Golden ratio nets and sequences

Christiane Lemieux

Department of Statistics and Actuarial Science

University of Waterloo

(joint work with Nathan Kirk (IIT) and Jaspar Wiart)

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Motivation

- van der Corput sequence in base b is a great tool to build digital nets and sequences
- As b gets larger, equidistribution properties hold for $n = b^m$, which can thus be large
- Causes deterioration of quality as s increases for Faure and Halton sequences
- Reason behind choice of $b = 2$ (Sobol') in many high-dimensional applications
- Smallest integer base is 2: is there a way to have a smaller base?

We propose to address this using nets and sequences defined over an **irrational base**, the golden ratio being the prime example...

$\rightarrow$ Equidistribution happens more often but is not as "perfect"

Agenda

1. Background and guiding examples
2. New equidistribution definitions
3. $(t, m, s)-$nets and $(t, s)-$sequences in base φ
4. Extension to other irrational bases
5. Interlaced Halton sequences and their scrambling

Sources for this work

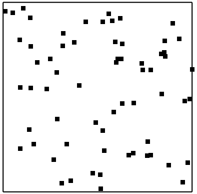
1-4: N. Kirk, C. Lemieux, J. Wiart. *Golden ratio nets and sequences*, Functiones et Approximatio, 2024.

5: N. Kirk and C. Lemieux. *An improved Halton Sequence for implementation in quasi-Monte Carlo Methods*, WSC 2024.

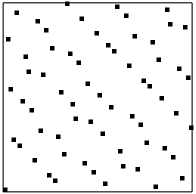
Related Work

1. C. Aistleitner, M. Hofer, V. Ziegler. *On the uniform distribution modulo 1 of multidimensional LS-sequences.* Ann. Mat. Pura Appl., 2014.
2. I. Carbone. *Comparison between LS-sequences and* $\beta-$*adic van der Corput sequences*, MCQMC 2014 Proceedings.
3. I. Carbone, M. R. Iacó and A. Volčič. *A LS-sequences of points in the unit square*, preprint, 2012.
4. S. Ninomiya. *Constructing a new class of low-discrepancy sequences by using the* β*-adic transformation*, Math. Comput. Simul., 1998.
5. S. Ninomiya. *On the discrepancy of the* $\beta-$*adic van der corput sequence*, J. Math. Sci. Univ. Tokyo, 1998.
6. C. Schretter, H. Zhijian, M. Gerber, N. Chopin, H. Niederreiter. Van der Corput and golden ratio sequences along the Hilbert sapce-filling curve, MCQMC 2014.

1. Low-discrepancy point sets



(Pseudo)random



Sobol'

Use these point sets P_n to form approximation $\hat{\mu}_n = \frac{1}{n}\sum_{i=1}^{n} f(\mathbf{u}_i)$ for $\mu = \int_{[0,1)^s} f(\mathbf{u} d\mathbf{u}$

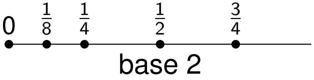
van der Corput sequence in integer base

In one dimension, we can construct a sequence of points $u_0, u_1, \ldots$ with a low discrepancy as follows:

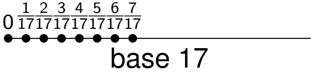
1. Choose integer base $b \geqslant 2$
2. To define u_i:
   - expand i in base b, i.e., write $i = \sum_{l=0}^{\infty} a_l b^l$:
   - apply *radical-inverse function*: $u_i = (0.a_0 a_1 \ldots)_b = \sum_{l=0}^{\infty} a_l b^{-l-1} \in [0, 1)$,

This yields the *van der Corput sequence in base* b*, denoted* Σ^b *(goes back to 1935)*

van der Corput Sequences in base b



As the base increases, the “space-filling” properties of the sequence deteriorate...



Can juxtapose van der Corput sequences in different bases to form s-dimensional construction: Halton sequence is $(\Sigma^2, \Sigma^3, \Sigma^5, \Sigma^7, \ldots)$

If we need n points in dimension s, can use n first points of Halton sequence in $s-1$ dimensions and add coordinate $u_{i,s} = i/n, i = 0, \ldots, n$ → **Hammersley point set**

Guiding Examples for Irrational Base Construction

Goal: define the
***van der Corput sequence in base** $\varphi = (1+\sqrt{5})/2$
***Hammersley point set in base** φ

Useful fact: any $x \in \mathbb{R}$ has unique base φ expanion:

$$x = \sum_{j=m-1}^{-\infty} d_j \varphi^j = (d_{m-1} \dots d_1 d_0 . d_{-1} d_{-2} \dots)_\varphi$$

where $d_j \in \{0,1\}$ and $d_j d_{j-1} = 0$ (i.e., no consecutive ones).

- can guarantee this *reduced form* because $\varphi^2 = \varphi + 1$
  $\Rightarrow$ can replace the string $(011)_\varphi$ by $(100)_\varphi$

Whole numbers in base φ

Expand $n \in \mathbb{N}_0$ using Fibonacci numbers (with $F^{-2} = 0$, $F^{-1} = 1$, $F^{j} = F^{j-1} + F^{j-2}$):

$$n = (d_{m-1} \dots d_1 d_0)_{\mathscr{F}} = \sum_{j=0}^{m-1} d_j F^j,$$

No i such that $d_i = d_{i-1} = 1$ (i.e., no consecutive ones). Can guarantee this *reduced form* because can replace the string $(011)_{\mathcal{F}}$ by $(100)_{\mathcal{F}}$. Then

$$\overline{n} = (d_{m-1} \dots d_1 d_0)_{\varphi} = \sum_{j=0}^{m-1} d_j \varphi^j,$$

is the n^{th} whole number in base φ.

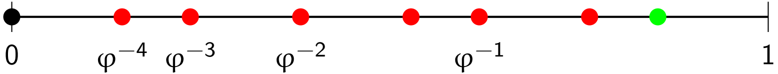
- The zeroth digit of either n or $\overline{n}$ is denoted by $|n| = |\overline{n}| = d_0$.

van der Corput sequence in base φ

Def: The n^{th} point of the *van der Corput sequence in base* φ is given by $g_n := (.d_0 d_1 \ldots d_{m-1})_\varphi$.

The first few points of this sequence are $g_0 = (.0)_\varphi = 0$, $g_1 = (.10)_\varphi = \varphi^{-1}$, $g_2 = (.010)_\varphi = \varphi^{-2}$, $g_3 = (.0010)_\varphi = \varphi^{-3}$, $g_4 = (.101)_\varphi = \varphi^{-1} + \varphi^{-3}$, etc.

ex: $4 = 1 + 3 = F^0 + F^2$ so $g_4 = (0.101)_\varphi = \varphi^{-1} + \varphi^{-3} = 0.854\ldots$



Hammersley point set in base φ

Def: The *Hammersley point set in base* φ with F^m points in $[0, 1)^2$ is defined as

$$H_m = \left\{ \left(g_n, \frac{\overline{n}}{\varphi^m} \right) : 0 \leqslant n < F^m \right\}$$

Example:

$$H_3 = \{(0,0), ((0.100)_\varphi, (0.001)_\varphi), ((0.010)_\varphi, (0.010)_\varphi), ((0.001)_\varphi, (0.100)_\varphi), ((0.101)_\varphi, (0.101)_\varphi)\}$$

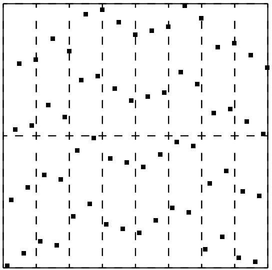
Note: Why F^m points? Because there are F^m $m-$digit binary strings corresponding to a whole number in base φ (i.e., with no consecutive ones)

Hammersley point sets in base φ

H_2, H_3, H_4, H_5 $\qquad$ H_{16} (contains $F^{16} = 2584$ pts)

2. New equidistribution definitions

Integer base b setup.



Elementary intervals of the form $\prod_{j=1}^{s}\left[\frac{a_j}{b^{m_j}}, \frac{a_j+1}{b^{m_j}}\right)$ with $0 \leqslant a_j < b^{m_j}$ for **partition** induced by $(m_1, \ldots, m_s)$

Irrational base setup

Will not get partition into congruent boxes.

Will not get local discrepancy of 0 over boxes.

Elementary intervals appear in more than one **partition**.

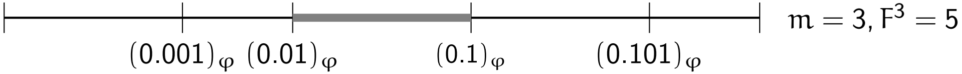
New equidistribution definitions

Def: An elementary m—interval I in base φ is a subinterval of $[0,1)$ of the form

$$I = \left[\frac{\overline{a}}{\varphi^m}, \frac{\overline{a+1}}{\varphi^m}\right)$$

for some $0 \leqslant a < F^m$ and $m \in \mathbb{N}_0$.

ex: $m = 3$ and $a = 2 = F^1$; $\overline{a} = \varphi$ and $\overline{a+1} = \varphi^2$ so $I = [\varphi^{-2}, \varphi^{-1})$

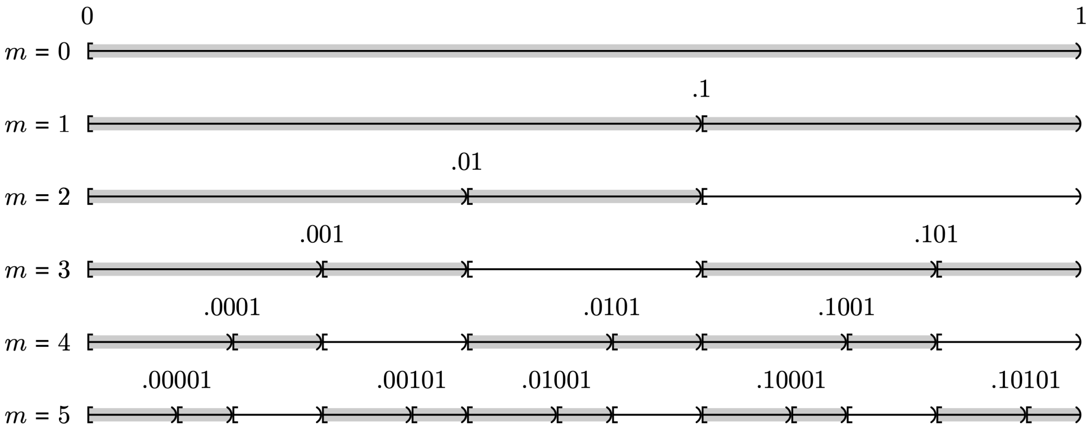


For given m, I can be of two different lengths. This is because

$$\overline{a+1} - \overline{a} = \varphi^{-|\overline{a}|}.$$

where $|\overline{a}| = |a| = d_0 \Rightarrow$ either of length φ^{-m} or φ^{-m-1}. Length depends on d_0

Elementary intervals



The first six $\mathfrak{m}$-partitions $\mathcal{P}_{\mathfrak{m}}$.

Prime elementary intervals

Def: An elementary interval I in base φ is called a prime elementary k–interval in base φ if k is the least positive integer such that there exists $0 \leqslant a < F^k$ such that

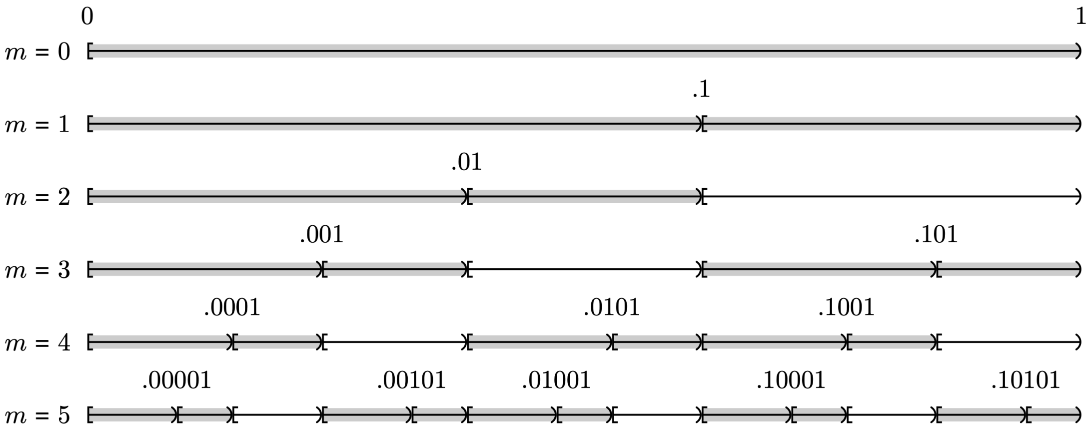
$$I = \left[\frac{\overline{a}}{\varphi^k}, \frac{\overline{a+1}}{\varphi^k}\right).$$

Holds iff $d_1 = 0$ (where $a = (d_{m-1} \ldots d_1 d_0)_{\mathcal{F}}$)

Means I is in $\mathcal{P}_k$ but not in $\mathcal{P}_{k-1}$.

$\rightarrow$ this def'n gives us a systematic way to check local discrepancy over I **only once**

Elementary intervals



The first six $\mathfrak{m}$-partitions $\mathcal{P}_{\mathfrak{m}}$, with the prime elementary intervals filled in gray.

Elementary intervals in dimension $s > 1$

Def: An elementary $(m_1, \ldots, m_s)-$interval I in base φ is a subinterval of $[0,1)^s$ of the form

$$I = \prod_{j=1}^{s} \left[\frac{\overline{a_j}}{\varphi^{m_j}}, \frac{\overline{a_j + 1}}{\varphi^{m_j}} \right)$$

where $0 \leqslant a_j \leqslant F^{m_j}$ and $m_j \in \mathbb{N}_0$ for each j.

Result: volume of I is $\varphi^{-|I|}$, where $|I| = \sum_{j=1}^{s} \left(m_j + |a_j|\right)$

Def: A prime elementary $(k_1, \ldots, k_s)-$interval in base φ is a subset of $[0,1)^s$ of the form

$$I = \prod_{j=1}^{s} \left[\frac{\overline{a_j}}{\varphi^{k_j}}, \frac{\overline{a_j + 1}}{\varphi^{k_j}} \right)$$

where $0 \leqslant a_j < F^{k_j}$ has its second-to-last digit d_1 equal to zero in its base $\mathscr{F}$ expansion.

Equidistribution

Definition needs two components:

1. total number points in point set
2. number of points we require in each elementary interval.

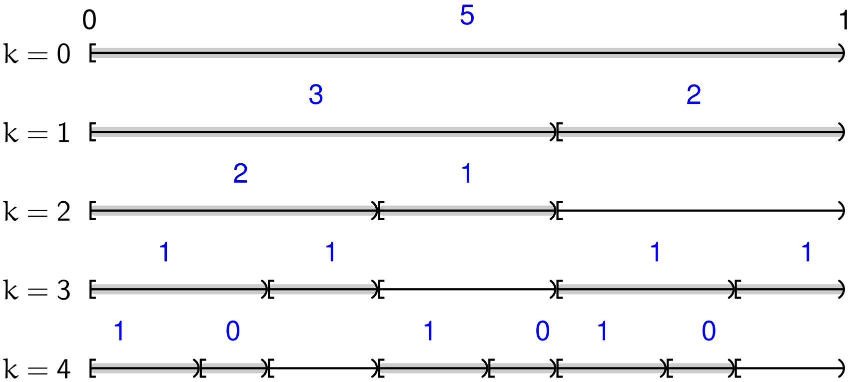
Volume $\varphi^{-|I|}$ is irrational, so **local discrepancy** can never be exactly 0.

Def: A point set P_m contained in $[0, 1)^s$ with F^m points is said to be $(k_1, \ldots, k_s)$-equidistributed in base φ if every **prime** elementary $(k_1, \ldots, k_s)$—interval in base φ, I, contains exactly $F^{m-|I|}$ points from P_m.

Why $F^{m-|I|}$ pts? Can prove **best rational approximation to** φ^{-k} with denominator F^m is F^{m-k}/F^m

Note: if we remove "**prime**" then we qualify equidistribution as **strong**

$F^3 = 5$ points being k-equidistributed for $k \leqslant 4$



3. Nets and sequences in base φ

Question: to define a $(t, m, s)-$net in base φ, what should be the volume cutoff for equidistribution (i.e., the "$b^{-(m-t)}$" required in base b)?

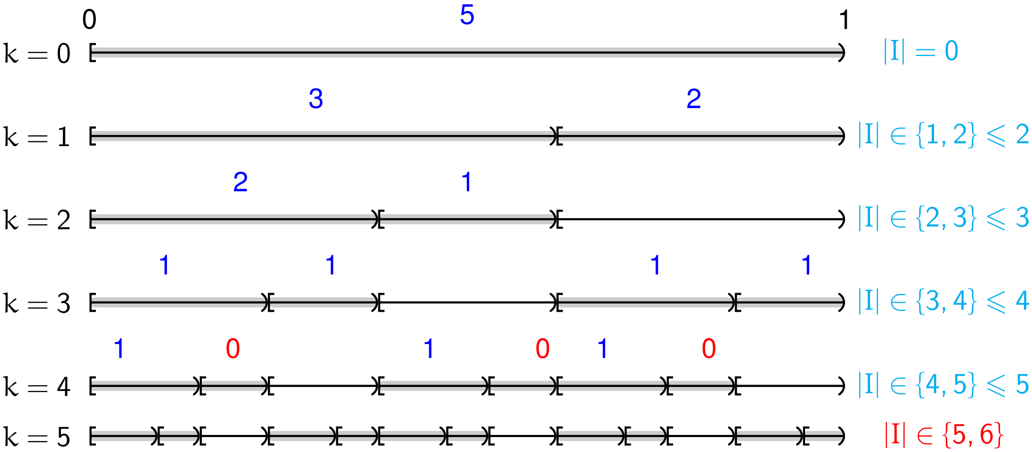
For I in an $\mathbf{m} = (m_1, \ldots, m_s)-$partition, have that

$$\sum_{j=1}^{s} m_j \leqslant |I| \leqslant \sum_{j=1}^{s} (m_j + \mathbf{1}_{m_j>0}) =: \rho(\mathbf{m})$$

Def: A point set P_m contained in $[0,1)^s$ with F^m points is called a $(t, m, s)-$net in base φ if it is $(k_1, \ldots, k_s)$-equidistributed in base φ for all $\mathbf{k} \in \mathbb{N}_0^s$ such that $\rho(\mathbf{k}) \leqslant m + 2 - t$.

Why $m+2-t$? Can show that for partition $\mathcal{P}_m$ where each $|I| \leqslant m+2$, we have $F^m = \sum_{I \in \mathcal{P}_m} F^{m-|I|}$.
$\Rightarrow$ F^m points can correctly be distributed among $I \in \mathcal{P}_m$

Cutoff to check quality parameter $t = 0$ when $m = 3$



(t, s)—sequence in base φ

Def: A sequence $\{x_0, x_1, \dots\}$ is called a (t, s)—sequence in base φ if for every $m \geqslant t$ and $k \in \mathbb{N}_0$, the set $\{x_{k \odot \varphi^{m+1}}, \dots x_{k \odot \varphi^{m+1} + F^m - 1}\}$ is a (t, m, s)—net in base φ.
(Here $n \odot \varphi^k = \sum_{j=0}^{m-1} d_j F^{j+k}$.)

Prop: If there exists a (t, s)—sequence in base φ, then for every $m > t$ there exists a $(t, m, s + 1)$—net in base φ.

Idea: add $\overline{n}/\varphi^m$ coordinate for $0 \leqslant n < F^m$, (i.e., "Hammersley" it)

Def: A sequence $\{x_0, x_1, \dots\}$ is called a weak (t, s)—sequence in base φ if for all $m \geqslant t$, $\{x_0, x_1, \dots, x_{F^m - 1}\}$ is a (t, m, s)-net in base φ.

Back to our constructions

Prop.: The van der Corput sequence in base φ is a $(0, 1)-$sequence in base φ.

Prop.: The Hammersley set H_m in base φ with F^m points is a $(0, m, 2)$-net in base φ.

Question: can we construct a $(t, s)-$sequence in base φ with small value of t?

Prop.: There exists weak $(1, 2)-$sequences in base φ.

4. Extensions to other irrational bases

- Can generalize the above constructions and definitions from φ to any irrational base γ being the **largest root of** $x^2 - px - q$ for $0 \leqslant q \leqslant p$.
- Work with $n \in \mathbb{N}_0$ s.t.

$$n = (\dots d_m \dots d_1 d_0)_{p+1} = \sum_{\ell=0}^{\infty} d_\ell (p+1)^\ell$$

satisfies condition $d_\ell < q$ if $d_{\ell-1} = p$ (condition $L_{p,q}$).

$$\Gamma_m^L = \text{set of } m\text{-digit numbers satisfying } L_{p,q} \quad \Rightarrow |\Gamma_m^L| =: G_m$$

Lemma: G_m is given by

$$G_m = \frac{(\gamma+1)\gamma^m + (\gamma - p - 1)(p-\gamma)^m}{2\gamma - p} (= F^m \text{ if } \gamma = \psi)$$

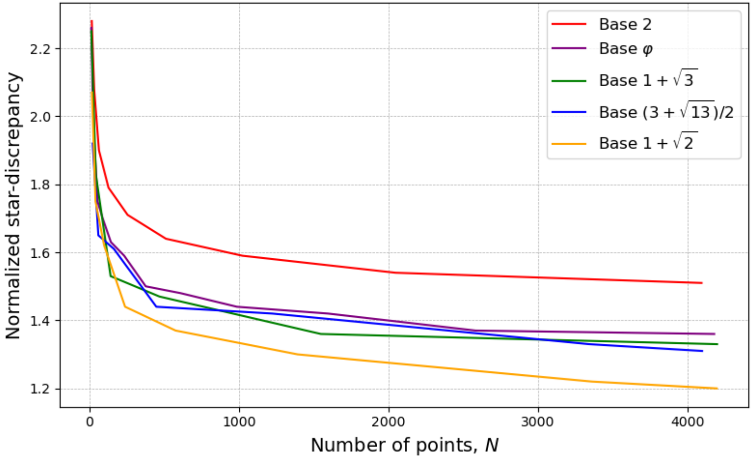
van der Corput sequence in base γ

Def: Let $n_i = (d_{m-1} \dots d_1 d_0)_{p+1}$ be the ith non-neg. integer satisfying condition $L_{p,q}$.
Then the i^{th} point of the van der Corput sequence (with parameters (p, q)) in base γ is

$$g_{i,\gamma} := (.d_0 d_1 \dots d_{m-1})_\gamma = \sum_{\ell=0}^{\infty} d_\ell \gamma^{-(\ell+1)}.$$

We also defined equidistribution, Hammersley point sets, $(t, m, s)-$nets and $(t, s)-$sequences in base γ (skip).

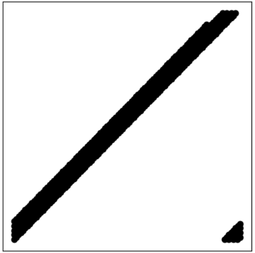
Star-discrepancy



The best performing two-dimensional Hammersley point sets in base γ with respect to the star discrepancy. All values are normalized by $\log N/N$.

5. Interlaced Halton sequences

Halton sequences are easy to implement and intuitive, but without any modification they do not work well in higher dimensions (see below first 500 points of coordinates (26,27))



Idea: *interlace* van der Corput sequences in appropriate irrational bases γ between the existing integer base coordinates of the original Halton sequence.

Guidance from previous work (Aistleitner et al. (2012))

Condition A. The two-dimensional sequence defined by the parameters (p_1, q_1) and (p_2, q_2) fails to be uniformly distributed in $[0, 1]^2$ if there exists $k, m \in \mathbb{N}$ such that $\frac{\gamma_1^k}{\gamma_2^m} \in \mathbb{Q}$.

E.g., fails with $(p_1, q_1) = (1, 1)$ and $(p_2, q_2) = (11, 1)$ since then $\gamma_1 = \varphi$ and $\gamma_2 = (11 + 5\sqrt{5})/2$, and we have $\gamma_1^5 = \gamma_2$.

Condition B. The two-dimensional sequence defined by the parameters (p_1, q_1) and (p_2, q_2) fails to be uniformly distributed in $[0, 1]^2$ if gcd$(p_1, q_1, p_2, q_2) > 1$.

E.g., fails with $p_1 = 2$, $q_1 = 0$ (i.e., $\gamma_1 = 2$) and $p_2 = 4$, $q_2 = 2$ (i.e., $\gamma_2 = 2 + \sqrt{6}$) since gcd$(2, 0, 4, 2) = 2 > 1$.

Interlaced Halton construction

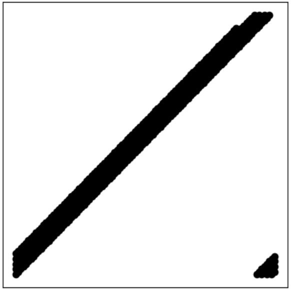
- Assume b_1 and b_2 are consecutive prime numbers used as bases for subsequent coordinates of the original Halton sequence.
- Σ^b be the vdc sequence in integer base b and $\Sigma_{p,q}$ be the vdc sequence in irrational base associated with (p, q)
- Then, for every natural number $b_1 \leqslant p < b_2$, we build $\Sigma_{p,1}$, unless p is prime when we take $\Sigma_{p,\lfloor p/2 \rfloor}$
- These sequences are subsequently inserted in order of increasing p between the base b_1 and b_2 van der Corput sequences.

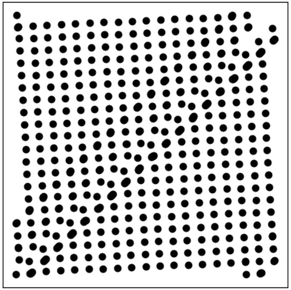
$$\text{(ex: } b_1 = 11, b_2 = 13) \qquad \Sigma^{11} \qquad \underset{\Sigma_{11,5}}{\downarrow} \qquad \underset{\Sigma_{12,1}}{\downarrow} \qquad \Sigma^{13}$$

- This is **if** the chosen parameters do not create two-dimensional projections meeting Conditions A or B.
- In the case that we are in breach of Condition A or B, we increase q until we find a

Example

Projection of the first 500 points of the 26^{th} and 27^{th} of the original Halton sequence (bases 101 and 103) and the interlaced Halton sequence (bases 19.462.. and 20.05..)





Scrambling irrational-base constructions

- Hard to scramble over elementary m-intervals in base γ because of varying interval sizes
- Instead we propose to use Owen's scrambling for each coordinate: for $\Sigma_{p,q}$, we scramble in base $p+1$, and for Σ^b in base b. Why?
- Motivation comes from dependence study of scrambled Halton sequences (Dong and Lemieux, 2022) where quantities $C_{\mathbf{b}}(\mathbf{k}; P_n)$ measures quality of a point set P_n after being scrambled in base $\mathbf{b} = (b_1, \ldots, b_s)$: small ($\leqslant 1$) values are good

Quality measure for a scrambling in base b $= (b_1, \ldots, b_s)$

Def.: Let P_n be a set of n points in $[0,1]^s$ and $b \geqslant 2$ be an integer. Define

$$C_{\mathbf{b}}(\mathbf{k}; P_n) := \frac{\prod_{j=1}^{d} b_j^{k_j} M_{\mathbf{b}}(\mathbf{k}; P_n)}{n(n-1)}$$

where $M_{\mathbf{b}}(\mathbf{k}; P_n)$ denotes the number of ordered pairs of distinct points from P_n that lie in the same elementary intervals induced by $\mathbf{k} \in \mathbb{N}_0^s$, i.e., of the form

$$\prod_{j=1}^{s} \left[\frac{a_j}{b_j^{k_j}}, \frac{a_j + 1}{b_j^{k_j}} \right),$$

Quality measure for a scrambling in base $\mathbf{b} = (b_1, \ldots, b_s)$

(From Dong and Lemieux (2022).

Def.: If $C_{\mathbf{b}}(\mathbf{k}; P_n) \leqslant 1$ for all $\mathbf{k}$ then we say P_n is completely quasi-equidistributed (c.q.e) in base $\mathbf{b} = (b_1, \ldots, b_s)$.

Prop: If P_n comes from a Halton sequence then it is c.q.e. in base $\mathbf{b} = (b_1, \ldots, b_s)$, where b_j is jth prime number

$C_2(\mathbf{k})$ values for van der Corput sequence in base golden ratio

k	1	2	3	4	5	6	7	8	9
$C_2(k; \cdot)$	0.998	0.994	0.986	0.971	0.939	0.885	0.773	0.607	0.226

Conjecture: Let γ be the largest root of the polynomial $x^2 - px - q$ for $1 \leqslant q \leqslant p$. The van der Corput sequence in base γ is c.q.e. in base $(p+1)$.

Integration results

Two test functions.

$$f_1(\mathbf{x}) = \prod_{j=1}^{s} \frac{|4x_j - 2| + a_j}{1 + a_j}$$

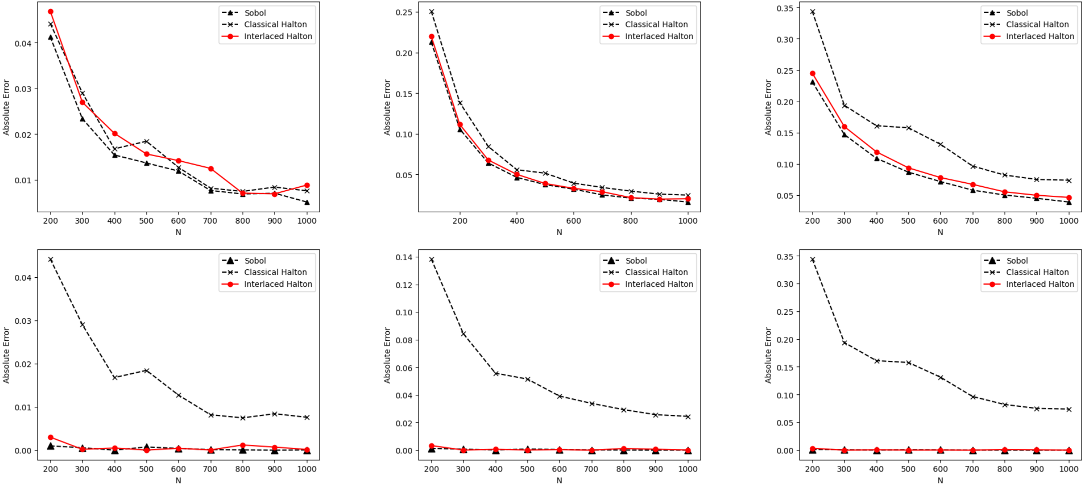
for $\mathbf{x} = (x_1, \ldots, x_d) \in [0,1]^s$ and coefficient vector $\mathbf{a} = (a_1, \ldots, a_s) \in \mathbb{R}^s$.

$$f_2(\mathbf{x}) = \prod_{j=1}^{s} 1 + c(x_j - 0.5)$$

where $c \in \mathbb{R}$.

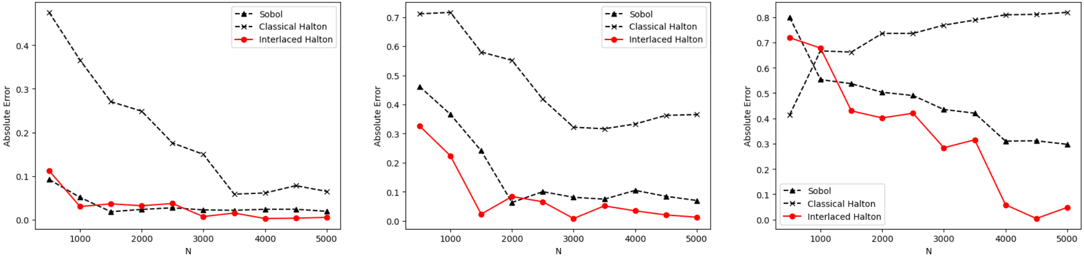
$\rightarrow$ Will compare interlaced Halton with above scrambling idea with Sobol' and original Halton (also scrambled)

Integration results with f_1



Integration error for $a_j \in \{j, j^2\}$ (top/bottom), and $s = 25, 50, 100$ (left/middle/right).

Integration results with f_2



Integration error with $c = 1$ for $s = 25, 50, 100$ (left/middle/right).

Future work

- Prove conjecture that van der Corput sequence $\Sigma_{p,q}$ is c.q.e. in base $p+1$
- Based on numerical experiments of the discrepancy of irrational based digital nets and sequences, why is a base chosen between 2 and 3 seemingly the best base for construction? What is the best base?
- Is there a better (systematic) way to choose pairs (p, q) to interlace with the Halton sequence?
- How should one construct digital nets and sequences in base φ or general base γ in more than two dimensions?