Extensions of Atanassov's methods for Halton sequences

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Basic things, contents will follow

The van der Corput sequence S_b in base b is defined as ($n \geq 1$)

$$S_b(n) = \sum_{r=0}^{\infty} \frac{a_r(n)}{b^{r+1}} \text{ with } n-1 = \sum_{r=0}^{\infty} a_r(n)\ b^r (\text{ b-adic expansion}).$$

An s-dimensional Halton sequence H in $I^s = [0,1)^s$ is defined as

$$H(n) = (S_{b_1}(n), \ldots, S_{b_s}(n)), \text{ with pairwise coprime } b_j\text{'s.}$$

A generalized van der Corput sequence associated with a sequence $\Sigma = (\sigma_r)_{r\geq 0}$ of permutations of $Z_b = \{0, 1, \ldots, b-1\}$ is defined as

$$S_b^{\Sigma}(n) = \sum_{r=0}^{\infty} \frac{\sigma_r\big(a_r(n)\big)}{b^{r+1}}.$$

A generalized Halton sequence GH, associated with s sequences of permutations, $\Sigma_j = (\sigma_{j,r})_{r\geq 0}$ of Z_{b_j}, $j = 1, \ldots, s$, is defined as

$$GH(n) = (S_{b_1}^{\Sigma_1}(n), \ldots, S_{b_s}^{\Sigma_s}(n)),\ n \geq 1.$$

Pairwise coprime bases b_j are usually chosen as the first s primes.

The concept of $(t,s)-$sequences in base b requires two definitions:

– An elementary interval E in I^s is defined as (a_i, d_i are integers)

$$E = \prod_{i=1}^{s} [a_i b^{-d_i}, (a_i+1)b^{-d_i}) \text{ with } 0 \leq a_i \leq b^{d_i} \text{ for } 1 \leq i \leq s.$$

– Given integers t, m with $0 \leq t \leq m$, a $(t,m,s)-$net in base b is an s-dimensional set with b^m points such that any elementary interval in base b with volume b^{t-m} contains exactly b^t points of the set.

An s-dimensional sequence X in I^s is a $(t,s)-$sequence if the subset $\{X(n) : kb^m < n \leq (k+1)b^m\}$ is a $(t,m,s)-$net in base b for all integers $k \geq 0$ and $m \geq t$.

Further generalizations by Niederreiter and Xing and more recently by Dick & all would require extensions of that definition. To avoid too much developments, we leave them out. In the following, we will only need the definition of $(t,s)-$sequences. The questions of the construction of such sequences and of the optimization of the quality parameter t are not relevant for our purpose in the present study.

For short, from now on, we will use the notation X_n instead of $X(n)$.

Discrepancy

For a point set $\mathcal{P}_N = \{X_1, X_2, ..., X_N\}$ in $I^s = [0,1)^s$ and a subinterval J of I^s, we define the discrepancy function as

$$E(J,N) = A(J,N) - NV(J) \quad \text{where}$$

$$A(J,N) = \#\{n; 1 \leq n \leq N, X_n \in J\} \text{ and } V(J) \text{ is the volume of } J.$$

Then, the star (extreme) discrepancy D^*, respectively the (extreme) discrepancy D of $\mathcal{P}_N$ are defined as

$$D^*(\mathcal{P}_N) = \sup_{J^*}|E(J^*,N)| \quad \text{and} \quad D(\mathcal{P}_N) = \sup_J|E(J,N)|$$

where J^* (resp. J) is of the form $\prod_{i=1}^s [0, y_i[$ (resp. $\prod_{i=1}^s [y_i, z_i[$).

For an infinite sequence X, we denote $D(N,X)$ and $D^*(N,X)$ the discrepancies of its first N points. Similarly, for the discrepancy function we will note $E(J,N,X) = A(J,N,X) - NV(J)$.

A sequence satisfying $D^*(N, X) \in O((\log N)^s)$ is typically considered to be a low-discrepancy sequence. But the constant hidden in the O notation needs to be made explicit to make comparisons possible across sequences. This is achieved in many papers with an inequality of the form

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

But this is still unsatisfactory and the constants hidden in the complementary term can be so huge that the leading term can lose any significance in applications. Nevertheless, improving the leading term c_s is still of interest from a number theory point of view.

Outline

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4. Improvement in the case of an even base

Part II : Scrambling Halton sequences

1. Atanassov's result with admissible permutations

2. Scrambling Halton sequences with lower triangular matrices

3. Scrambling Halton sequences with admissible matrices

Part I : Extending Atanassov's method for Halton sequences to (t, s)–sequences

1. Atanassov's result for Halton sequences

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

if all b_j's are odd and with additional term u if b_j is the even base

$$u = \frac{b_j}{2(s-1)!} \prod_{1 \leq i \leq s, i \neq j} \left(\frac{(b_i - 1)\log N}{2\log b_i} + s - 1 \right).$$

Hence the leading constant is $c_s = \frac{1}{s!} \prod_{j=1}^{s} \frac{b_j - 1}{2\log b_j}$ (the old one$/s!$).

2. Leading constant for $(t, s)-$ sequences

$c_s = \frac{b^t}{s!}\frac{b-1}{2\lfloor\frac{b}{2}\rfloor}\left(\frac{\lfloor\frac{b}{2}\rfloor}{\log b}\right)^s$. Complementary term can be given explicitely.

The formula goes back to Niederreiter (after special cases by Sobol' and Faure).

Quality parameter t depends on b and s. While $t \in O(s \log s)$ for the Sobol' and Niederreiter constructions, $t \in O(s)$ for the constructions of Niederreiter-Xing.

Note also that Kritzer recently improved the constants c_s by a factor $1/2$ for odd $b \geq 3$ and $s \geq 2$, and by a factor $1/3$ for $b = 2$ and $s \geq 5$ (a similar result holds for even $b > 2$).

3. Atanassov's method applied to $(t, s)-$seq.

A careful examination of Atanassov's lemmas for pairwise coprime bases shows they can be adapted to a single base b, leading to

Theorem 1 *The discrepancy of a $(t, s)-$sequence X in base b satisfies*

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

Corollary *The leading constant c_s satisfies*

$$c_s = \begin{cases} \frac{b^t}{s!}\left(\frac{b-1}{2\log b}\right)^s & \text{if } b \text{ is odd} \\ \frac{b^t}{s!}\left(\frac{b}{2\log b}\right)^s & \text{if } b \text{ is even.} \end{cases}$$

For an odd b the constant c_s is the same as above, and for an even b it is larger by a factor $b/(b-1)$.

Idea of the proof

(1) Use numeration in base b with signed digits: $z \in [0,1)$ is writen as

$$z = \sum_{j=0}^{\infty} a_j b^{-j} \begin{cases} \text{with } |a_j| \leq \frac{b-1}{2} \text{ if } b \text{ is odd} \\ \text{with } |a_j| \leq \frac{b}{2} \text{ and } |a_j| + |a_{j+1}| \leq b-1 \text{ if } b \text{ is even.} \end{cases}$$

(2) Use signed splittings of an interval $J \in I^s$, i.e any collection of intervals $J_1, \dots, J_n$ and respective signs $\epsilon_1, \dots, \epsilon_n$ (± 1), such that for any additive function ν on intervals in I^s, we have $\nu(J) = \sum_{i=1}^{n} \epsilon_i \nu(J_i)$.

(3) Get discr. fct., with $I(\boldsymbol{j}) = I(j_1, \dots, j_s)$ sign.splitting. from (1):

$$A(J,N) - NV(J) = \sum_{j_1=0}^{n} \cdots \sum_{j_s=0}^{n} \epsilon(\boldsymbol{j}) \left(A(I(\boldsymbol{j}),N) - NV(I(\boldsymbol{j}))\right) =: \Sigma_1 + \Sigma_2$$

In Σ_1, put the terms $\boldsymbol{j}$ such that $b^{j_1} \dots b^{j_s} \le N$, and in Σ_2 the rest. Hence, Σ_1 deals with the coarser part whereas Σ_2 deals with the finer.

(4) Main ingredient to bound Σ_1 and Σ_2 (from elementary diophantine geometry): $\# \left\{ (j_1, \dots, j_k); b^{j_1} \dots b^{j_k} \le N \right\} \le \frac{1}{k!} \left(\frac{\log N}{\log b} \right)^k$.

Σ_1 gives the leading part of the bound in $(\log N)^s$ and Σ_2 the other part in $(\log N)^{s-1}$.

A refinement of the method is possible for even b, thanks to a deeper investigation of Σ_1 with the numeration system using signed digits:

4. Improvement in the case of an even base

Theorem 2 *The discrepancy of a (t,s)–sequence X in an even base b satisfies*

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

Recall that for even b, the known leading constant is

$$c_s = \frac{b^t}{s!}\frac{b-1}{b}\left(\frac{b}{2\log b}\right)^s .$$

This improvement is especially interesting in small bases: for instance, for $b=2$, c_s is divided by 2^{s-1} about.

Part II : Scrambling Halton sequences with admissible matrices

1. Atanassov's result with admissible permutations

In the same paper, Atanassov obtains a further improvement for the leading constant c_s of a sub-class of generalized Halton (GH) sequences which he calls modified Halton sequences (MH). Requires an auxiliary definition:

Admissible integers. Let $p_1, \ldots, p_s$ be distinct primes. The integers $k_1, \ldots, k_s$ are called admissible for them if $p_i \nmid k_i$ and for each set of integers $b_1, \ldots, b_s$ such that $p_i \nmid b_i$, we have

$$k_i^{\alpha_i} \prod_{1 \le j \le s, j \neq i} p_j^{\alpha_j} \equiv b_i \pmod{p_i}, \quad i = 1, \ldots, s.$$

Sets of admissible integers are easy to obtain (amounts to solving linear equations).

A modified Halton sequence in bases (p_i) associated with admissible integers (k_i) is a generalized Halton sequence $GH = (S_{p_1}^{\Sigma_1}, \ldots, S_{p_s}^{\Sigma_s})$ where the sequence of permutations $\Sigma_i = (\sigma_{i,r})_{r \geq 0}$ is defined by

$$\sigma_{i,r}(a) = a k_i^r \pmod{p_i} \qquad \text{for all } 0 \leq a < p_i,\ r \geq 0,\ i = 1, \ldots, s.$$

Such sequences are low discrepancy sequences with upper bound

$$D^*(N, MH) \leq \frac{1}{s!} \sum_{i=1}^{s} \log p_i \prod \frac{p_i(1 + \log p_i)}{(p_i - 1) \log p_i} (\log N)^s + O((\log N)^{s-1}).$$

The leading constant is very low (MH sequences compete with Niederreiter–Xing $(t, s)-$sequences), but the constant in the complementary term is very huge. In applications taking $r \geq 1$ (instead of $r \geq 0$) is highly recommended.

2. Scrambling Halton sequences with matrices

This is the analog of generalized $(0, s)-$sequences from Tezuka (1994), first mentioned by Lemieux (2009, book,App. B, Springer).

A linearly scrambled Halton (LSH) sequence X based on nonsingular lower triangular (NLT) matrices $A_1, \ldots, A_s$, where A_i has entries in $\mathbb{Z}_{p_i}$, is defined as

$$X = (S_{p_1}^{A_1}, \ldots, S_{p_s}^{A_s}),$$

in which, for an $\infty \times \infty$ matrix $C = (C_{r,l})_{r\geq 0, l\geq 0}$ with elements in $\mathbb{Z}_b$ (b prime), S_b^C is the sequence

$$S_b^C(n) = \sum_{r=0}^{\infty} y_{n,r} b^{-(r+1)} \quad \text{with} \quad y_{n,r} = \sum_{l=0}^{\infty} C_{r,l} a_l(n),$$

(the $a_l(n)$ are the digits of the b-adic expansion of $n-1$ as stated previously). Requires truncation as for generalized $(0, s)-$sequences.

Theorem 3 *A LSH sequence satisfies the same discrepancy bound as a GH sequence (hence with the same leading constant c_s):*

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

if all b_j's are odd and with additional term u if b_j is the even base

$$u = \frac{b_j}{2(s-1)!} \prod_{1 \leq i \leq s, i \neq j} \left(\frac{(b_i - 1)\log N}{2\log b_i} + s - 1 \right).$$

The proof follows closely that of Atanassov, but requires a new fundamental lemma taking into account the action of NLT matrices and the necessity of the truncation operator.

3. Scrambling Halton sequences with admissible matrices

This is the generalisation of modified Halton sequences, using powers of admissible integers on the diagonal entries.

Let $A_1, \ldots, A_s$ be invertible NLT matrices in distinct prime bases $p_1, \ldots, p_s$ and let $k_1, \ldots, k_s$ be admissible integers for $p_1, \ldots, p_s$. Then the matrices $A_1, \ldots, A_s$ are admissible if they have the form

$$\begin{pmatrix} k_i^{\beta_i} & 0 & 0 & \cdots \\ * & k_i^{\beta_i+1} & 0 & \cdots \\ * & * & k_i^{\beta_i+2} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

where $\beta_1, \ldots, \beta_s$ are non-negative integers. A LSH sequence based on admissible matrices $A_1, \ldots, A_s$ is called a modified linearly scrambled Halton (MLSH) sequence.

Original Atanassov's modified Halton sequences correspond to diagonal admissible matrices A_j and to $\beta_j = 0$ for all j.
The sequences used in the experiments by Atanassov–Durchova (2003) and Faure–Lemieux (2009) correspond to diagonal admissible matrices A_j and to $\beta_j = 1$.

Theorem 4 *A modified linearly scrambled Halton sequence associated to distinct primes $p_1, \ldots, p_s$ with admissible matrices $A_1, \ldots, A_s$ and to non-negative integers $\beta_1, \ldots, \beta_s$ satisfies the same discrepancy bound as a modified Halton sequence:*

$$D^*(N, MLSH) \leq \frac{1}{s!} \sum_{i=1}^{s} \log p_i \prod \frac{p_i(1 + \log p_i)}{(p_i - 1) \log p_i} (\log N)^s + O((\log N)^{s-1}).$$

The proof is adapted from that of Atanassov to take into account the addition of non-negative integers $\beta_1, \ldots, \beta_s$ and the truncation involved by NLT matrices.

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