for the three families of sequences applies and leads to [10, Theorem 1] for (t, s) -sequences which is an improvement on [9, Theorems 2 and 3]. Summarizing, we get the following result:

Theorem 2. *(i) For any (t, s) -sequence X in an odd base b and for any $N \geq 1$ (FL14-odd)*

$$D^*(N, X) \leq \frac{b^t}{s!} \left(\frac{b-1}{2} \right)^s \prod_{k=1}^s \left(\frac{\log N}{\log b} + k \right) + b^t \sum_{k=0}^{s-1} \frac{b}{k!} \left(\frac{b-1}{2} \right)^k \prod_{l=1}^k \left(\frac{\log N}{\log b} + l \right).$$

(ii) For any (t, s) -sequence X in an even base b and any $N \geq 1$ (FL14-even)

$$D^*(N, X) \leq \frac{b^t}{s!} \left(\frac{b-1}{2} \right)^s \prod_{k=1}^s \left(\frac{\log N}{\log b} + 2k \right) + b^t \sum_{k=0}^{s-1} \frac{b}{k!} \left(\frac{b-1}{2} \right)^k \prod_{l=1}^k \left(\frac{\log N}{\log b} + 2l \right).$$

Proof. For the odd b case and as mentioned above, the result can be proved following the same steps as the proof of Theorem 1 up until (6), where we use (8) instead of Lemma 3 with $c = (b-1)/2$ since $a_{j_i}^{(i)} \leq (b-1)/2$ when b is odd. Thus we get

$$|\Sigma_1| \leq \frac{b^t}{s!} \left(\frac{b-1}{2} \right)^s \prod_{k=1}^s \left(\frac{\log N}{\log b} + k \right).$$

The same argument is used to handle the bound on Σ_2 , the result being that each term in the sum over k for the bound in (7) is replaced by an expression of the form

$$\frac{b}{k!} \left(\frac{b-1}{2} \right)^k \prod_{l=1}^k \left(\frac{\log N}{\log b} + l \right).$$

For the even b case, the proof also mimics the one for Theorem 1 up to (6), where instead of using Lemma 3, we use (9) to bound $|\Sigma_1|$, with c and c' given respectively by $(b-2)/2$ and $b/2$, as can be inferred from the comments at the beginning of the proof of Theorem 1, when bounds on $a_j^{(i)}$ are given. As in the odd b case, we also apply this argument to obtain a bound on $|\Sigma_2|$ where Inequality (9) is applied to each term over k in that bound. \square

Finally, as alluded to in the presentation of our *variant* in the introduction, we discuss its adaptation that led to an improvement of the leading constant c_s in [17, Theorem 2]. This application to (t, \mathbf{e}, s) -sequences will be improved in Section 4. The main ingredient is the following inequality, established in [10, Lemma 7]. It is based on the diophantine argument (3) combined with the idea already used for the proof of (9):

$$\sum_{\{\mathbf{j}; e_1 j_1 + \dots + e_k j_k \leq n\}} \prod_{i=1}^k c_{j_i}^{(i)} \leq \frac{1}{k!} \prod_{i=1}^k \left(\frac{f_i + f'_i}{e_i} \left\lfloor \frac{n + \sum_{i=1}^k e_i}{2} \right\rfloor + k \right), \quad (10)$$

in which the numbers $c_j^{(i)} \geq 0$ satisfy $c_0^{(i)} \leq 1$, $c_{2h+1}^{(i)} \leq f_i$ for any $h \geq 0$ and $c_{2h}^{(i)} \leq f'_i$ for any $h \geq 1$ (and where $f_i, f'_i \geq 0$ are some fixed numbers).

Applying again the scheme presented for the three families in the proof of Theorem 1, but with Inequality (10) in place of Lemma 3, our *variant* leads to [10, Theorem 2] for (t, \mathbf{e}, s) -sequences, as given below.

Theorem 3. *For any (t, \mathbf{e}, s) -sequence X in base b and $N \geq 1$, we have (FLtes14)*

$$D^*(N, X) \leq \frac{b^t}{s!} \prod_{i=1}^s \left(\frac{b^{e_i} - 1}{2e_i} \left(\frac{\log N}{\log b} + \sum_{i=1}^s e_i \right) + s \right) + \sum_{k=0}^{s-1} \frac{b^{t+e_{k+1}}}{k!} \prod_{i=1}^k \left(\frac{b^{e_i} - 1}{2e_i} \left(\frac{\log N}{\log b} + \sum_{i=1}^k e_i \right) + k \right).$$

Proof. Here as well, the proof proceeds as in the proof of Theorem 1 up until (6), where instead of Lemma 3 we apply (10) with $n = \lfloor \log N / \log b \rfloor$, $f_i = \lfloor (b^{e_i} - 1)/2 \rfloor$ and $f'_i = \lfloor b^{e_i}/2 \rfloor$. (These values for f_i and f'_i come from the bounds for the digits $a_j^{(i)}$ mentioned at the beginning of the proof of Theorem 1.) Applying (10) also to the terms in the sum over k that bounds $|\Sigma_2|$ in (7) gives us the result. \square

3. Improving bounds for (t, s) -sequences

In this section, as announced in Section 1, we revisit our *variant* of the first At.M. for (t, s) -sequences. We start by presenting in Section 3.1 a new bound that holds for odd bases, and then in Section 3.2 we focus on the case of even bases. An explicit comparison between the new bound obtained there and the one obtained in our *variant* for the case $b = 2$ is studied in Section 3.3.

Before presenting these results, we first give the improved bound on Σ_2 that was mentioned at the end of our proof of Theorem 1, as it will be used throughout this section to provide smaller complementary terms in the different bounds we present. The proof of this result (and of the original bound (7)) is given in the appendix. Note that the improved bound is given in terms of the product $\prod_{i=1}^k |a_{j_i}^{(i)}|$ which can then be bounded according to the different approaches considered in this paper, including (t, \mathbf{e}, s) -sequences (Section 4) and Halton sequences (Section 5).

Proposition 1. Let $N \geq 1, s \geq 1$ and b_1, \dots, b_s ($b_i \geq 2$) be integers. Let Σ_2 and the integers $a_j^{(i)}$ for $i = 1, \dots, s$ be defined as in the proof of Theorem 1. Then

$$|\Sigma_2| \leq b^t \sum_{k=0}^{s-1} \left\lfloor \frac{b_{k+1}}{2} + 1 \right\rfloor \sum_{\{\mathbf{j}; b_1^{j_1} \dots b_k^{j_k} \leq N\}} \prod_{i=1}^k |a_{j_i}^{(i)}|.$$

3.1. The case of an odd base

Starting from another combinatorial property, namely *the number of positive integer solutions of the equation $x_1 + \dots + x_k = n$ is equal to $\binom{n-1}{k-1}$* (see the proof of [10, Lemma 4]), we have found an inequality even more precise than Inequalities (2) used for [9, Theorem 1] and (8) used for [10, Theorem 1] (see [10, Third point of Remark 2]):

Lemma 5. Let the quantities $c_j^{(i)}$ and $c_i = c$ be as in Lemma 3. Then we have

$$\sum_{\{\mathbf{j}; 0 \leq j_1 + \dots + j_k \leq n\}} \prod_{i=1}^k c_{j_i}^{(i)} \leq \sum_{m=0}^k c^m \binom{n}{m} \binom{k}{m} = \sum_{m=0}^{\min(k,n)} c^m \binom{n}{m} \binom{k}{m}. \quad (11)$$

Proof. We give the proof for the sake of completeness. We first partition the set $\{\mathbf{j}; 0 \leq j_1 + \dots + j_k \leq n\}$ into $k+1$ subsets as follows: $\cup_{m=0}^k T_m$, where $T_m = \{\mathbf{j}; 0 \leq j_1 + \dots + j_k \leq n \text{ and } \sum_{i=1}^k \mathbf{1}_{j_i > 0} = m.\}$ Since $c_0^{(i)} \leq 1$, we have that

$$\sum_{\{\mathbf{j}; 0 \leq j_1 + \dots + j_k \leq n\}} \prod_{i=1}^k c_{j_i}^{(i)} \leq \sum_{m=0}^k \sum_{\mathbf{j} \in T_m} c^m.$$

We then note that $|T_m| = \binom{k}{m} \sum_{l=m}^n \binom{l-1}{m-1} = \binom{k}{m} \binom{n}{m}$, where the first equality comes from the combinatorial property mentioned before the statement of Lemma 5, and the second equality follows from a well-known combinatorial identity involving binomial coefficients. \square

In the case of an *odd* base, we then apply the scheme presented in Theorem 2, but with (11) instead of Lemma 4, and Proposition 1 to handle Σ_2 , and get the following improved bound:

Theorem 4. For any (t, s) -sequence X in odd base b and for any $N \geq 1$

$$D^*(N, X) \leq b^t \sum_{m=0}^{\min(s,n)} \frac{1}{m!} \binom{s}{m} \left(\frac{b-1}{2}\right)^m \prod_{l=0}^{m-1} \left(\frac{\log N}{\log b} - l\right) +$$

$$b^t \sum_{k=0}^{s-1} \sum_{m=0}^{\min(k,n)} \frac{b+1}{2m!} \binom{k}{m} \left(\frac{b-1}{2}\right)^m \prod_{l=0}^{m-1} \left(\frac{\log N}{\log b} - l\right) \text{ (newFL-odd)},$$

where $n = \lfloor \log N / \log b \rfloor$.

This new bound improves upon FL14-odd because in the latter, we replace $((b-1)/2)^m$ in the above bound by $((b-1)/2)^s$ to simplify it. Hence the improvement will be more significant as b increases. The new bound also improves upon FL12-gen because in the latter, the term $\binom{n}{m}$ in the above bound is replaced by $n^m s^{s-m}/s!$ to simplify it. Thus the improvement of the above bound is more significant when n and s are small.

3.2. The case of an even base

The case of an *even* base needs a new version of inequality (11), i.e., an analogue of (9) with two constants c, c' instead of one. To this end, we proceed as in [10, Lemma 7], but with all $e_i = 1$. The idea is then to replace the argument from diophantine geometry used in the proof of that lemma by the other combinatorial property we just evoked for the proof of (11). Details are given in the proof of the following result:

Lemma 6. *With the notations of Inequality (10), but based on common values $f_i = f$ and $f'_i = f'$ for all i , we have*

$$\sum_{\{(j_1, \dots, j_k) : 0 \leq j_1 + \dots + j_k \leq n\}} \prod_{i=1}^k c_{j_i}^{(i)} \leq \sum_{m=0}^k (f + f')^m \binom{\lfloor \frac{n+m}{2} \rfloor}{m} \binom{k}{m}. \quad (12)$$

Proof. In the same manner as in [1, Lemma 3.3], [9, Lemma 3] and [17, Lemma 2], we split up the sum on the left-hand side (LHS) of (12) along subsets u of $\{1, \dots, k\}$ with $j_i > 0$ if $i \in u$ and $j_i = 0$ if $i \notin u$, and with $m = |u|$, but we add a new splitting according to the parity of the j_i 's. To this end, we consider subsets \mathcal{L} of u with $i \in \mathcal{L}$ if j_i is even and $i \in u \setminus \mathcal{L}$ if j_i is odd:

$$\sum_{(j_1, \dots, j_k) \in S'} \prod_{i=1}^k c_{j_i}^{(i)} = \sum_{u \subseteq \{1, \dots, k\}} \sum_{l=0}^m \sum_{\mathcal{L} \subseteq u, |\mathcal{L}|=l} \sum_{\substack{j \in S'_u \\ j_i \text{ even} \Leftrightarrow i \in \mathcal{L}}} \prod_{i=1}^k c_{j_i}^{(i)},$$

where $S'_u = \{(j_1, \dots, j_k) \in S'; e_{i_1}j_{i_1} + \dots + e_{i_m}j_{i_m} \leq n \text{ and } j_i = 0 \Leftrightarrow i \notin u\}$. According to the hypothesis on the coefficients $c_{j_i}^{(i)}$, we obtain

$$\begin{aligned} \sum_{(j_1, \dots, j_k) \in S'} \prod_{i=1}^k c_{j_i}^{(i)} &\leq \sum_{u \subseteq \{1, \dots, k\}} \sum_{l=0}^m \sum_{\mathcal{L} \subseteq u, |\mathcal{L}|=l} \sum_{\substack{\mathbf{j} \in S'_u \\ j_i \text{ even} \Leftrightarrow i \in \mathcal{L}}} \left[\prod_{i \in \mathcal{L}} f'_i \prod_{i \in u \setminus \mathcal{L}} f_i \right] \\ &\leq \sum_{u \subseteq \{1, \dots, k\}} \sum_{l=0}^m \sum_{\mathcal{L} \subseteq u, |\mathcal{L}|=l} N(u, \mathcal{L}, k, n) (f')^l f^{m-l}, \end{aligned}$$

where $N(u, \mathcal{L}, k, n)$ is the cardinality of the set $\{\mathbf{j} \in S'_u; j_i \text{ even} \Leftrightarrow i \in \mathcal{L}\}$.

For short, we write $|u| = m$ and $|u \setminus \mathcal{L}| = m - l$. Adding the numbers of solutions to $\sum_{i \in u} h_i = g$ with g going from m to $\lfloor \frac{n+m-l}{2} \rfloor$ (recall that $h_i > 0$ if $i \in u$, so that $\sum_{i \in u} h_i \geq m$), we get:

$$N(u, \mathcal{L}, k, n) = \binom{\lfloor \frac{n+m-l}{2} \rfloor}{m}$$

instead of the bound $N(u, \mathcal{L}, k, n) \leq \frac{1}{m!} \lfloor \frac{n+m-l}{2} \rfloor^m$ that was used to get [10, Lemma 7], recalled here via (10).

Putting this all together, and using the simplification that here the numbers f_i and f'_i take the respective common values f and f' , we get

$$\begin{aligned} \sum_{(j_1, \dots, j_k) \in S'} \prod_{i=1}^k c_{j_i}^{(i)} &\leq \sum_{u \subseteq \{1, \dots, k\}} \sum_{l=0}^m \binom{m}{l} \binom{\lfloor \frac{n+m-l}{2} \rfloor}{m} (f')^l f^{m-l} \\ &\leq \sum_{m=0}^k \binom{k}{m} \binom{\lfloor \frac{n+m}{2} \rfloor}{m} (f + f')^m. \end{aligned}$$

□

Using this result, we again apply the scheme used in Theorem 1 and bound Σ_1 and Σ_2 in the same way – with Σ_2 handled via Proposition 1 – arriving to:

Theorem 5. *For any (t, s) -sequence X in an even base b and any $N \geq 1$ we have*

$$D^*(N, X) \leq b^t \sum_{m=0}^{\min(s, n)} \frac{1}{m!} \binom{s}{m} \left(\frac{b-1}{2}\right)^m \prod_{l=0}^{m-1} \left(\frac{\log N}{\log b} + m - 2l\right) +$$

$$b^t \sum_{k=0}^{s-1} \sum_{m=0}^{\min(k,n)} \frac{b+2}{2m!} \binom{k}{m} \left(\frac{b-1}{2}\right)^m \prod_{l=0}^{m-1} \left(\frac{\log N}{\log b} + m - 2l\right) \quad (\text{newFL-even}),$$

where $n = \lfloor \log N / \log b \rfloor$.

3.3. Comparisons between new and variant-based bounds for the case $b = 2$

Since the proof for the new bound relies on an entirely different argument than what is used for FL14-even (Theorem 2 (ii)) and FL12-even (Theorem 1 (iii)), it is more difficult to make comparisons than in the b odd case. When $b \geq 4$, the new bound is based on a sum of smaller powers of $(b-1)/2$ than the other two bounds, but this is no longer an advantage when $b = 2$. In that case, the bound FL14-even is never larger than the newFL-even bound from Theorem 5, as shown in the following result.

Proposition 2. *For a (t, s) -sequence X in base $b = 2$ and with $s \geq 2$, the bound on $D^*(N, X)$ given in Theorem 2 (FL14-even) is never larger than the one given in Theorem 5 (newFL-even) for any $N \geq b^s$.*

Proof. Looking at these two bounds, it should be clear that the required result is obtained if we can prove that $g_s(n) \leq h_s(n)$ for $n = \log N / \log b \geq s$, where

$$g_s(n) = \frac{1}{2^s s!} (n+2s)(n+2s-2) \cdots (n+2) = \frac{1}{s!} \frac{\Gamma(\frac{n}{2} + s + 1)}{\Gamma(\frac{n}{2} + 1)}$$

$$h_s(n) = \sum_{m=0}^s h_{s,m}(n), \quad \text{where } h_{s,m}(n) = \frac{\binom{s}{m} \Gamma(\frac{n+m}{2} + 1)}{m! \Gamma(\frac{n-m}{2} + 1)}.$$

To do so, we first rewrite $g_s(n)$ in the same form as $h_s(n)$ by grouping the terms having the same power of $s/2$:

$$g_s(n) = \frac{1}{s!} \left(\frac{n+s}{2} + \frac{s}{2}\right) \left(\frac{n+s}{2} - 1 + \frac{s}{2}\right) \cdots \left(\frac{n-s}{2} + 1 + \frac{s}{2}\right)$$

$$= \sum_{m=0}^s g_{s,m}(n) \quad \text{where } g_{s,m}(n) = \frac{1}{s!} \binom{s}{m} \left(\frac{s}{2}\right)^{s-m} \mu(n, s, m),$$

where

$$\mu(n, s, m) := \frac{1}{\binom{s}{m}} \sum_{\mathcal{I} \subseteq \mathcal{B}(n,s), |\mathcal{I}|=m} \prod_{i_j \in \mathcal{I}} i_j \quad (13)$$

and $\mathcal{B}(n, s) := \{\frac{n+s}{2}, \frac{n+s}{2} - 1, \dots, \frac{n-s}{2} + 1\}$. Indeed, $\binom{s}{m}\mu(n, s, m)$ is the product of m distinct terms of the form $(n+s)/2 - j$ for $0 \leq j < s$, which are exactly the elements of $\mathcal{B}(n, s)$.

To help us compare the terms $h_{s,m}(n)$ and $g_{s,m}(n)$, the following lemma will be useful. It shows that the average product $\mu(n, s, m)$ defined in (13) is bounded from above by the product of the m “middle” terms in the set $\mathcal{B}(n, s)$. Its proof is in the appendix.

Lemma 7. *For $n \geq s \geq 2$ and $0 \leq m \leq s$, where $m, s \in \mathbb{N}$ and $n \in \mathbb{R}$, we have that $\mu(n, s, m) \leq \Gamma(\frac{n+m}{2} + 1)/\Gamma(\frac{n-m}{2} + 1)$.*

Based on Lemma 7, we see that if m is large enough, then $g_{s,m}(n) \leq h_{s,m}(n)$. More precisely, if we let k_s^* be the smallest integer such that

$$\left(\frac{s}{2}\right)^{s-k_s^*} \leq \frac{s!}{k_s^{*!}}, \quad (14)$$

then $g_{s,m}(n) \leq h_{s,m}(n)$ for $m \geq k_s^*$. On the other hand, when m is small, we cannot infer from Lemma 7 that $g_{s,m}(n) \leq h_{s,m}(n)$. However by pairing the terms appropriately, in the end it is possible to obtain that the terms coming from $h_s(n)$ dominate the ones from $g_s(n)$. First, we will show the following result, whose proof is in the appendix.

Lemma 8. *Let $w = \lceil s/2 \rceil$ and k_s^* be defined as in (14). Then we have that*

$$g_{s,k}(n) + g_{s,k+w}(n) \leq h_{s,k+w}(n) \text{ for } 0 \leq k < k_s^*. \quad (15)$$

Next, from Lemma 8, since $g_{s,k}(n) \leq h_{s,k}(n)$ (and $g_{s,w+k}(n) \leq h_{s,w+k}(n)$) for $k \geq k_s^*$, and since all terms $g_{s,k}(n)$ and $h_{s,k}(n)$ are non-negative, we get as required

$$\begin{aligned} g_s(n) &= \sum_{k=0}^s g_{s,k}(n) = \sum_{k=0}^{k_s^*-1} (g_{s,k}(n) + g_{s,w+k}(n)) + \sum_{k=k_s^*}^{w-1} g_{s,k}(n) + \sum_{k=w+k_s^*}^s g_{s,k}(n) \\ &\leq \sum_{k=0}^{k_s^*-1} h_{s,w+k}(n) + \sum_{k=k_s^*}^{w-1} h_{s,k}(n) + \sum_{k=w+k_s^*}^s h_{s,k}(n) \leq \sum_{k=0}^s h_{s,k}(n) = h_s(n). \end{aligned}$$

Hence, Proposition 2 is proved. \square

4. Improving bounds for (t, \mathbf{e}, s) -sequences

4.1. Overview on the current state of results on (t, \mathbf{e}, s) -sequences

The original result of Tezuka [17, Theorem 2] was recalled in Theorem 1, and the one based on our variant [10, Theorem 2] in Theorem 3. The main difference between these two results is in the leading term with a smaller asymptotic constant c_s for even bases in [10], whose online version was published in March 2014. Several months later, in 2014 Tezuka published a new paper [18] where he obtained the same constant c_s for even bases as the one we obtained in [10], using an approach that we proposed for (t, s) -sequences in an even base in [9, Section 4] (see [18, Theorem 2]). These various bounds are stated and discussed in Section 4.3 and Section 6.

4.2. On the range of validity of bounds for (t, \mathbf{e}, s) -sequences

The other difference between [10, Theorem 2] and [17, Theorem 2] is in the range of N : indeed, the bound (FLtes14) is interesting only if $N > b^t$ since trivially $D^*(N, X) \leq N$ for any N whereas this bound is always larger than b^t . But in QMC methods where, until now, the only (t, \mathbf{e}, s) -sequences used are generalized Niederreiter sequences, i. e., $(0, \mathbf{e}, s)$ -sequences, the difference on the range of N disappears. In the end, as to the non-asymptotic regime, the bound (Tez13) seems better without the quantity $\sum_{i=1}^s e_i$ appearing in the products, in spite of a smaller c_s in (FLtes14) for even b . This is the case in our numerical experiments (Section 6), which confirm that an improvement of the leading constant c_s is often obtained at the expense of complementary terms (as already noticed in [11, Section 5], especially with the bound from [6] which gives the currently best c_s for (t, s) -sequences).

The difference is even more striking when considering the new bound from [18], which has the same improved value for c_s as (FLtes14), but at the expense of an extra complementary term that appears to grow quickly with the dimension, leading to a larger bound than both (FLtes14) and (Tez13).

In any case, the discussion vis-a-vis the significance about the range of N in both theorems is pointless since our proof of [10, Theorem 2] also works with the hypothesis $N > b^t$ and gives $(\log N / \log b - t)$ in place of $(\log N / \log b)$ in our bound (FLtes14). Indeed, this is achieved by defining Σ_1 to be over the vectors \mathbf{j} such that $e_1 j_1 + \dots + e_s j_s \leq n - t$ (as done in [17]) rather than using $e_1 j_1 + \dots + e_s j_s \leq n$, as done in (10). While this means there are now more vectors in Σ_2 , this split still allows Lemma 1 to be applied in the same way in the argument used to bound the sums over each

B_k (see Remark 1 in the appendix), and thus the same bound is obtained at the end. Furthermore, the new bound for Σ_2 given in Proposition 1 leads to the following slight effective improvement of [17, Theorem 2].

Theorem 6. *For any (t, \mathbf{e}, s) -sequence X in any base b and any $N > b^t$ we have (newTez13)*

$$D^*(N, X) \leq \frac{b^t}{s!} \prod_{i=1}^s \left(\frac{\lfloor b^{e_i}/2 \rfloor}{e_i} \left(\frac{\log N}{\log b} - t \right) + s \right) + b^t \sum_{k=0}^{s-1} \frac{\lfloor \frac{b^{e_{k+1}}}{2} + 1 \rfloor}{k!} \prod_{i=1}^k \left(\frac{\lfloor b^{e_i}/2 \rfloor}{e_i} \left(\frac{\log N}{\log b} - t \right) + k \right).$$

Similarly, we can improve [10, Theorem 2], where we use the “ $N > b^t$ ” version discussed in the preceding paragraph, and focus on the case where b is even (the only case susceptible of interest for this result):

Theorem 7. *For any (t, \mathbf{e}, s) -sequence X in an even base b and any $N > b^t$ we have (newFLtes-even)*

$$D^*(N, X) \leq \frac{b^t}{s!} \prod_{i=1}^s \left(\frac{b^{e_i} - 1}{2e_i} \left(\frac{\log N}{\log b} - t + \sum_{i=1}^s e_i \right) + s \right) + b^t \sum_{k=0}^{s-1} \frac{\lfloor \frac{b^{e_{k+1}}}{2} + 1 \rfloor}{k!} \prod_{i=1}^k \left(\frac{b^{e_i} - 1}{2e_i} \left(\frac{\log N}{\log b} - t + \sum_{i=1}^k e_i \right) + k \right).$$

4.3. Discussion of the result [18, Theorem 2]

Now, recall [18, Theorem 2]: *For any (t, \mathbf{e}, s) -sequence X in any base b and any $N > b^t$ we have (Tez14)*

$$D^*(N, X) \leq \frac{b^t}{s!} \prod_{i=1}^s \left(\frac{b^{e_i} - 1}{2e_i} \left(\frac{\log N}{\log b} - t \right) + s \right) + \frac{b^{t+e_s} \sum_{i=1}^s e_i}{2} \prod_{i=1}^{s-1} \left(\frac{\lfloor b^{e_i}/2 \rfloor}{e_i} \left(\frac{\log N}{\log b} - t \right) + \lfloor b^{e_i}/2 \rfloor \right) + \sum_{k=0}^{s-1} \frac{b^{t+e_{k+1}}}{k!} \prod_{i=1}^k \left(\frac{\lfloor b^{e_i}/2 \rfloor}{e_i} \left(\frac{\log N}{\log b} - t \right) + k \right).$$

For an odd base, this bound has no improvement on [17, Theorem 2]. In the case of an even base, it provides another proof for the leading term and the asymptotic constant c_s we already obtained in [10, Theorem 2] and in Theorem 7. Hence, it is of interest to compare in the non asymptotic regime these two methods leading to the same c_s . However, in order to get a fair comparison, we will compare the bounds of Theorem 6 (b odd) and Theorem 7 with the following slight improvement of [18, Theorem 2] using our Proposition 1:

Theorem 8. *For any (t, \mathbf{e}, s) -sequence X in any base b we have (newTez14)*

$$D^*(N, X) \leq \frac{b^t}{s!} \prod_{i=1}^s \left(\frac{b^{e_i} - 1}{2e_i} \left(\frac{\log N}{\log b} - t \right) + s \right) + \frac{b^{t+e_s} \sum_{i=1}^s e_i \prod_{i=1}^{s-1} \left(\frac{\lfloor b^{e_i}/2 \rfloor}{e_i} \left(\frac{\log N}{\log b} - t \right) + \lfloor b^{e_i}/2 \rfloor \right) + b^t \sum_{k=0}^{s-1} \frac{\lfloor \frac{b^{e_{k+1}}}{2} + 1 \rfloor}{k!} \prod_{i=1}^k \left(\frac{\lfloor b^{e_i}/2 \rfloor}{e_i} \left(\frac{\log N}{\log b} - t \right) + k \right)}{2}$$

Because Theorems 7 and 8 are mainly interesting in number theory, for their improvement of the leading term with the constant c_s , it might seem useless to improve a part of the complementary terms, all the more since the methods imply further restrictions for the range of N . But, as already observed, bounds in the finite range are mainly useful in applied mathematics (QMC Methods); and there, all (t, \mathbf{e}, s) -sequences of interest (until now) belong to the sub-family of generalized Niederreiter sequences for which $t = 0$. Hence, the range for N is the interval $[1, \infty)$ and it makes sense to use the bounds (newFLtes-even) and (newTez14) in numerical experiments for comparisons with other bounds.

5. Improving bounds for Halton sequences

In Theorem 1 we recalled the bound established in [1] for Halton sequences. The term u in that bound arises from Atanassov's trick to get the desired bound on Σ_1 , as mentioned in Section 2: see [19, page 15] for complete details. However, an alternative approach is to use a bound similar to (10), using the analogy between the bases b_i and the powers b^{e_i} stated earlier. This leads to the following lemma.

Lemma 9. *Let $N \geq 1$, $k \geq 1$ and b_1, \dots, b_k be pairwise coprime integers with b_r even for some r . Then*

$$\sum_{\mathbf{j}; b_1^{j_1} \dots b_k^{j_k} \leq N} \prod_{i=1}^k c_{j_i}^{(i)} \leq \frac{1}{k!} \prod_{i=1, i \neq r}^k \left(\frac{f_i \log(b_r N)}{\log b_i} + k \right) \left(\frac{(f_r + f'_r) \log(b_r N)}{2 \log b_r} + k \right), \quad (16)$$

in which the numbers $c_{j_i}^{(i)}$ satisfy $c_0^{(i)} \leq 1$, $c_{j_i}^{(i)} \leq f_i$ for $i \neq r$, $c_{2h+1}^{(r)} \leq f_r$, and $c_{2h}^{(r)} \leq f'_r$.

Proof. For $u \subseteq \{1, \dots, k\}$, let $S_u = \{\mathbf{j} = (j_1, \dots, j_k) \in S; j_i > 0 \Leftrightarrow i \in u\}$ and let $e_i = \log b_i$. We split the sum over the vectors in S according to the cases: (1) $r \in u, \mathbf{j} \in S_u, j_r$ even; (2) $r \in u, \mathbf{j} \in S_u, j_r$ odd, and (3) $r \notin u, \mathbf{j} \in S_u$. In order to bound these sums, we need to count how many vectors \mathbf{j} there are in each of the three inner sums. We get $\frac{1}{2^{|u|}} \prod_{i \in u} \log N / e_i$ for the first one, $\frac{1}{2^{|u|}} \prod_{i \in u} (\log N + e_r) / e_i$ for the second, and $\frac{1}{|u|!} \prod_{i \in u} \log N / e_i$ for the third. Hence we can bound the LHS of (16) by

$$\begin{aligned} & \sum_{u: r \in u} \frac{1}{2^{|u|}} \left(\prod_{i \in u} \frac{\log N}{e_i} \right) f'_r \prod_{i \in u, i \neq r} f_i + \sum_{u: r \in u} \frac{1}{2^{|u|}} \left(\prod_{i \in u} \frac{\log N + e_r}{e_i} \right) f_r \prod_{i \in u, i \neq r} f_i \\ & + \sum_{u: r \notin u} \frac{1}{|u|!} \left(\prod_{i \in u} \frac{\log N}{e_i} \right) \prod_{i \in u} f_i \\ & \leq \sum_{u: r \in u} \frac{1}{|u|!} \prod_{i \in u} \frac{\log N + e_r}{e_i} \left(\prod_{i \in u, i \neq r} f_i \right) \left(\frac{f_r + f'_r}{2} \right) + \sum_{u: r \notin u} \frac{1}{|u|!} \prod_{i \in u} \frac{\log N}{e_i} \prod_{i \in u} f_i, \end{aligned}$$

where u runs over all subsets of $\{1, \dots, k\}$. Next, using the notation $\tilde{f}_i = f_i$ if $i \neq r$ and $\tilde{f}_r = (f_r + f'_r)/2$, and the inequality $1/|u|! \leq k^{k-|u|}/k!$, we bound the above by

$$\sum_u \frac{k^{k-|u|}}{k!} \prod_{i \in u} \frac{\tilde{f}_i}{e_i} \log(b_r N) \leq \frac{1}{k!} \prod_{i=1, i \neq r}^k \left(\frac{(\log b_r N) f_i}{e_i} + k \right) \left(\frac{(f_r + f'_r) (\log b_r N)}{2 e_r} + k \right).$$

□

The following new bound for Halton sequences is obtained by applying Lemma 9 with $f_i = (b_i - 1)/2$, $f_r = b_r/2$ and $f'_r = (b_r - 2)/2$, and by using our improved bound for Σ_2 , presented in Proposition 1.

Theorem 9. For any Halton sequence X in bases b_i , where b_r is even for some r , and any $N \geq 1$ with $n_r = \log(b_r N)$, we have (newFLHa)

$$D^*(N, X) \leq \frac{1}{s!} \prod_{i=1}^s \left(\frac{(b_i - 1)n_r}{2 \log b_i} + s \right) + \sum_{k=0}^{s-1} \frac{\lfloor \frac{b_{k+1}}{2} + 1 \rfloor}{k!} \prod_{i=1}^k \left(\frac{(b_i - 1)n_r}{2 \log b_i} + k \right).$$

6. Numerical comparisons

We now wish to compare some of the bounds discussed in this paper for given values of N and s , and for some specific LDS. Rather than comparing $D^*(N, X)$ or $D^*(N, X)/N$ directly as we did in [11], we follow an approach proposed by P. Kritzer [14] and motivated by a question by H. Woźniakowski: we instead consider the quantity

$$\sigma_{s,p}^* = \sup_{N \geq p} \frac{D^*(N, X)}{(\log N)^s}.$$

The definition of $\sigma_{s,p}^*$ is motivated by the fact that the Koksma-Hlawka bound [15] on the integration error obtained by using the first $N \geq p$ points of the sequence can be written as $\sigma_{s,p}^* ((\log N)^s / N) \|f\|_1$, where $\|f\|_1$ is the variation of f in the sense of Hardy and Krause. As done by Kritzer, we then plot $\sigma_{s,p}^*$ on graphs for which p ranges between 1000 and 10,000 in Figures 1, 2, and 3, and between 10,000 and 100,000 in Figure 4. We chose this approach over the one in [11] because the bounds are more easily (and more compactly) compared via graphs than tables of numbers, and the quantity $\sigma_{s,p}^*$ has the advantage of providing a nice connection with the use of LDS for QMC methods. We also note that here as in [11], we show values of $\sigma_{s,p}^*$ even when they correspond to discrepancy values worse than the trivial bound of N , as this still allows us to compare the behaviour of the different bounds and infer how they may eventually reach values of N where they become non-trivial.

For (t, s) -sequences, for a given s and base b , we consider the sequence with the smallest known value of t (obtained via MinT), and then compare bounds from Thm 1 (FL12-gen), Thm 2 (FL14-odd), Thm 3 (FL12-even), Thm 4 (FL14-even), FK from [6] with our new bounds from Thm 5 (newFL-odd) and Thm 6 (newFL-even). We note that although the bound FK from [6] gives the best constant c_s for (t, s) -sequences, the bound itself is typically larger than the newer FL14 and newFL. Due to space constraints, we show graphs only for a few pairs (b, s) , but they are fairly representative of the results we obtained overall.

In Figures 1 and 2, first we see that for $(b = 2, s = 5)$, the bound FL14-even is the smallest, followed closely by our new bound newFL-even, and that when we increase to $s = 10$, newFL-even and FL14-even are by far much better than the other bounds (some of them are not shown because they are too large). On the other hand, we show that for the base $(b = 4, s = 4)$, the best bound is newFL-even, while FL14-even is better than FL12-gen only for smaller values of N . Finally, with a larger base $b = 11$ and in dimension $s = 10$, our new bound newFL-odd and FL12-gen outperform the others (not shown on the graph), with the new one being clearly the smallest one.

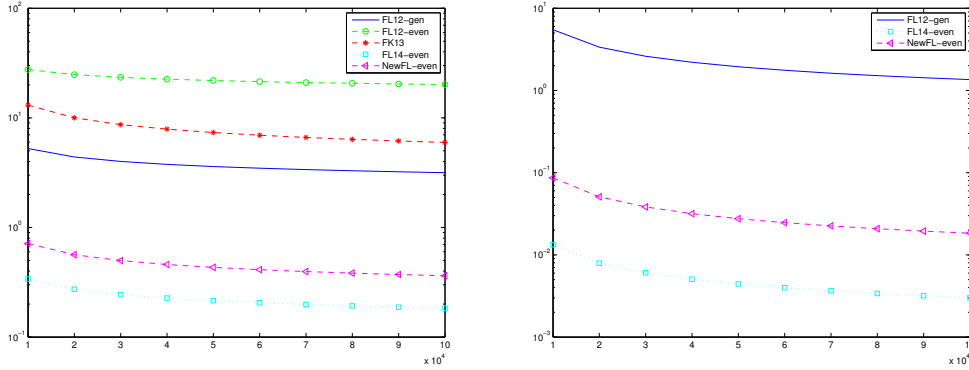


Figure 1: (t, s) -sequences: $b = 2, s = 5$ (left), $b = 2, s = 10$ (right)

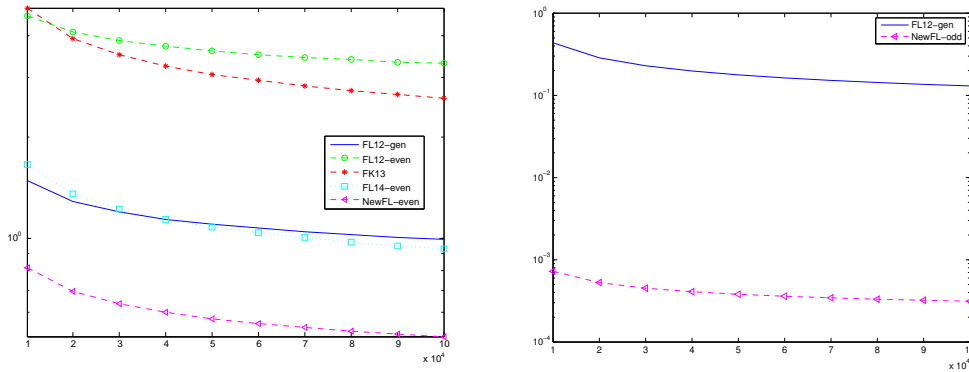


Figure 2: (t, s) -sequences: $b = 4, s = 4$ (left), $b = 11, s = 10$ (right)

Next for (t, e, s) -sequences, in base $b = 2$ and for generalized Niederreiter sequences, where $t = 0$, our new bound specialized to the case b even (newFLtes-even) provides some improvement over newTez13 – which is the

same as the bound from [17], except for the slight improvement to handle Σ_2 – for small dimensions, e.g., when $s = 4$, as seen on top of Figure 3.

Both bounds are much better than the one from [18], even if we used the version newTez14 from Theorem 8 that incorporates the slight improvement from Proposition 1. However, newFLtes-even is clearly outperformed by newTez13 in larger dimensions. In such cases, what is more interesting is to compare the bound Tez13 with newTez13, which are the same except that newTez13 handles the Σ_2 term using a tighter bound. Here as well the bound from [18] is the largest. Comparisons between these four bounds are provided in the lower left part of Figure 3, for $b = 2$ and $s = 10$. For the case $b = 3$ and $s = 20$, we only show the bound Tez13 of [17] and newTez13, i.e., the effect of Proposition 1, as the one from [18] is dramatically large and off scale.

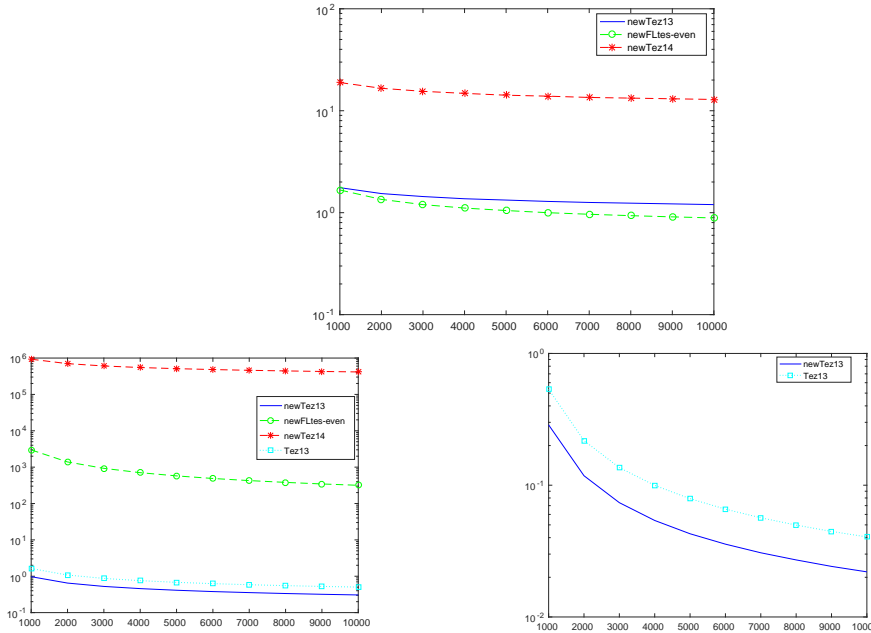


Figure 3: (t, e, s) -sequences: $b = 2, s = 4$ (top), $b = 2, s = 10$ (bottom left), $b = 3, s = 20$ (bottom right)

As for the Halton sequences, we compare five different bounds: in addition to AtHa04 and our new bound newFLHa, we also consider AtHaBk (AtHa04 with improved term Σ_2 as proposed here), a “brute” method where in (1) we replace the term $(b_i - 1)/2$ by $\lfloor b_i/2 \rfloor$ and thus do not need the u term; brutBk is the same as this brute method but where the bound on Σ_2 is improved

as proposed in our new bound. The results shown on Figure 4 suggest that our new bound newFLHa outperforms AtHa04 from [1] in lower dimensions, but eventually, as s increases, the latter becomes smaller. Typically, we see that AtHaBk gives the lowest bound, followed very closely by BrutBk when $s = 50$.

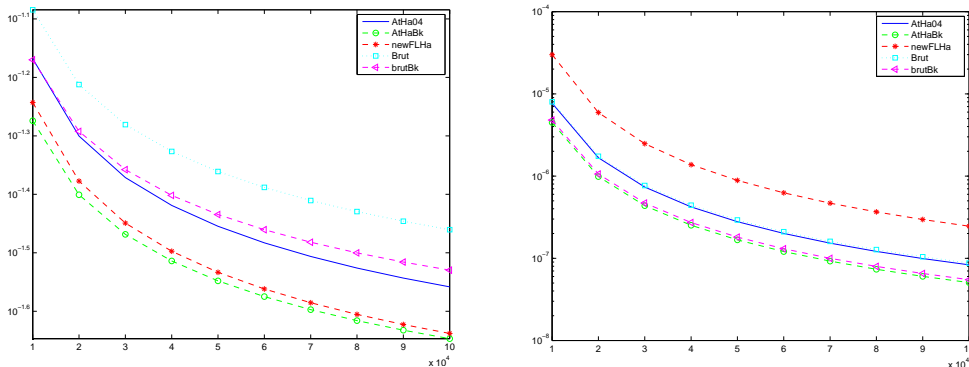


Figure 4: Halton sequences: $s = 10$ (left), $s = 50$ (right)

Acknowledgements

We thank the two anonymous reviewers for their helpful comments. In particular, we thank the anonymous reviewer who mentioned the publication [18] to us, as we were not aware of its existence at the time the present paper was originally submitted. The second author was supported by NSERC grant RGP238959.

Appendix

Proof of the bound (7) for Σ_2 . The way we obtain (7) is similar to what is done in the proof of Theorems 1 and 2 in [10]. First, we split the sum over $\{\mathbf{j}; b_1^{j_1} \dots b_s^{j_s} > N\}$ into subsets B_0, \dots, B_{s-1} where $B_0 = \{\mathbf{j}; b_1^{j_1} > N\}$ and $B_k = \{\mathbf{j}; b_1^{j_1} \dots b_k^{j_k} \leq N, b_1^{j_1} \dots b_{k+1}^{j_{k+1}} > N\}$ for $k = 1, \dots, s-1$. We note that $B_0 \neq \emptyset$ since we must have $j_1 = n_1 + 1$. In order to evaluate its contribution to Σ_2 , we proceed as follows. Let $r \geq 1$ be the largest integer such that $b_1^{r-1} \leq N$, so that $r = n_1 + 1$. Hence, $\mathbf{j} \in B_0$ if and only if $j_1 = r, j_2, \dots, j_s$ being arbitrary in $[0, n_i + 1]$. Recall that $J = \prod_{i=1}^s [0, z^{(i)}]$, and set

$$J' = [0, z_r^{(1)}] \times \prod_{i=2}^s [0, z^{(i)}] \text{ and } K = [\min(z_r^{(1)}, z^{(1)}), \max(z_r^{(1)}, z^{(1)})] \times \prod_{i=2}^s [0, z^{(i)}].$$

If $z^{(1)} > z_r^{(1)}$, then we have $J = J' \cup K$, and otherwise we have $J' = J \cup K$ (disjoint unions), so that

$$\operatorname{sgn}(z^{(1)} - z_r^{(1)})E(K; [\mathcal{P}_N(X)]) = E(J; [\mathcal{P}_N(X)]) - E(J'; [\mathcal{P}_N(X)]).$$

Therefore, we have $\pm E(K; [\mathcal{P}_N(X)]) = \sum_{\mathbf{j} \in B_0} \epsilon(\mathbf{j})E(I(\mathbf{j}); [\mathcal{P}_N(X)])$ and so, $E(K; [\mathcal{P}_N(X)])$ is the contribution of B_0 to Σ_2 . Now since $b_1^{r-1}z_r^{(1)} \in \mathbb{Z}$ and

$$|z^{(1)} - z_r^{(1)}| = \left| \sum_{j=r}^{\infty} a_j^{(k+1)} b_1^{-j} \right| \leq \left\lfloor \frac{b_1}{2} \right\rfloor \frac{1}{b_1^r} \frac{b_1}{b_1 - 1} \leq \frac{1}{b_1^{r-1}}, \quad (17)$$

we get $[\min(z_r^{(1)}, z^{(1)}), \max(z_r^{(1)}, z^{(1)})] \subseteq [m_1 b_1^{-r}, m_2 b_1^{-r}]$ for some non-negative integers m_1, m_2 satisfying $0 \leq m_2 - m_1 \leq b_1$. Hence, $K \subset [m_1 b_1^{-r}, m_2 b_1^{-r}] \times [0, 1)^{s-2}$ and so, using Lemma 1 (observe that $N < b_1^r \leq b^t b_1^r$) we have $A(K; [\mathcal{P}_N(X)]) \leq b^t(m_2 - m_1) \leq b^t b_1$. But we also have $NV(K) \leq b^t b_1^r(m_2 - m_1) b_1^{-r} \leq b^t b_1$ which in the end gives the bound $|E(K; [\mathcal{P}_N(X)])| \leq b^t b_1$ for the contribution of B_0 .

We can then deal with the sets B_k for $1 \leq k \leq s-1$ in a similar fashion to what we did for B_0 (see [19] (and [9, p. 72] for the special case of (t, s) -sequences) for complete details), so that we get

$$|\Sigma_2| \leq b^t \sum_{k=0}^{s-1} b_{k+1} \sum_{\{(j_1, \dots, j_k); b_1^{j_1} \dots b_k^{j_k} \leq N\}} \prod_{i=1}^k |a_{j_i}^{(i)}|. \quad (18)$$

Finally, we bound the $a_{j_i}^{(i)}$'s using Lemma 3. Hence, we get the bound

$$|\Sigma_2| \leq b^t \sum_{k=0}^{s-1} \frac{b_{k+1}}{k!} \prod_{l=1}^k \left(\left\lfloor \frac{b_l}{2} \right\rfloor \frac{\log N}{\log b_l} + k \right). \quad (19)$$

□

Remark 1. Note that the argument used to handle B_0 above can easily be adapted to the alternative split of Σ_1 and Σ_2 based on $b_1^{j_1} \dots b_s^{j_s} \leq \log_b N - t$, because in that case, when we first use Lemma 1 we would have $N/b^t < b_1^r$, which still leads to $N < b^t b_1^r$ and thus the rest of the argument follows.

Proof of Proposition 1. To get the improved bound in Proposition 1, we go back to the step where we bound, for each set $B_k, 0 \leq k < s$, the b_{k+1} -adic expansion of the real number $z^{(k+1)}$ starting from the r th digit, i.e., $z^{(k+1)} - z_r^{(k+1)} = \sum_{j=r}^{\infty} a_j^{(k+1)} b_{k+1}^{-j}$. In the above proof (see (17) for the case $k = 0$), this term is bounded by b_{k+1}^{-r+1} .

- When b_{k+1} is odd, it is easy to show that a bound of $b_{k+1}^{-r+1}/2$ can instead be obtained. The rest of the proof shows that the constant that must then appear in the bound for Σ_2 restricted to B_k – which, in the different bounds for $D^*(N, X)$ that we have given in Theorem 1, appears inside the sum over k from 0 to $s - 1$ in the second term – is the smallest integer larger than b_{k+1}^r times this bound. Hence for an odd base, we get that this constant is $(b_{k+1} + 1)/2$ instead of b_{k+1} for each B_k .

- When b_{k+1} is even, we must split the expansion over odd and even indices:

$$|z^{(k+1)} - z_r^{(k+1)}| \leq \sum_{j=r}^{\infty} |a_j^{(k+1)}| b_{k+1}^{-j} \leq b_{k+1}^{-r} \left(\sum_{j=0}^{\infty} |a_{r+2j}^{(k+1)}| b_{k+1}^{-2j} + \sum_{j=0}^{\infty} |a_{r+2j+1}^{(1)}| b_{k+1}^{-2j-1} \right),$$

and then consider the case r even and odd independently, using the worst configuration as in the proofs of Theorems 1 and 2 in [10]. Simple calculations respectively yield

$$|z^{(k+1)} - z_r^{(k+1)}| \leq \frac{1}{b_{k+1}^{r-1}} \frac{b_{k+1} + 2}{2(b_{k+1} + 1)} \text{ and } |z^{(k+1)} - z_r^{(k+1)}| \leq \frac{1}{b_{k+1}^{r-1}} \frac{b_{k+1}}{2(b_{k+1} + 1)}.$$

Hence for an even base, the constant b_{k+1} in the bound for each B_k can be replaced by $(b_{k+1} + 2)/2$ (the largest of these two bounds), so that overall we obtain a single upper bound for odd and even bases:

$$|\Sigma_2| \leq b^t \sum_{k=0}^{s-1} \left\lfloor \frac{b_{k+1}}{2} + 1 \right\rfloor \sum_{\{\mathbf{j}; b_1^{j_1} \dots b_k^{j_k} \leq N\}} \prod_{i=1}^k |a_{j_i}^{(i)}|.$$

At this point, we mention that, for an even base b , summing over odd and even digits leads to $b^{-r+1} \sum_{j=0}^{\infty} \left(\frac{b}{2b^j} + \frac{b-2}{2b^{j+1}} \right) = b^{-r+1} \frac{b^2+b-2}{2(b^2-1)} = b^{-r+1} \frac{b+2}{2(b+1)}$, a formula invoqued by Atanassov to justify the existence of signed numeration systems in even bases [1, p. 21-22], but not to bound more closely Σ_2 as we did above. \square

Proof of Lemma 7. We note that $\mu(n, s, 0) = 1$ and proceed by induction on $s \geq 2$, with the exact statement used for induction being

$$\mu(n, s, m) \leq \frac{\Gamma(\frac{n+m}{2} + 1)}{\Gamma(\frac{n-m}{2} + 1)} \quad \text{for all } 1 \leq m \leq s \text{ and } n \geq s. \quad (20)$$

To start the recursion, we need to show that $\mu(n, 2, m) \leq \Gamma(\frac{n+m}{2} + 1)/\Gamma(\frac{n-m}{2} + 1)$ for $m = 1, 2$ and $n \geq 2$. Indeed, we have

$$\mu(n, 2, 1) = \frac{1}{2} \left(\frac{n+2}{2} + \frac{n}{2} \right) = \frac{\Gamma(\frac{n+1}{2} + 1)}{\Gamma(\frac{n-1}{2} + 1)}, \quad \mu(n, 2, 2) = \binom{n+2}{2} \frac{n}{2} = \frac{\Gamma(\frac{n+2}{2} + 1)}{\Gamma(\frac{n-2}{2} + 1)}.$$

We also note that for any $s \geq 2$, the cases $m = s$ and $m = 1$ are easily seen to be true since both the LHS and RHS of (20) are given by

$$\frac{\Gamma(\frac{n+s}{2} + 1)}{\Gamma(\frac{n-s}{2} + 1)} \quad \text{and} \quad \frac{1}{s} \sum_{j=0}^{s-1} \binom{n+s}{2} - j = \frac{n+s}{2} - \frac{s-1}{2} = \frac{n+1}{2}.$$

Proceeding to the induction step, we now assume that (20) holds for $s-1 \geq 2$ and we want to show it also holds for s and $1 < m < s$. To do so, we split the sum over \mathcal{I} in the definition (13) of $\mu(n, s, m)$ into two sums based on the decomposition

$$\mathcal{B}(n, s) = \frac{n+s}{2} \cup \mathcal{B}(n-1, s-1).$$

The first sum is over the subsets \mathcal{I} included in $\mathcal{B}(n-1, s-1)$ (which contains the $s-1$ numbers $(n+s)/2 - 1, \dots, (n-s)/2 + 1$) and the second over the subsets that include $(n+s)/2$ and $m-1$ other elements from $\mathcal{B}(n-1, s-1)$. Applying the induction hypothesis on both sums and using the fact that $\binom{s-1}{m}/\binom{s}{m} = (s-m)/m$ and $\binom{s-1}{m-1}/\binom{s}{m} = \frac{m}{s}$, we get

$$\begin{aligned} \mu(n, s, m) &= \frac{s-m}{s} \mu(n-1, s-1, m) + \frac{m}{s} \frac{n+s}{2} \mu(n-1, s-1, m-1) \\ &\leq \frac{s-m}{s} \frac{\Gamma(\frac{n-1+m}{2} + 1)}{\Gamma(\frac{n-1-m}{2} + 1)} + \frac{m}{s} \binom{n+s}{2} \frac{\Gamma(\frac{n-1+m-1}{2} + 1)}{\Gamma(\frac{n-1-(m-1)}{2} + 1)}. \end{aligned}$$

Hence to show that this is bounded from above by $\Gamma(\frac{n+m}{2} + 1)/\Gamma(\frac{n-m}{2} + 1)$, we need to show that

$$\left(\frac{s-m}{s} \right) \frac{\Gamma(\frac{n-1+m}{2} + 1)}{\Gamma(\frac{n-1-m}{2} + 1)} \left(\frac{\Gamma(\frac{n+m}{2} + 1)}{\Gamma(\frac{n-m}{2} + 1)} \right)^{-1} \leq 1 - \frac{m}{s} \binom{n+s}{2} \frac{2}{n+m} = \frac{n(s-m)}{s(n+m)},$$

which is equivalent to prove by induction on $m \geq 1$ that

$$G(n, m) := \frac{n-1+m}{n} \frac{\Gamma(\frac{n-1+m}{2})}{\Gamma(\frac{n-1-m}{2} + 1)} \left(\frac{\Gamma(\frac{n+m}{2})}{\Gamma(\frac{n-m}{2} + 1)} \right)^{-1} \leq 1.$$

First, as easily seen, $G(n, 1) = 1$ and $G(n, 2) \leq 1$. Then, it's not difficult to show that $G(n, m) = G(n, m-2)((n^2 - (m-1)^2)/((n^2 - (m-2)^2))$ which in turn is bounded by 1 since $1 < m < s \leq n$. \square

Proof of Lemma 8. We prove this lemma by successive reductions of the inequality $g_{s,k}(n) + g_{s,k+w}(n) \leq h_{s,k+w}(n)$ for $0 \leq k < k_s^*$ (Equation (15)), where $w = \lceil s/2 \rceil$. For future use, observe (by elementary case analysis) that $(s-1)/2 < w \leq (s+1)/2$.

First, multiplying both sides by $s!$ and using Lemma 7, it is sufficient to prove

$$\binom{s}{k} \frac{\Gamma(\frac{n+k}{2})}{\Gamma(\frac{n-k}{2})} \left[\left(\frac{s}{2} \right)^{s-k} \right] \leq \frac{\Gamma(\frac{n+k+w}{2} + 1)}{\Gamma(\frac{n-(k+w)}{2} + 1)} \binom{s}{k+w} \left[\frac{s!}{(k+w)!} - \left(\frac{s}{2} \right)^{s-(k+w)} \right]. \quad (21)$$

This is a first reduction. The next ones are detailed in the following Claims 1, 3, 4 (Claim 2 being required for Claims 3, 4).

Claim 1: The case where $k = 0$. Noting that $\mu(n, s, 0) = 1$ and that the RHS of (21) (in which $k = 0$) increases with $n \geq s$, it is clear that (21) reduces to

$$\left(\frac{s}{2} \right)^s \leq \frac{\Gamma(\frac{s+w}{2} + 1)}{\Gamma(\frac{s-w}{2} + 1)} \binom{s}{w} \left(\frac{s!}{w!} - \left(\frac{s}{2} \right)^{s-w} \right). \quad (22)$$

Now, simple computations on the RHS of (22) show that

$$\left(\frac{s!}{w!} - \left(\frac{s}{2} \right)^{s-w} \right) \geq \left(\frac{s}{2} \right)^{s-w}, \quad \frac{\Gamma(\frac{s+w}{2} + 1)}{\Gamma(\frac{s-w}{2} + 1)} \geq w! \quad \text{and} \quad \binom{s}{w} \geq \frac{1}{w!} \left(\frac{s}{2} \right)^w$$

(hints: for the first bound compute $\frac{s!}{w!} \left(\frac{s}{2} \right)^{s-w}$ and note that $2 \left(1 + \frac{2}{s} \right)^{s-w-1} \geq 2$ since $s \geq 2$; for the second bound, simplify and use $(s+w)/2 \geq w$; for the third bound, use $s-w+1 \geq s/2$). Thus, (21) is true for $k = 0$ and hence Lemma 8 reduces to (21) with $1 \leq k < k_s^*$, a second reduction.

Claim 2: An upper bound for k_s^* . For all $s \geq 2$, we have $k_s^* \leq \max(2, \lfloor (s-1)/7 \rfloor)$.

We first note that $k_s^* \leq \lfloor s/2 \rfloor$ as easily seen from its definition given by (14). On the other hand, it is also easy to check the claim for all $s \geq 2$ up to several thousands of integers by comparing numerically $\prod_{j=0}^{s-k-1} s/(2(s-j))$ to 1. But the proof requires more attention and efforts since the bound is almost sharp as can be seen by investigation of numerical results. The first values are $k_s^* = 1$ for $2 \leq s \leq 13$ and $k_s^* = 2$ for $14 \leq s \leq 21$.

Let $s = 7l + j$ for $0 \leq j \leq 6$. We proceed by induction on l and we first check numerically that $k_s^* \leq \lfloor l + (j-1)/7 \rfloor =: l_j$ for small $l \geq 1$ and $1 \leq j \leq 6$, i. e., that

$$A := \left(\frac{7l+j}{2} \right)^{7l+j-l_j} \leq \frac{(7l+j)!}{l_j!}. \quad (23)$$

Then, we assume (23) holds for a given l and want to show that

$$\left(\frac{7(l+1)+j}{2} \right)^{7(l+1)+j-(l_j+1)} = A \frac{\left(\frac{7(l+1)+j}{2} \right)^{7(l+1)+j-(l_j+1)}}{\left(\frac{7l+j}{2} \right)^{7l+j-l_j}} \leq \frac{(7(l+1)+j)!}{(l_j+1)!} \quad (24)$$

Applying the induction hypothesis to A and simplifying the ratio, we see that to obtain (24) it is sufficient to show that

$$\frac{(7l+j)!}{l_j!} \left(1 + \frac{7}{7l+j} \right)^{7l+j-l_j} \left(\frac{7(l+1)+j}{2} \right)^6 \leq \frac{(7(l+1)+j)!}{(l_j+1)!}. \quad (25)$$

From this point, we separate the cases $j = 0$ where $l_0 = l - 1$ and $j \geq 1$ where $l_j = l$.

- For $j = 0$, (25) becomes

$$\frac{(7l)!}{(l-1)!} \left(1 + \frac{1}{l} \right)^{6l+1} \left(\frac{7(l+1)}{2} \right)^6 \leq \frac{(7(l+1))!}{l!}, \quad \text{i. e.,}$$

$$\left(1 + \frac{1}{l} \right)^{6l} \leq \left(\frac{2}{7(l+1)} \right)^6 7(7l+6) \dots (7l+1).$$

Now, we have $(1 + 1/l)^l \leq e$ and $7l + j \geq 7l$, so (25) will be true if l satisfies $e^6 \leq 7 \cdot 2^6 (l/(l+1))^6$, i. e., $(2^{\sqrt[6]{7}} - e)l \geq e$. With $e \leq 2.72$ and $2^{\sqrt[6]{7}} \geq 2.76$ we obtain $l \geq 2.72/0.04 = 68$.

- For $j \geq 1$, (25) becomes

$$\frac{(7l+j)!}{l!} \left(1 + \frac{7}{7l+j}\right)^{6l+j} \left(\frac{7(l+1)+j}{2}\right)^6 \leq \frac{(7(l+1)+j)!}{(l+1)!}, \text{ i. e. ,}$$

$$\left(1 + \frac{7}{7l+j}\right)^{6l+j} \leq \left(\frac{2}{7l+j+7}\right)^6 \frac{(7l+j+7)\dots(7l+j+1)}{l+1}.$$

But, $7l+j+7 = (7l+j)(1+7/(7l+j))$, thus (25) will be true if l satisfies

$$\left(1 + \frac{7}{7l+j}\right)^{6l+j-1} \leq \left(\frac{2}{7l+j+7}\right)^6 \frac{(7l+j)(7l+j+6)\dots(7l+j+1)}{l+1}.$$

Now, it is easy to see that $7(6l+j-1) \leq 6(7l+j)$, so that

$$\left(1 + \frac{7}{7l+j}\right)^{6l+j-1} \leq \left(1 + \frac{6}{6l+j-1}\right)^{6l+j-1} \leq e^6.$$

Hence, (25) will be true if l satisfies $e \leq 2\sqrt[6]{\frac{7l+j}{l+1} \frac{7l+j+1}{7l+j+7}}$. In addition, since $(7l+j)/(l+1)$ increases up to 7 when $l \rightarrow \infty$, we can choose the same lower bound as for $j = 0$ with l such that $2\sqrt[6]{\frac{7l+j}{l+1}} \geq 2.76$ for all $1 \leq j \leq 6$, i. e., $l \geq 119$. Finally, (25) will be true if $l \geq 119$ satisfies

$$e \leq 2.76 \frac{7l+j+1}{7l+j+7} = 2.76 \left(1 - \frac{6}{7l+j+7}\right), \text{ i. e., } 0.04(7l+j+7) \geq 6 \cdot 2.76,$$

which requires only $l \geq 60$ (of course, it could be possible to optimize the least l satisfying both conditions).

Claim 3: A third reduction. Coming back to (21) with $1 \leq k < k_s^*$ and dealing with the last term of its RHS, in the same way as in the proof of (22) for the same term but with $k = 0$, we first obtain

$$\frac{s!}{(k+w)!} - \left(\frac{s}{2}\right)^{s-(k+w)} \geq \left(\frac{s}{2}\right)^{s-(k+w)}$$

since from Claim 2, we have $k+w < k_s^*+w \leq s$ and so $\left(1 + \frac{2k}{s}\right)^{s-(k+w)-1} \geq 1$.

Next, set $v = \lfloor \frac{w}{2} \rfloor$ and notice for future use that $(s-2)/4 \leq v \leq (s+1)/4$ (by simple case analysis). Since $w/2 - v \geq 0$, we obtain

$$\frac{\Gamma(\frac{n+k}{2} + 1)}{\Gamma(\frac{n-k}{2} + 1)} \leq \frac{\Gamma(\frac{n+w+k}{2} - v + 1)}{\Gamma(\frac{n+w-k}{2} - v + 1)}.$$

Thus the RHS of (21) times the ratio $\Gamma(\frac{n-k}{2})/\Gamma(\frac{n+k}{2})$ is bounded from below by

$$\binom{s}{k+w} \left(\frac{s}{2}\right)^{s-(k+w)} \times \frac{\Gamma(\frac{n+k+w}{2} + 1)}{\Gamma(\frac{n+w+k}{2} - v + 1)} \times \frac{\Gamma(\frac{n+w-k}{2} - v + 1)}{\Gamma(\frac{n-w-k}{2} + 1)}.$$

Hence a sufficient condition to obtain (21) is to establish the bound

$$\binom{s}{k} \left(\frac{s}{2}\right)^w \leq \binom{s}{k+w} \frac{\Gamma(\frac{n+k+w}{2} + 1)}{\Gamma(\frac{n+w+k}{2} - v + 1)} \times \frac{\Gamma(\frac{n+w-k}{2} - v + 1)}{\Gamma(\frac{n-w-k}{2} + 1)}. \quad (26)$$

Claim 4: A last reduction. First, we note that the product of ratios in the RHS of (26) is increasing in n , and thus it suffices to prove (26) with $n = s$. Then, we observe that the first ratio is the product of v terms larger than $n/2$, hence (26) reduces to

$$\left(\frac{s}{2}\right)^{w-v} \leq \binom{s}{k}^{-1} \binom{s}{k+w} \frac{\Gamma(\frac{s+w-k}{2} - v + 1)}{\Gamma(\frac{s-w-k}{2} + 1)}. \quad (27)$$

To achieve the proof of Lemma 8, we need the explicit forms of $R := \frac{\Gamma(\frac{s+w-k}{2} - v + 1)}{\Gamma(\frac{s-w-k}{2} + 1)}$ and $B := \binom{s}{k}^{-1} \binom{s}{k+w}$ in the RHS of (27):

$$R = \left(\frac{s+w-k}{2} - v\right) \left(\frac{s+w-k}{2} - v - 1\right) \cdots \left(\frac{s-(w+k)}{2} + 1\right) \text{ and}$$

$$B = \binom{s}{k}^{-1} \binom{s}{k+w} = \frac{(s-k)(s-k-1)\cdots(k+w+1)}{(s-(k+w))(s-(k+w)-1)\cdots(k+1)}, \text{ where}$$

we used the fact that $s-k \geq k+w$ since $2k \leq 2(k_s^* - 1) \leq 2(\lfloor s/7 \rfloor - 1) \leq s-w$.

There are two cases to consider, depending on which of R and B has the most terms ($w-v$ and $s-w-2k$, respectively).

• **Case 1:** $w-v \leq s-w-2k$. We see that the $w-v$ terms of R clearly dominate the $w-v$ largest terms of the denominator of B since $(s+w-k)/2 - v \geq s-k-w$, i. e., $3w+k-2v \geq s$, because $w \geq (s-1)/2$ (as already noted) and $k \geq 1$. The remaining $s-w-2k-(w-v)$ (smallest) terms of the denominator of B are clearly dominated by the $s-w-2k-(w-v)$ smallest terms of its numerator, and then the remaining $w-v$ (largest) terms

of the numerator of B are all at least $s/2$, so that overall, we indeed have $B \cdot R \geq (s/2)^{w-v}$.

• **Case 2:** $w - v > s - 2k - w$ (i. e., more terms in R than in B).

First, we note that $1 \leq k < k_s^*$ implies $k_s^* \geq 2$; so, as seen in Claim 2, $s \geq 14$. But $s = 14$ cannot occur in Case 2 since $w - v = 4 \leq s - 2k - w \leq 5$. Hence Claim 2 applies with $s \geq 15$ and $k_s^* \leq \lfloor (s-1)/7 \rfloor$.

Then, as argued in Case 1, the $s - 2k - w$ smallest terms in R dominate the terms in the denominator of B if $(s - w - k)/2 + 1 \geq k + 1$, i. e., $3k \leq s - w$. But, from Claim 2, $3k \leq 3((s-1)/7 - 1) = 3(s-8)/7 \leq (s-1)/2 \leq s - w$ (since $w \leq (s+1)/2$).

Next, we observe that all the terms in the numerator of B are at least $s/2$ since $k + w + 1 \geq s/2$. So it is sufficient to show that each of the $w - v - (s - 2k - w)$ largest terms of R can be paired in the reverse order with the largest terms from the numerator of B so that their product is at least $(s/2)^2$.

To this end, we first need to check that $l := w - v - (s - 2k - w) \leq s - 2k - w$, the number of terms in B . This is true if $2s - 3w + v - 4k \geq 2s - 3(s + 1)/2 + (s - 2)/4 - 4k \geq 0$, i. e., if $8k \leq (3s - 8)/2$, which is clearly satisfied because $k \leq ((s-1)/7 - 1)$.

Next, to verify that the above property holds, it is sufficient to check that it is satisfied for the first product, i.e.,

$$\left(\frac{s + w - k}{2} - v - (w - v - (s - 2k - w) - 1) \right) (s - k) \geq \frac{s^2}{4},$$

i. e., $((3s - 3w - 5k)/2 + 1)(s - k) \geq s^2/4$, because if $xy \geq z$ then $(x+1)(y-1) \geq z$ if $y \geq x+1$; and this last condition is verified with $x+1 = (3s - 3w - 5k)/2 + 2$ and $y = s - k$ because $w \geq (s-1)/2$ implies $(s-3)/4 + 3k/2 \geq 2$, true since $s \geq 15$.

Finally, using again that $w \leq (s+1)/2$ and $k \leq (s-1)/7 - 1$, we obtain after a simple computation $(3s - 3w - 5k + 2)(s - k) \geq (s(11/14) + 87/14)(6s + 8)/7 \geq s^2/2$, since $(11/14)(6/7) = 33/49 \geq 1/2$. Overall, we indeed have $B \cdot R \geq (s/2)^{w-v}$ in Case 2, just like for Case 1 and this ends the proof of Lemma 8. \square

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