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Generalized von Neumann–Kakutani transformation and random-start scrambled Halton sequences

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ABSTRACT

It is a well-known fact that the Halton sequence exhibits poor uniformity in high dimensions. Starting with Braaten and Weller in 1979, several researchers introduced permutations to scramble the digits of the van der Corput sequences that make up the Halton sequence, in order to improve the uniformity of the Halton sequence. These sequences are called scrambled Halton, or generalized Halton sequences. Another significant result on the Halton sequence was the fact that it could be represented as the orbit of the von Neumann–Kakutani transformation, as observed by Lambert in 1982. In this paper, I will show that a scrambled Halton sequence can be represented as the orbit of an appropriately generalized von Neumann–Kakutani transformation. A practical implication of this result is that it gives a new family of randomized quasi-Monte Carlo sequences: random-start scrambled Halton sequences. This work generalizes random-start Halton sequences of Wang and Hickernell. Numerical results show that random-start scrambled Halton sequences can improve on the sample variance of random-start Halton sequences by factors as high as 7000.

0. Introduction

The van der Corput sequence, and its generalization to higher dimensions, the Halton sequence, are among the best known low-discrepancy sequences. The nth term of the van der Corput sequence in base b, $\phi_b(n)$, is defined as follows: First, write n in its base b expansion:

$$n = (a_k \cdots a_1 a_0)_b = a_0 + a_1 b + \cdots + a_k b^k,$$

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then compute

$$\phi_b(n) = (.a_0a_1\cdots a_k)_b = \frac{a_0}{b} + \frac{a_1}{b^2} + \cdots + \frac{a_k}{b^{k+1}}. \tag{1}$$

The Halton sequence in the bases $b_1, \ldots, b_s$ is $(\phi_{b_1}(n), \ldots, \phi_{b_s}(n))_{n=0}^{\infty}$. This is a uniformly distributed mod 1 (u.d. mod 1) sequence if the bases are relatively prime. In practice, b_i is usually chosen as the ith prime number.

There is a well-known defect of the Halton sequence: in higher dimensions, certain components of the sequence exhibit very poor uniformity—this is sometimes stated as high correlation between components. This fact was observed by several authors, and as a remedy, *scrambled Halton sequences* were introduced [1–10]. The scrambled van der Corput sequence generalizes Eq. (1) as

$$\phi_b(n) = \frac{\sigma(a_0)}{b} + \frac{\sigma(a_1)}{b^2} + \cdots + \frac{\sigma(a_k)}{b^{k+1}}$$

where σ is a permutation on the digit set $\{0, \ldots, b-1\}$. By considering different permutations σ_{b_i} for the corresponding bases b_i, one can define the scrambled Halton sequence in the bases $b_1, \ldots, b_s$ in the usual way.

In this paper, we will consider a generalization of the above scrambling that allows the use of different permutations at each digit. This generalization was considered by Faure in [11]. We obtain the following definition for the nth term of the scrambled van der Corput sequence. The scrambled Halton sequence is defined similarly.

Definition 1. The scrambled van der Corput sequence in base b and permutations $\sigma_1, \sigma_2, \ldots$, is $(\phi_b(n))_{n=0}^{\infty}$, where

$$\phi_b(n) = \frac{\sigma_1(a_0)}{b} + \frac{\sigma_2(a_1)}{b^2} + \cdots + \frac{\sigma_k(a_{k-1})}{b^k} \tag{2}$$

and $n = (a_k \cdots a_1a_0)_b$.

There have been other methods introduced in the literature to reduce the correlation in the Halton sequence. For example, Hess and Polak [12] shuffle the one-dimensional van der Corput sequences that make up the Halton sequence, using independent random permutations. The "scrambled" strategy of Spanier [13] uses random permutations to scramble the order of the Halton sequences across different random walks so that a lower dimensional Halton sequence can be used in a high dimensional problem. Similar ideas appear in the "renumbering" and "continuation" methods used by Moskowitz [14], and numbering techniques used by Coulibaly and Lécot [15], and Morokoff and Caflisch [16].

1. The von Neumann–Kakutani transformation and a generalization

The van der Corput sequence can be obtained from the von Neumann–Kakutani transformation, as was first observed by Lambert [17,18]. The ergodic theory connection to van der Corput sequences was also explored in detail by Hellekalek [19]. Here we will give a brief description of the von Neumann–Kakutani transformation, and later discuss a modification of it in more detail. A thorough analysis of this transformation can be found in [20].

The von Neumann–Kakutani transformation is an ergodic and measure preserving transformation $T : [0, 1) \to (0, 1)$, and it is constructed inductively. At the nth stage of this construction, a mapping T_n with domain D_n is defined. D_n is a proper subset of $[0, 1)$, and the next stage constructs a mapping T_{n+1} with domain D_{n+1} such that $D_n \subsetneqq D_{n+1}$, $D_{n+1} \subsetneqq (0, 1)$, and the restriction of T_{n+1} onto D_n is T_n. The construction is such that $\cup_{n=1}^{\infty} D_n = [0, 1)$. The transformation T is defined as $T(x) = \lim_{n\to\infty} T_n(x)$.

At the first stage of the construction we split $[0, 1)$ into two subintervals, $[0, 1/2)$ and $[1/2, 1)$, and define T_1 as the translation of the first subinterval onto the second one. This is illustrated in the first diagram in Fig. 1: the action of T_1 is simply mapping a point in $[0, 1/2)$ to the point directly above in $[1/2, 1)$. The second stage of the construction cuts these intervals in half, takes the second

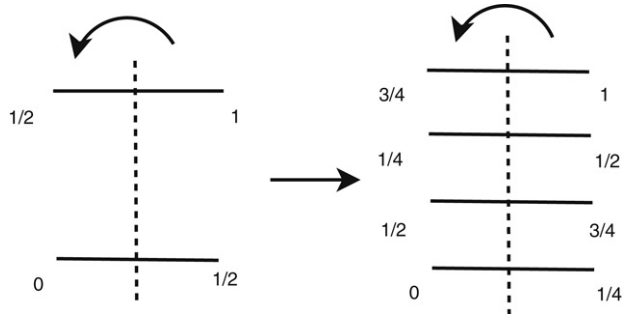

Fig. 1. Construction of the von Neumann–Kakutani transformation.

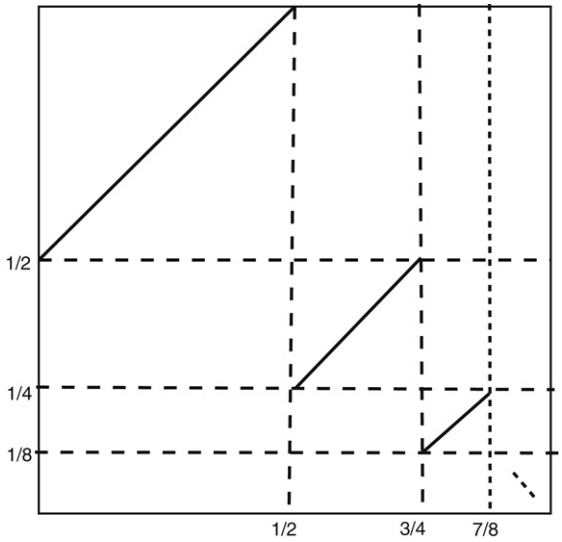

Fig. 2. Plotting the von Neumann–Kakutani transformation.

(right) half and stacks it onto the top of the first (left) half. This splitting and stacking is shown by the arrows and the dashed lines in Fig. 1. This diagram also shows how T_2 is defined: T_2 translates $[0, 1/4)$ onto $[1/2, 3/4)$, $[1/2, 3/4)$ onto $[1/4, 1/2)$, and $[1/4, 1/2)$ onto $[3/4, 1)$. Note that T_2 extends T_1 by mapping $[1/2, 3/4)$ onto $[1/4, 1/2)$. Also note the progression of domains: $D_1 = [0, 1/2)$ and $D_2 = [0, 1/2) \cup (1/2, 3/4)$. The splitting and stacking process continues in this manner.

In Fig. 2, we plot T_1, T_2 and T_3, to visualize the inductive construction of the limiting transformation T. The graph of T_1 is the line segment between $(0, 1/2)$ and $(1/2, 1)$, excluding the point $(1/2, 1)$. The graph of T_2 is the union of the graph of T_1 and the line segment between $(1/2, 1/4)$ and $(3/4, 1/2)$, excluding the point $(3/4, 1/2)$. The graph of T_3, adds to the graph of T_2, the line segment between $(3/4, 1/8)$ and $(7/8, 1/4)$, excluding the point $(7/8, 1/4)$. The construction continues in this manner.

Observe that the orbit of 0 under T, $0 \to 1/2 \to 1/4 \to 3/4 \to \cdots$, (see Fig. 1) is the van der Corput sequence in base 2. The splitting and stacking construction we discussed above can be done in any base b, in the following way. At each stage, the intervals will be cut into b subintervals of equal size, and stacking will be done from right to left: If we number the "stacks" as $0, 1, \ldots, b-1$, starting with the left-most stack, and if $x \prec y$ means stack y moves to the top of stack x, then stacking is done in the order $0 \prec 1 \prec \cdots \prec b-1$. The orbit of 0 under T in this general setting is the van der Corput sequence in base b.

Although the inductive definition of T by splitting and stacking is what we will examine in this paper, here we note an algebraic definition for T, in base b, using the "rightward carry addition" operation $\bigoplus$. If x is given as

$$x = \sum_{k=0}^{\infty} \frac{u_k}{b^{k+1}}$$

then

$$T(x) := x \bigoplus \frac{1}{b} = \frac{1+u_m}{b^{m+1}} + \sum_{k>m} \frac{u_k}{b^{k+1}}$$

where

$$m = \min\{k \mid u_k \neq b-1\}.$$

Since T_{n+1} is an extension of T_n for all n, this definition also gives an algebraic description for the mappings T_n. For example, the translations that were described in Fig. 1 are obtained by rightward carry addition by $1/2 = (0.1)_2$. In particular, $0 \bigoplus 1/2 = 1/2$, $1/2 \bigoplus 1/2 = 1/4$, and $1/4 \bigoplus 1/2 = 3/4$.

There are advantages of approaching the van der Corput sequence using the von Neumann–Kakutani transformation. The transformation T is ergodic and measure preserving, and $\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} f(T^{n-1}(\omega)) = \int_0^1 f(x)dx$ for almost all ω, where f is an integrable function on $[0, 1)$, from Birkhoff's ergodic theorem (see, for example, Friedman [21]). In other words, the orbit of ω, $\{\omega, T(\omega), T^2(\omega), \ldots\}$, is a u.d. mod 1 sequence for almost all ω. If $\omega = 0$, this orbit coincides with the van der Corput sequence in base b. If ω is a b-adic rational, then it will appear as the left-end of an interval in the splitting and stacking process, and thus $T^k(0) = \omega$ for some k. Therefore, the orbit of ω will be the van der Corput sequence in base b skipped by k terms.

We next describe a generalization of the splitting and stacking process. This new process will help us to analyze scrambled van der Corput sequences using ergodic theory.

Definition 2. A ladder L of height h and width w is an ordered set of h disjoint subintervals I_i contained in $[0, 1)$. The subintervals are left-closed and right-open, and have width w. We write $L = (I_0, I_1, \ldots, I_{h-1})$.

Definition 3. Let $\sigma_1, \sigma_2, \ldots$ be a sequence of permutations on $\{0, 1, \ldots, b-1\}$. The scrambled splitting and stacking process for $[0, 1)$ in base b is an inductive construction of a sequence of ladders L_n, where L_n has height b^n and width b^{-n}. The first ladder L_1 is obtained by stacking the subintervals $I_0 = [0, 1/b), I_1 = [1/b, 2/b), \ldots, I_{b-1} = [\frac{b-1}{b}, 1)$ as follows: If we number the subintervals $I_0, I_1, \ldots, I_{b-1}$ as $0, 1, \ldots, b-1$, then stacking is done in the order $\sigma_1(0) \prec \sigma_1(1) \prec \cdots \prec \sigma_1(b-1)$. Ladder L_n is obtained from L_{n-1} by splitting the subintervals of L_{n-1} into b subintervals of equal width. This divides the ladder L_{n-1} into b stacks, which are then arranged in the order $\sigma_n(0) \prec \sigma_n(1) \prec \cdots \prec \sigma_n(b-1)$, where $0, 1, \ldots, b-1$ is the numbering of the stacks from left to right.

An example will be helpful. Let $b = 3$ and all permutations equal to $\sigma = (0\ 2\ 1)$ (i.e., $\sigma(0) = 0, \sigma(1) = 2, \sigma(2) = 1$). The first ladder is obtained by stacking $\underbrace{[0, 1/3)}_{0}, \underbrace{[1/3, 2/3)}_{1}, \underbrace{[2/3, 1)}_{2}$ in the order $\sigma(0) = 0 \prec \sigma(1) = 2 \prec \sigma(2) = 1$ (see the first diagram in Fig. 3). The second ladder is obtained by splitting the first ladder into thirds (see the dashed lines in Fig. 3), labeling the resulting stacks as 0, 1, 2 (from left to right), and then stacking in the order $0 \prec 2 \prec 1$. The lower arrow in the figure shows that stack number 2 goes to the top of stack number 0, and the top arrow shows stack number 1 goes to the top of stack number 2. Fig. 4 plots the resulting transformations: T_1 maps $[0, 1/3)$ onto $[2/3, 1)$, and $[2/3, 1)$ onto $[1/3, 2/3)$, and T_2 extends T_1 by mapping $[1/3, 4/9)$ onto $[2/9, 1/3)$, and $[5/9, 2/3)$ onto $[1/9, 2/9)$.

At each stage of its construction, the scrambled splitting and stacking process defines a linear mapping T_n, as in the original von Neumann–Kakutani construction: T_n maps each subinterval in the

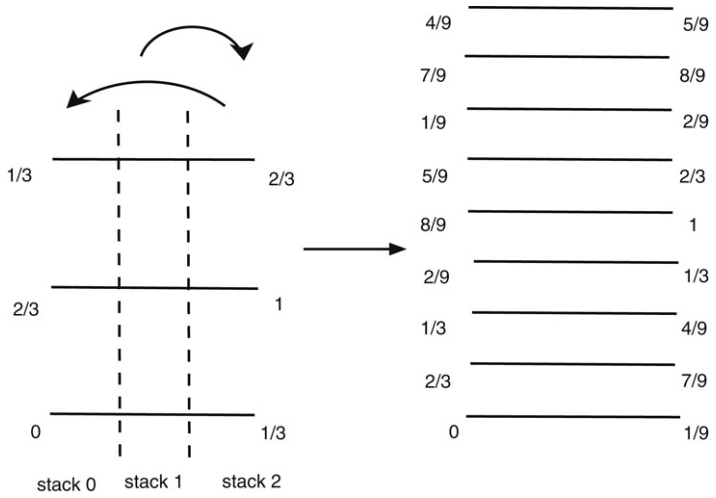

Fig. 3. Scrambled splitting and stacking.

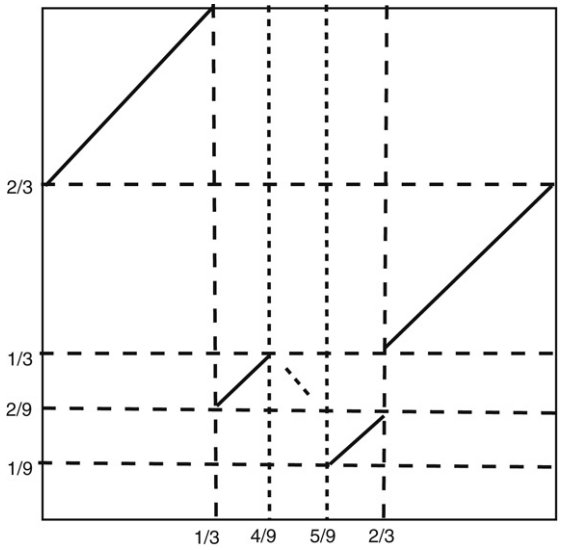

Fig. 4. Plotting the von Neumann–Kakutani transformation for $b = 3$ and $\sigma = (0\,2\,1)$.

ladder L_n onto the subinterval above by translation. This is possible since the intervals are disjoint and have equal width. We will call T_n the mapping induced by L_n. It is also clear that T_{n+1} is an extension of T_n. Indeed, T_n is defined everywhere in $[0, 1)$ except for the top interval of its ladder, and after splitting and stacking, this top interval will contain the top interval of the next ladder (where T_{n+1} is *not* defined) as a proper subset. Moreover, since stacking preserves the ordering of subintervals in each "stack", T_{n+1} reduces to T_n on the domain D_n of T_n. The limiting mapping, $T(x) = \lim_{n\to\infty} T_n(x)$, can be defined just as before, provided the union of the domains D_n is $[0, 1)$. We will prove that T as defined is ergodic and measure preserving, after we make a few more observations.

The orbit of 0 under the mapping T in the above example is $\{0, 2/3, 1/3, 2/9, 8/9, 5/9, 1/9, 7/9, 4/9, \ldots\}$. This is precisely the scrambled van der Corput sequence in base 3 with all permutations

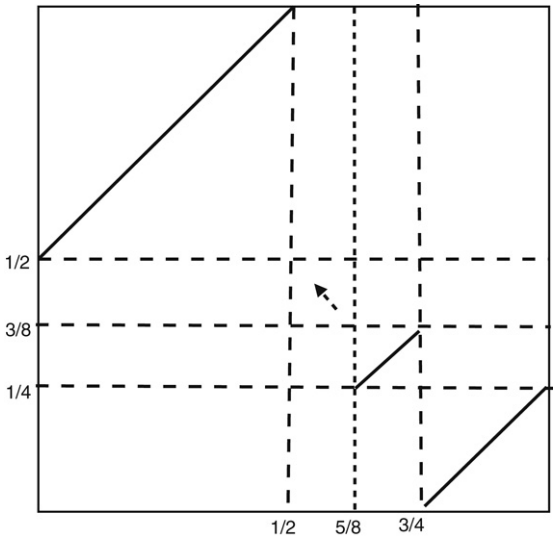

Fig. 5. Plotting the von Neumann–Kakutani transformation for $b = 2$ and $\sigma_1 = (0\ 1), \sigma_2 = \sigma_3 = \cdots = (1\ 0)$.

equal to $\sigma = (0\ 2\ 1)$ in (2). This choice of permutation for scrambled van der Corput sequence was used by Braaten and Weller [2].

Not all scrambled splitting and stacking transformations yield a transformation T on $[0, 1)$: it is possible to obtain domains D_n whose union miss a point of $[0, 1)$. For example, consider the transformation in base 2, with $\sigma_1 = (0\ 1), \sigma_2 = \sigma_3 = \cdots = (1\ 0)$. Since stacking is done from left to right after the first stage, $1/2$ appears as the left-end point of all the top intervals of the ladders. Therefore, $1/2$ does not belong to the domain of any of the T_n's. Fig. 5 plots the translations: T_1 maps $[0, 1/2)$ onto $[1/2, 1)$, T_2 extends T_1 by mapping $[3/4, 1)$ onto $[0, 1/4)$, and T_3 extends T_2 by mapping $[5/8, 3/4)$ onto $[1/4, 3/8)$. The arrow in Fig. 5 indicates the "direction" of the limiting process for T_n: note that $x = 1/2$ will not appear as the left-end point of any domain (interval) of a translation.

This kind of behavior can be observed in any base b, if the left-most stack is stacked at the top of another stack indefinitely, after a certain stage. In terms of permutations, this type of stacking corresponds to having a sequence of permutations $\sigma_k, \sigma_{k+1}, \ldots$, such that all permutations map 0 to a nonzero value. Although redefining T on a set of measure 0 does not change any of the properties such as ergodicity or measure preservation, not having a b-adic rational in the orbit of 0 is not desirable.

There is another disadvantage of having permutations that map 0 to a nonzero value. Let σ_k be the first permutation that stacks the left-most stack to the top of another stack. Then, 0 will appear as the left-end point of a subinterval other than the bottom interval, in the kth ladder. For example, if $\sigma_1 = (0\ 1)$ and $\sigma_2 = (1\ 0)$, then the left-end points of the subintervals in the first and second ladders are $(0, 1/2)$ and $(1/4, 3/4, 0, 1/2)$. This destroys the sequential construction of the orbit of 0. Even if we did not care about constructing a sequence, but only wanted to have a scrambled net (finite point set), having 0 at any other location than the beginning is not desirable, since 0 is often avoided (skipped) when its orbit is used in simulation.

For the reasons explained above, in the rest of the paper we will consider only scrambled splitting and stacking processes where σ_k maps 0 to 0 for all k.

Definition 4. A scrambled splitting and stacking process for $[0, 1)$ in base b, with permutations $\sigma_1, \sigma_2, \ldots$, is called normal if σ_k maps 0 to 0 for all k.

Lemma 5. *Consider a normal scrambled splitting and stacking process in base b, and let T_n be the mapping induced by the ladder L_n. Let $T(x) = \lim_{n\to\infty} T_n(x)$. Then, T is an ergodic and measure preserving transformation on* $[0, 1)$.

Proof. Let intervals I_n and J_n denote the domain and range of T_n. From the definition of the scrambled splitting and stacking process, I_n and J_n are disjoint, they have the same length b^{-n}, and T_n translates I_n onto J_n. Moreover, $\cup_{n=1}^{\infty} I_n = [0, 1)$. Indeed, observe that T_n is not defined on a left-closed right-open interval of width b^{-n}; the top interval of the ladder L_n. Denote this interval as $[l_n, r_n)$. The next phase of the process constructs T_{n+1}, which is undefined on an interval $[l_{n+1}, r_{n+1})$ with width b^{-n-1}. Clearly, $[l_n, r_n) \supsetneqq (l_{n+1}, r_{n+1})$, and since the process is normal, $l_{n+1} \neq l_n$. Therefore $\cap_{n=1}^{\infty}[l_n, r_n)$ is the empty set, proving the assertion. Similarly, in a normal process, the intervals that are not contained in the range of T_n (i.e., $[0, 1) - J_n$) are the bottom intervals of ladders: $[0, 1/b)$, $[0, 1/b^2)$, ... The intersection of these sets is $\{0\}$. Therefore, $\cup I_n = \cup J_n = [0, 1)$, except for a set of measure 0. The properties we have verified so far show that T is a σ-translation, and all σ-translations are measure preserving (see Friedman [20]). The proof that T is ergodic follows the ergodicity proof of the von Neumann–Kakutani transformation given in Friedman [20]. All the arguments made in the proof in Friedman [20] are still valid, once the binary intervals of the proof are replaced by b-adic intervals. □

Lemma 6. *The orbit of* 0 *under a normal scrambled splitting and stacking process in base b with permutations* $\sigma_1, \sigma_2, \ldots$*, coincides with the scrambled van der Corput sequence in base b with the same permutations.*

Proof. Proof is by induction on the stage number n of the scrambled splitting and stacking process. We will show that for any n, the left-end points of the intervals of L_n are the scrambled van der Corput numbers. At the first stage $n = 1$, the subintervals $[i/b, (i + 1)/b) i = 0, \ldots, b - 1$, are arranged in the order $\sigma_1(0) = 0 \prec \sigma_1(1) \prec \cdots \prec \sigma_1(b - 1)$ to construct L_1. Therefore the left-end points are $0, \sigma_1(1)/b, \ldots, \sigma_1(b - 1)/b$. These are exactly the first b terms of the scrambled van der Corput sequence in base b since $\phi_b(0) = \sigma_1(0)/b = 0, \phi_b(1) = \sigma_1(1)/b, \ldots, \phi_b(b - 1) = \sigma_1(b - 1)/b$.

Now assume that the induction hypothesis is true for the ladder L_{k-1}. The left-end points of L_{k-1} are $(0, T(0), \ldots, T^{b^{k-1}-1}(0))$, and the induction hypothesis implies $T^j(0) = \phi_b(j)$, for $j = 0, \ldots, b^{k-1} - 1$ (T^0 is the identity map). To construct L_k, we divide L_{k-1} into b equal subintervals and stack according to the permutation $\sigma_k = (0, \sigma_k(1), \ldots, \sigma_k(b - 1))$. By construction, the first interval that moves to the top of the ladder is the bottom interval of the stack numbered as $\sigma_k(1)$ (see Fig. 6). This interval is $[\frac{\sigma_k(1)}{b^k}, \frac{\sigma_k(1)+1}{b^k})$. Therefore, $T(T^{b^{k-1}-1}(0)) = T^{b^{k-1}}(0) = \frac{\sigma_k(1)}{b^k}$ which is nothing but $\phi_b(b^{k-1})$. The next $b^{k-1} - 1$ points in the orbit of 0 are the left-end points of the intervals in the rest of the stack. These points are, $T^{b^{k-1}+1}(0), T^{b^{k-1}+2}(0), \ldots, T^{2b^{k-1}-1}(0)$, and thus they are obtained from $\sigma_k(1)/b^k$ by translating by $T(0), T^2(0), \ldots, T^{b^{k-1}-1}(0)$. Therefore, $T^{b^{k-1}+j}(0) = \sigma_k(1)/b^k + T^j(0) = \sigma_k(1)/b^k + \phi_b(j) = \phi_b(b^{k-1} + j)$, where $0 \leq j \leq b^{k-1} - 1$. The next stack, stack number $\sigma_k(2)$, will determine the next b^{k-1} points in the orbit: $T^{2b^{k-1}}(0), T^{2b^{k-1}+1}(0), \ldots, T^{3b^{k-1}-1}(0)$. Now the bottom interval of the stack numbered as $\sigma_k(2)$ goes to the top, and thus, $T^{2b^{k-1}}(0) = \sigma_k(2)/b^k$, and the rest of the orbit is obtained by translating $\sigma_k(2)/b^k$ by $T(0), T^2(0), \ldots, T^{b^{k-1}-1}(0)$ as before. Then $T^{2b^{k-1}+j}(0) = \sigma_k(2)/b^k + T^j(0) = \sigma_k(2)/b^k + \phi_b(j) = \phi_b(2b^{k-1} + j)$, where $0 \leq j \leq b^{k-1} - 1$. In general, stack number $\sigma_k(i)$ determines the points $T^{ib^{k-1}}(0), T^{ib^{k-1}+1}(0), \ldots, T^{(i+1)b^{k-1}-1}(0)$, by translating $T^{ib^{k-1}}(0) = \sigma_k(i)/b^k$ by $T(0), T^2(0), \ldots, T^{b^{k-1}-1}(0)$. Therefore

$$T^{ib^{k-1}+j}(0) = \sigma_k(i)/b^k + T^j(0) = \sigma_k(i)/b^k + \phi_b(j) = \phi_b(ib^{k-1} + j)$$

for $1 \leq i \leq b - 1$ and $0 \leq j \leq b^{k-1} - 1$. This proves the lemma. □

2. A randomization of the scrambled van der Corput and Halton sequences

The quasi-Monte Carlo method, which uses low-discrepancy sequences such as the Halton sequence in estimating integrals, has the following drawback: using one low-discrepancy sequence in simulation gives a single estimate for the integral, and there is no practical way of assessing the error of this estimate. Indeed, although the Koksma–Hlawka inequality (or, its generalizations) provides an upper bound for the error, the upper bound itself needs to be estimated numerically, in

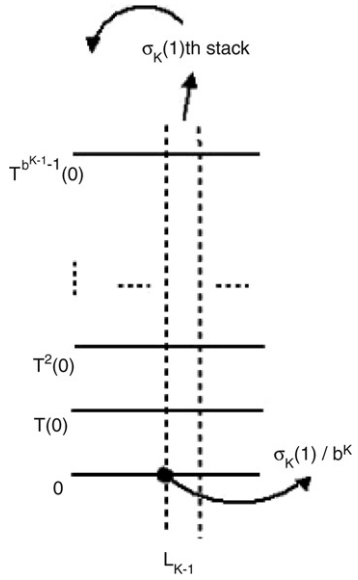

Fig. 6. Constructing L_k from L_{k-1}.

general. Moreover, for a given function, we do not know how tight the upper bound is. To address this drawback, researchers have introduced the so-called *randomized quasi-Monte Carlo* (RQMC) methods in the last decade. RQMC methods construct a family of low-discrepancy sequences, from which one can draw a sequence at random and use it to obtain an estimate for the integral. Statistical analysis can be applied to multiple estimates obtained this way, to measure error. For recent surveys of RQMC methods, see Ökten and Eastman [22] and L'Ecuyer and Lemieux [23]. In this section we will discuss a randomization of the scrambled Halton sequence.

Let T be an ergodic and measure preserving transformation obtained from a normal scrambled splitting and stacking process in base b. The permutations $\sigma_1, \sigma_2, \ldots$, are used in the splitting and stacking process. A word about the notation: Since all results of this section, except for one, are true for arbitrary sequences of permutations, we will suppress the permutations in the notation for T.

From the ergodic theorem, we have the following result.

Theorem 7. *For almost all* $x \in (0, 1)$*, the orbit of* x *under* T*, i.e., the sequence* $\{T^n(x)\}_{n=0}^{\infty}$*, is a u.d.* mod 1 *sequence in* $[0, 1)$.

Lemma 8. *If* X *is a random variable with the uniform distribution on* $[0, 1)$*, then so is* $T(X)$.

Proof. T is a σ-translation, and thus, measure preserving (a proof can be found in Friedman [20]). Therefore, $\lambda(T(B)) = \lambda(B)$ for any Borel measurable set $B \subset (0, 1)$, where λ is the Lebesgue measure on $[0, 1)$. Finally, for any such subset B, we observe that

$$P(T(X) \in B) = P(X \in T^{-1}(B)) = \lambda(T^{-1}(B)) = \lambda(B)$$

where the last equality holds since λ is measure preserving. □

Now define a random variable θ_N as

$$\theta_N(X) = \frac{1}{N}\sum_{i=0}^{N-1} f(T^i(X))$$

where f is a function defined on $[0, 1)$, and let $I = \int_0^1 f(x)\mathrm{d}x$.

Theorem 9. *The random variable $\theta_N(X)$ is an unbiased estimator for $I = \int_0^1 f(x)\mathrm{d}x$.*

Proof. For a given $x \in (0, 1)$, Theorem 7 implies that $\theta_N(x) \to I$ as $N \to \infty$, for almost all x. Moreover, for a given N, we have

$$\mathbf{E}[\theta_N] = \frac{1}{N}\sum_{i=0}^{N-1} \mathbf{E}[f(T^i(X))] = I$$

since $T^i(X)$ has the uniform distribution on $[0, 1)$, for any i, as implied by Lemma 8. □

Let $T_{b_1}, \ldots, T_{b_s}$ be the ergodic and measure preserving transformations obtained from normal scrambled splitting and stacking processes in relatively prime bases $b_1, \ldots, b_s$. For $\mathbf{x} = (x_1, \ldots, x_s) \in (0, 1)^s$, define

$$\mathbf{T}(\mathbf{x}) = (T_{b_1}(x_1), \ldots, T_{b_s}(x_s)).$$

Theorem 10. *For almost all $\mathbf{x} \in (0, 1)^s$, the orbit of $\mathbf{x}$ under $\mathbf{T}$, i.e., the sequence $\{\mathbf{T}^n(\mathbf{x})\}_{n=0}^{\infty}$, is a u.d.* mod 1 *sequence in $[0, 1)^s$.*

Proof. The eigenvalues for the von Neumann–Kakutani transformation in base b are $\exp(2\pi \mathrm{i}k/b^n)$, $0 \le k \le b^n$, $n \in \mathbf{N}$ (see [21]), and the Cartesian product of ergodic transformations is ergodic, as long as the only common eigenvalue of the transformations is one (see [24]). The generalized von Neumann–Kakutani transformation can be viewed as an adic system or generalized odometer (see [25]), and have the same eigenvalues as the von Neumann–Kakutani transformation.[1] Given relatively prime numbers $b_1, \ldots, b_s$, the only common eigenvalue for $T_{b_1}, \ldots, T_{b_s}$ is one. Therefore $\mathbf{T}$ is ergodic. The conclusion follows from the ergodic theorem. □

Let $\mathbf{X} = (X_1, \ldots, X_s)$ be a random variable with the uniform distribution on $[0, 1)^s$. Lemma 8 implies that $T_{b_i}(X_i)$ has the uniform distribution on $[0, 1)$ for any $i = 1, \ldots, s$, and thus, $\mathbf{T}(\mathbf{X})$ has the uniform distribution on $[0, 1)^s$. This fact enables us to generalize the estimator θ_N and Theorem 9 to multidimensions.

Theorem 11. *The random variable $\theta_N(\mathbf{X}) = \frac{1}{N}\sum_{i=0}^{N-1} f(\mathbf{T}^i(\mathbf{X}))$ is an unbiased estimator for $I = \int_{[0,1)^s} f(x)\mathrm{d}x$.*

To study the variance of θ_N, it suffices to know the discrepancy of the sequence $\{\mathbf{T}^n(\mathbf{x})\}_{n=0}^{\infty}$. This is known for the special case when the permutations used in the scrambled splitting and stacking process are the identity. The following result is by Lapeyre and Pagès [26], which generalizes the corresponding discrepancy bound for a one-dimensional van der Corput sequence of Pagès [27] (a proof of this result is sketched in [26]; personal communication with Dr. Lépingle and Dr. Pagès).

Theorem 12 (*Lapeyre and Pagès*). *Consider the sequence $\{\mathbf{T}^n(\mathbf{x})\}_{n=0}^{\infty}$ where all the permutations used in the scrambled splitting and stacking process are the identity. Then*

$$D_N^*(\mathbf{T}^n(\mathbf{x})) \le \frac{1}{N}\left[1 + \prod_{i=1}^{s}(b_i - 1)\frac{\log b_i N}{\log b_i}\right]$$

where D_N^* is the star discrepancy.

If $\mathbf{x} = \mathbf{0} = (0, \ldots, 0)$ and the permutations are arbitrary, in other words, if $\{\mathbf{T}^n(\mathbf{x})\}_{n=0}^{\infty}$ is simply the scrambled Halton sequence, then the following result by Atanassov [1] applies (this is the best known bound for the star discrepancy of an arbitrary scrambled Halton sequence):

[1] I am grateful to Dr. Karl Petersen for pointing this out.

Theorem 13 (*Atanassov*). *Consider the sequence* $\{\mathbf{T}^n(\mathbf{0})\}_{n=0}^{\infty}$ *where arbitrary permutations are used in the scrambled splitting and stacking process. Then*

$$D_N^*(\mathbf{T}^n(\mathbf{0})) \leq \frac{1}{N}\frac{1}{s!}\prod_{i=1}^{s}\frac{b_i-1}{\log b_i}(\log N)^s + O(N^{-1}(\log N)^{s-1}). \tag{3}$$

Therefore, in the special cases when (i) the sequence is the orbit of **x,** but the permutations are the identity, or (ii) the permutations are arbitrary, but the sequence is the orbit of **0,** the star discrepancy is $O(N^{-1}(\log N)^s)$. We think this result is true for any **x**, and for arbitrary permutations, but unable to prove it.

Conjecture 14. $D_N^*(\mathbf{T}^n(\mathbf{x}))$ *is* $O(N^{-1}(\log N)^s)$ *for arbitrary permutations used in the scrambled splitting and stacking process, arbitrary* **x,** *and any relatively prime bases* $b_1, \ldots, b_s$.

If this conjecture is true, then we can prove that

$$\sigma^2(\theta_N(\mathbf{X})) = O(N^{-2}(\log N)^{2s})$$

if f has bounded variation in the sense of Hardy and Krause, and **X** is a random variable with the uniform distribution on $[0,1)^s$. Indeed, this simply follows from the Koksma–Hlawka inequality:

$$\sigma^2(\theta_N(\mathbf{X})) = \int_{[0,1)^s} |\theta_N(\mathbf{x}) - I|^2 \, d\mathbf{x} \leq V(f)^2 D_N^*(\mathbf{T}^n(\mathbf{x}))^2 = O(N^{-2}(\log N)^{2s}),$$

where $V(f)$ is the variation of f in the sense of Hardy and Krause.

Remark 15. As we mentioned earlier, if x_i is a b_i-adic rational, then the orbit of x_i is the (scrambled) van der Corput sequence in base b_i skipped by k_i terms where k_i is such that $T^{k_i}(0) = x_i$. Similarly, for $\mathbf{x} = (x_1, \ldots, x_s)$, and each x_i is a b_i-adic rational, $\{\mathbf{T}^n(\mathbf{x})\}_{n=0}^{\infty}$ is the (scrambled) Halton sequence in bases $b_1, \ldots, b_s$, skipped by the integer vector $(k_1, \ldots, k_s)$, where k_i is such that $T^{k_i}(0) = x_i$ for $i = 1, \ldots, s$. The bound $O(N^{-1}(\log N)^s)$ is valid for the star discrepancy of these skipped sequences.

The idea of randomizing the starting point in the orbit of an ergodic transformation for the original Halton sequence first appeared in Struckmeier [28]. The theoretical analysis of this idea, including the unbiasedness of the estimator as well as an estimate for its variance was established by Wang and Hickernell [29]. We call the sequence $\{\mathbf{T}^n(\mathbf{x})\}_{n=0}^{\infty}$, random-start scrambled Halton sequence, adapting the terminology used in [29].

The results of this section show that we can randomize any scrambled Halton sequence using the random-start approach, and analyze the estimates obtained from independent randomizations statistically. This will provide significant error reduction in especially high dimensional problems where the standard Halton sequence fails. Next we present some examples.

3. Numerical results

In the numerical results that follow, we consider two test problems, and two scrambled Halton sequences (via deterministic permutations); one by Faure [5], and the other by Kocis and Whiten [7]. Permutations of Faure [5] are constructed recursively, and they are designed to minimize the extreme discrepancy of the one-dimensional van der Corput sequences. An algorithm to compute these permutations is given in [9]. Permutations of Kocis and Whiten [7] are constructed following a heuristic argument; the authors provide examples in [7].

Both of these sequences (Faure and Kocis & Whiten scrambled Halton sequences) are randomized using the random-start method we discussed in the previous section. We compare them with some other randomized quasi-Monte Carlo methods and standard Monte Carlo. The computer implementation of the random-start method is based on Remark 15. Specifically, to generate a random-start scrambled van der Corput sequence in base b, we first generate a random number u from the uniform distribution on $(0,1)$. We then compute a b-adic rational x such that $|x-u| < \varepsilon$, for

Table 1
Sample standard deviations for the test integral.

a_k	N (K)	σ_H	σ_{FH}	σ_{LSF}	σ_{MC}	$\frac{\sigma^2_{MC}}{\sigma^2_H}$	$\frac{\sigma^2_{MC}}{\sigma^2_{FH}}$	$\frac{\sigma^2_H}{\sigma^2_{FH}}$	$\frac{\sigma^2_{LSF}}{\sigma^2_{FH}}$
k^2	10	14.8e−6	11.8e−6	5.7e−5	1129e−6	5859	9152	1.6	23
k^2	20	7.5e−6	6.3e−6	3.0e−5	760.4e−6	10,354	14,592	1.4	22
k^2	30	3.0e−6	3.3e−6	1.5e−5	574e−6	35,792	29,534	0.8	21
k^2	40	3.1e−6	3.8e−6	1.3e−5	562.5e−6	32,075	22,135	0.7	12
k^2	50	3.2e−6	2.7e−6	1.0e−5	404.5e−6	15,840	23,300	1.5	15
$(s-k)^2$	10	2970e−6	36.7e−6	2.1e−5	556.4e−6	0.04	230	6542	0.3
$(s-k)^2$	20	1185e−6	20.2e−6	1.1e−5	378.5e−6	0.1	353	3458	0.3
$(s-k)^2$	30	535e−6	13.4e−6	4.3e−6	327.9e−6	0.4	595	1584	0.1
$(s-k)^2$	40	768.4e−6	9.1e−6	4.3e−6	270.3e−6	0.1	880	7113	0.2
$(s-k)^2$	50	145.2e−6	8.1e−6	4.1e−6	253.1e−6	3.0	984	324	0.3
1	10	31.20e−3	9.73e−3	1.0e−2	10.53e−3	0.1	1.2	10.3	1.1
1	20	13.29e−3	6.70e−3	6.7e−3	7.54e−3	0.3	1.3	3.9	1.0
1	30	13.43e−3	7.20e−3	4.7e−3	5.49e−3	0.2	0.6	3.5	0.4
1	40	14.12e−3	5.26e−3	4.1e−3	5.80e−3	0.2	1.2	7.2	0.6
1	50	8.69e−3	3.43e−3	3.0e−3	4.93e−3	0.3	2.1	6.4	0.8

some predetermined small tolerance ε. In our numerical results, we chose $\varepsilon = b^{-20}$, in other words, we let the b-adic rational x be the number obtained from the first twenty digits of u in base b. Then, $\phi_b^{-1}(x)$ gives the number of terms that will be skipped in the van der Corput sequence.

3.1. A test integral

We consider a numerical integration test problem proposed in Radović, Sobol' and Tichy [30]. This problem was also considered by Wang and Hickernell [29]. The function to be integrated is $f(x) = \prod_{k=1}^{s} \frac{|4x_k-2|+a_k}{1+a_k}$ over $[0,1)^s$. The true value of the integral is 1 for any s. The constant a_k determines the "importance" of the kth dimension. If a_k is larger, then the importance, or sensitivity, of f with respect to its kth component is smaller. The definition of sensitivity, in the sense of the ANOVA decomposition of functions, can be found in Sobol' [31].

In Table 1, we compute forty estimates $e_1, \ldots, e_{40}$ for the integral, using the random-start Halton sequence, random-start Faure-scrambled Halton sequence, the random linear scrambled Faure sequence (see Matoušek [32]) and the Monte Carlo method. Each estimate is obtained by using N vectors of the underlying s-dimensional quasi-Monte Carlo sequence $\{\mathbf{q}_i\}$ in computing the standard Monte Carlo estimator for the integral, i.e., $e_i = \sum_{i=1}^{N} f(\mathbf{q}_i)/N$. We use the same methodology as Wang and Hickernell [29], and report the sample standard deviation of the sample mean estimator, $\sqrt{\sum_{i=1}^{M}(e_i-\bar{e})^2/[M(M-1)]}$, where $\bar{e} = (e_1+\cdots+e_M)/M$ and $M = 40$. The last four columns of the table display the ratios of sample variances of the sample mean estimator for the sequences. In the table, the abbreviations H, FH, LSF and MC correspond to random-start Halton, random-start Faure-scrambled Halton, linear scrambled Faure, and Monte Carlo. The dimension of the problem is $s = 50$. We use different choices for a_k and N, the number of fifty-dimensional quasi-Monte Carlo vectors used in estimating the integral. In the table **K** stands for 1000.

We make the following observations:

(1) When $a_k = k^2$, the importance of the components quickly decreases as the dimension increases. The problem is essentially low dimensional, and the important dimensions are the early dimensions. In such a problem, one would not expect the Halton sequence to perform badly, and this is reflected in the numerical results. Both the sequences (random-start Halton and random-start Faure-scrambled Halton) improve on the Monte Carlo error in factors between 20,000 and 30,000. The random-start Faure-scrambled Halton sequence is better than the random-start Halton sequence in three out of five samples, but the differences between these two sequences are

very small. The random-start Faure-scrambled Halton sequence improves on the linear scrambled Faure sequence by factors ($\sigma^2_{LSF}/\sigma^2_{FH}$) between 12 and 23.

(2) When $a_k = (s-k)^2$, the importance of the components decreases at the same rate as before, but in different order: now the higher dimensions are more important than lower dimensions. We would expect the Halton sequence to perform poorly in such a problem (for small to moderate N), since the high prime bases that cause correlation now contribute heavily to the solution of the problem. In fact, the column σ^2_{MC}/σ^2_H shows that Monte Carlo is more accurate than random-start Halton, up to a factor of 25, except for $N = 50\mathbf{K}$. The advantages of random-start Faure-scrambled Halton sequence over Monte Carlo and random-start Halton sequence are impressive: improvements are by factors as high as 1000 over Monte Carlo, and 7000 over random-start Halton sequence. Linear scrambled Faure is better than random-start Faure-scrambled Halton though the improvements are modest: factor of improvements are 3, 3, 3, 5, 10.

(3) When $a_k = 1$, all components have the same importance, and the effective dimension of the problem is quite high compared to the first two cases: this can be deduced by observing that the sample standard deviation of the estimates increases by a factor of 10^3. The random-start Halton sequence is worse than Monte Carlo for all N. The random-start Faure-scrambled Halton sequence is better than Monte Carlo in four out of five choices for N, but the improvements are small. There is not a significant separation between the linear scrambled Faure and random-start Faure-scrambled Halton sequences.

3.2. Asian geometric call option

Here we consider a problem from computational finance: the pricing of Asian geometric call options under the lognormal model. The price of the option can be computed exactly. Details on Asian options, including its analytical solution, can be found in Glasserman [33]. The pricing problem amounts to evaluating an integral, and the dimension of the integral in the numerical results reported below is 30 and 50.

In a recent paper, Faure and Lemieux [6] compared several scrambled (via deterministic permutations) Halton sequences, and the random-start Halton sequence, by an extensive set of numerical experiments. They considered different scramblings by Atanassov (see [1,34]), Faure and Lemieux [6], Kocis and Whiten [7], Vandewoestyne and Cools [9], and Chi, Mascagni and Warnock [4]. These sequences were compared deterministically, by the actual estimation error, as well as statistically, by the sample variance of their estimates when each method was randomized using the random-shift method.

Two main conclusions were made in [6], based on the numerical results. The scrambled Halton sequences by Atanassov, Faure & Lemieux, Kocis & Whiten, and Chi, Mascagni & Warnock, had a similar performance, and they all outperformed the (standard) Halton sequence, random-start Halton sequence, and the scrambled Halton sequence by Vandewoestyne & Cools.

Here we want to answer the following questions:

(1) One of the better scrambled Halton sequences tested in [6] was the one by Kocis & Whiten. This sequence can be randomized using the random-shift method (considered in [6]) as well as the random-start method as we have explained in this paper. How do these different randomizations compare?

(2) The Faure-scrambled Halton sequence was not tested in [6]. How does this sequence compare with the Kocis–Whiten-scrambled Halton sequence?

(3) How do these sequences compare with other randomized quasi-Monte Carlo methods, for example, the random linear scrambling of the Faure sequence (also called generalized Faure, or GFaure) which was considered by Tezuka [35], and Matoušek [32]?

In Tables 2 and 3, we compute twenty-five estimates for the option price, $e_1, \ldots, e_{25}$, and report their root mean square error, $\sqrt{\sum_{i=1}^{25}(e_i - e)^2/25}$, where e is the true option price. The estimates for the option price are obtained using (i) random-shift scrambled Halton by Kocis–Whiten (Rshift-KW), (ii) random-start scrambled Halton by Kocis–Whiten (Rstart-KW), (iii) random-start scrambled Halton

Table 2
Root mean square error. Dimension is 30.

N	Rshift-KW	Rstart-KW	Rstart-Faure	LinScrFaure	MC
500	1.48e−1	1.32e−1	1.24e−1	2.52e−1	4.09e−1
5 K	3.81e−2	3.25e−2	3.16e−2	3.24e−2	1.17e−1
10 K	1.85e−2	1.82e−2	1.84e−2	2.67e−2	8.04e−2

Table 3
Root mean square error. Dimension is 50.

N	Rshift-KW	Rstart-KW	Rstart-Faure	LinScrFaure	MC
500	1.92e−1	1.89e−1	1.64e−1	2.36e−1	3.61e−1
5 K	4.57e−2	3.34e−2	4.24e−2	5.55e−2	1.21e−1
10 K	2.73e−2	2.54e−2	2.56e−2	3.52e−2	7.72e−2

by Faure (Rstart-Faure), (iv) random linear scrambled Faure sequence (LinScrFaure), and (v) Monte Carlo. Each estimate is obtained using N vectors of the underlying quasi-Monte Carlo sequence. In Table 2 the dimension is 30, and in Table 3 the dimension is 50. We are especially interested in the performance of the methods when N is small, and the dimension is large, for this makes the problem, in general, harder for quasi-Monte Carlo.

As the results indicate, Rstart-KW gives a lower root mean squared error than Rshift-KW, for all N, although the improvement is small. Rstart-Faure also provides lower error than Rshift-KW. There is no clear separation between Rstart-KW and Rstart-Faure. All methods based on scrambled Halton sequences provide smaller error than the linear scrambled Faure sequence, except for $N = 5\mathbf{K}$ (Rshift-KW and Rstart-KW) in Table 2.

The random-start Faure-scrambled Halton sequence was applied to another problem from finance, computation of the endogenous mortgage rates, and favorable numerical results were obtained compared to random-start Halton sequence. See Goncharov, Ökten, Shah [36] for details.

4. Conclusion

Numerical results suggest that scrambled Halton sequences randomized by the random-start method can improve error significantly, or stay competitive, when compared to various other randomizations. Future numerical work will help in assessing the true benefits of these sequences.

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