A theoretical view on transforming low-discrepancy sequences from a cube to a simplex

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Abstract

Sequences of points with a low discrepancy are the basic building blocks of quasi-Monte Carlo methods. Traditionally these points are generated in a unit cube. Not much theory exists on generating low-discrepancy point sets on other domains, for example a simplex. We introduce a variation and a star discrepancy for the simplex and derive a Koksma-Hlawka inequality for point sets on the simplex.

Keywords : Multi-dimensional integration, quasi-Monte Carlo, discrepancy, simplex, Koksma-Hlawka inequality

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Sequences of points with a low discrepancy are the basic building blocks of quasi-Monte Carlo methods. Traditionally these points are generated in a unit cube. Not much theory exists on generating low-discrepancy point sets on other domains, for example a simplex. We introduce a variation and a star discrepancy for the simplex and derive a Koksma-Hlawka inequality for point sets on the simplex.

1 Quasi-Monte Carlo on a hypercube

1.1 Introduction

Traditionally quasi-Monte Carlo (qMC) methods evaluate the integrand of a function f over the unit cube

$$I[f] := \int_{I_s} f(\mathbf{x})\mathsf{d}\mathbf{x}$$

$$I_s := \{\mathbf{x} = (x_1, \dots, x_s) : 0 \le x_i \le 1, i = 1, \dots, s\}$$

by a cubature rule of the form

$$I[f] \approx Q[f] := \frac{1}{N} \sum_{\mathbf{x}_i \in P} f(\mathbf{x}_i)$$

where P is a low-discrepancy point set in I_s. We will always interpret 'point set' in the sense of the combinatorial notion of 'multiset,' i.e., a set in which the multiplicity of elements matters. In this section we first repeat the classical definitions of discrepancy and variation and the Koksma-Hlawka theorem on the error of a qMC approximation. Several options for defining the discrepancy of a point set exist. In this article we choose the star discrepancy.

Definition 1.1. *Let Υ be the set of all hyper-rectangles containing the origin $\mathbf{o} = (0, 0, \dots, 0)$,*

$$\Upsilon := \{\prod_{i=1}^{s} [0, x_i] : x_i \in (0, 1), \}$$

then the star discrepancy can be defined as

$$D^*(P) := \sup_{U \in \Upsilon} \left| \frac{A(U)}{N} - vol(U) \right|$$

with $A(U)$ the number of points of P inside U.

Let C be a hypercube

$$C := [a_1, b_1] \times [a_2, b_2] \times \cdots \times [a_s, b_s]$$

and define the s-dimensional difference operator $\Delta(f; C)$ as

$$\Delta(f; C) := \sum_{j_1=0}^{1} \cdots \sum_{j_s=0}^{1} (-1)^{|j|} f(j_1 a_1 + (1 - j_1) b_1, \ldots, j_s a_s + (1 - j_s) b_s)$$

where $|j| = \sum_{k=1}^{s} j_k$. Then the absolute value $|\Delta(f; C)|$ can be taken as a discrete measure of the variation of f on C.

For a partition

$$\Psi := \{[x_{l_1}^{(1)}, x_{l_1+1}^{(1)}] \times \cdots \times [x_{l_s}^{(s)}, x_{l_s+1}^{(s)}] : l_k = 0, \ldots, m_k - 1, k = 1, \ldots, s\}$$

of I_s, based on s partitions

$$0 = x_0^{(k)} < x_1^{(k)} < \cdots < x_{m_k}^{(k)} = 1, \qquad k = 1, 2, \ldots, s$$

of the interval $[0, 1]$,

$$V(f; \Psi) := \sum_{C \in \Psi} |\Delta(f; C)|$$

measures the variation of f with respect to Ψ. The variation of f in the sense of Vitali is the supremum over all partitions of this variation $V(f; \Psi)$.

Definition 1.2 (Variation in the sense of Vitali). *The variation $V^{Vitali}(f)$ of a function $f : I_s \to \mathbb{R}$ in the sense of Vitali is defined by*

$$V^{Vitali}(f) := \sup_{\Psi} \left(\sum_{C \in \Psi} |\Delta(f; C)| \right) \tag{1}$$

where the supremum is extended over all partitions Ψ of I_s. If $V^{Vitali}(f)$ is finite, then f is said to be of bounded variation on I_s in the sense of Vitali.

Using the variation in the sense of Vitali, we can define the variation in the sense of Hardy and Krause.

Definition 1.3 (Variation in the sense of Hardy and Krause). *Let $V^{(k)}(f; i_1, \ldots, i_k)$ denote the k-dimensional variation in the sense of Vitali of the restriction of f to the face*

$$I_s^{i_1, \ldots, i_k} := \{\mathbf{x} = (x_1, \ldots, x_s) \in I_s : x_j = 1 \text{ for } j \notin \{i_1, \ldots, i_k\}\}$$

of I_s, then the variation $V(f)$ of a function $f : I_s \to \mathbb{R}$ in the sense of Hardy and Krause is defined by

$$V(f) := \sum_{k=1}^{s} \sum_{1 \le i_1 \le \cdots \le i_k \le s} V^{(k)}(f; i_1, \ldots, i_k).$$

If $V(f)$ is finite then f is said to be of bounded variation in the sense of Hardy and Krause.

The following classical theorem gives an upper bound for the error of the approximation.

Theorem 1.1 (Koksma-Hlawka). *For $f : I_s \to \mathbb{R}$ a function of bounded variation*

$$|I[f] - Q[f]| = \left| \int_{I_s} f(\mathbf{x}) \mathrm{d}\mathbf{x} - \sum_{\mathbf{x}_i \in P} f(\mathbf{x}_i) \right| \le D^*(P)\ V(f).$$

1.2 An alternative definition for the variation in the sense of Vitali on I_s

The definition of the variation in the sense of Vitali on a hypercube can be simplified by considering only partitions based on the same one-dimensional partition in each dimension, we will call these partitions *equipartitions*. These partitions can be written as

$$\Psi := \{[x_{l_1}, x_{l_1+1}] \times \cdots \times [x_{l_s}, x_{l_s+1}] : l_k = 0, \ldots, m-1\ ,\ k = 1, \ldots, s\}.$$

The alternative definition of the variation will be easier to generalize.

Let C be a hypercube

$$C := [a_1, b_1] \times [a_2, b_2] \times \cdots \times [a_s, b_s]$$

and let C_1 and C_2 be two hypercubes which do not overlap (the s-volume of their intersection is 0) and which have C as their union

$$C_1 := [a_1, b_1] \times [a_2, b_2] \times \cdots \times [a_i, c] \times \cdots \times [a_s, b_s]$$

$$C_2 := [a_1, b_1] \times [a_2, b_2] \times \cdots \times [c, b_i] \times \cdots \times [a_s, b_s]$$

with $c \in (a_i, b_i)$. We say that C_1 and C_2 are a *refinement* of C. To reduce the weight on the notation we assume, without loss of generality, that $i = 1$, i.e.,

$$C_1 := [a_1, c] \times [a_2, b_2] \times \cdots \times [a_s, b_s] \text{ and } C_2 := [c, b_1] \times [a_2, b_2] \times \cdots \times [a_s, b_s].$$

Then, for any $f : I_s \to \mathbb{R}^s$

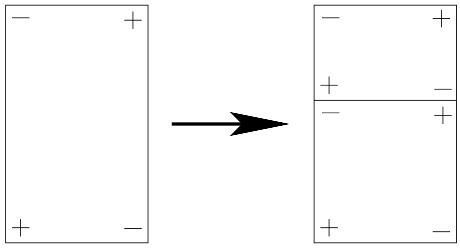
$$\begin{aligned}
|\Delta(f;C)| &= \left| \sum_{j_1=0}^{1} \cdots \sum_{j_s=0}^{1} (-1)^{|j|} f(j_1a_1 + (1-j_1)b_1,\ j_2a_2 + (1-j_2)b_2,\ \ldots,\ j_sa_s + (1-j_s)b_s) \right| \\
&= \left| \sum_{j_1=0}^{1} \cdots \sum_{j_s=0}^{1} (-1)^{|j|} f(j_1a_1 + (1-j_1)c,\ j_2a_2 + (1-j_2)b_2,\ \ldots,\ j_sa_s + (1-j_s)b_s) \right. \\
&+ \left. \sum_{j_1=0}^{1} \cdots \sum_{j_s=0}^{1} (-1)^{|j|} f(j_1c + (1-j_1)b_1,\ j_2a_2 + (1-j_2)b_2,\ \ldots,\ j_sa_s + (1-j_s)b_s) \right| \\
&\leq \left| \sum_{j_1=0}^{1} \cdots \sum_{j_s=0}^{1} (-1)^{|j|} f(j_1a_1 + (1-j_1)c,\ j_2a_2 + (1-j_2)b_2,\ \ldots,\ j_sa_s + (1-j_s)b_s) \right| \\
&+ \left| \sum_{j_1=0}^{1} \cdots \sum_{j_s=0}^{1} (-1)^{|j|} f(j_1c + (1-j_1)b_1,\ j_2a_2 + (1-j_2)b_2,\ \ldots,\ j_sa_s + (1-j_s)b_s) \right| \\
&= |\Delta(f;C_1)| + |\Delta(f;C_2)|.
\end{aligned}$$

This is illustrated in Fig.1. Thus, if partition Ψ' is a *refinement* of Ψ, then

$$V(f;\Psi) \leq V(f;\Psi').$$

For every partition of I_s there exists a refinement which is an equipartition. Choose for example the union of all partitions of the separate dimensions as base partition in all dimensions. Therefore, since the variation is a supremum, instead of using all possible partitions in (1), we can restrict this to equipartitions.

Figure 1: A refinement of C in two dimensions



Definition 1.4 (Alternative definition of the variation in the sense of Vitali). *The variation $V^{Vitali}(f)$ of a function $f : I_s \to \mathbb{R}$ in the sense of Vitali is defined by*

$$V^{Vitali}(f) := \sup_{\Psi} \left(\sum_{C \in \Psi} |\Delta(f; C)| \right)$$

where the supremum is extended over all equipartitions Ψ of I_s. If $V(f)$ is finite, then f is said to be of bounded variation on I_s in the sense of Vitali.

2 Quasi-Monte Carlo on a simplex

The focus of this text is the development of a qMC method to integrate over a simplex. We consider an integral of the form

$$I[f] = \int_{T_s} f(\mathbf{x}) \mathsf{d}\mathbf{x} \tag{2}$$

where

$$T_s := \{(x_1, \dots, x_s) \in \mathbb{R}^s : 0 \le x_1 \le x_2 \le \dots \le x_s \le 1\}.$$

For three dimensions, T_3 is illustrated in Fig. 2. The integral (2) can also be written as:

$$I[f] = \int_0^1 \int_{x_1}^1 \dots \int_{x_{s-1}}^1 f(\mathbf{x}) \mathsf{d}x_s \dots \mathsf{d}x_1.$$

We consider a numerical approximation for this integral of the form

$$\begin{aligned} I[f] \approx Q[f] \quad &:= \quad \frac{vol(T_s)}{N} \sum_{\mathbf{x}_i \in P} f(\mathbf{x}_i) \\ &= \quad \frac{1}{s!\; N} \sum_{\mathbf{x}_i \in P} f(\mathbf{x}_i) \end{aligned}$$

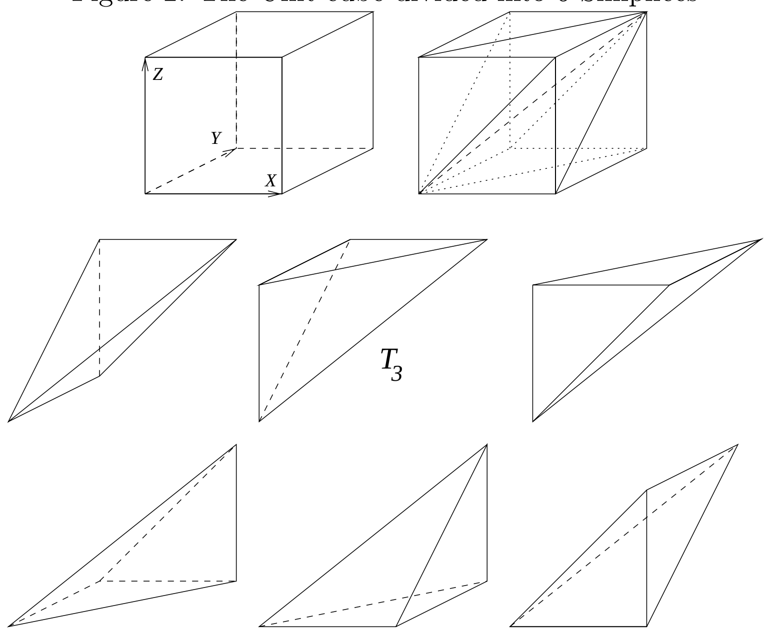
where P is a point set of N points in T_s.

For all possible s-dimensional permutations $(x_{i_1}, \dots, x_{i_s})$ of $(x_1, \dots, x_s)$ we define

$$S_i := \{(x_1, \dots, x_s) \in I_s | x_{i_1} \le \dots \le x_{i_s}\}.$$

Each of these simplices is equal to the original simplex T_s after a rotation. Observe that these simplices do not overlap (the s-dimensional volume of their conjunctions is 0) and their union is equal to the unit cube (see Fig. 2). Our aim is to prove a Koksma-Hlawka inequality on a simplex. Therefore, we need to define a (star) discrepancy and a variation on a simplex.

Figure 2: The Unit cube divided into 6 Simplices



3 A variation on the simplex

The simplex T_s cannot be divided into a finite collection of hypercubes. There will always be some uncovered space left along the 'diagonals'. Therefore the variation on a hypercube must be adjusted before we can generalize it to a simplex. In the first part of this section, we prove several properties of equipartitions of a simplex. These properties are then used to define a variation in the sense of Vitali and Hardy and Krause.

3.1 Exploring the equipartition of a simplex

To define a variation in the sense of Vitali on T_s we first need to prove some properties.

Lemma 3.1. *Let Ψ be an equipartition of I_s, then for every $C \in \Psi$ and for every edge of C, there exists an S_i such that the edge is entirely part of S_i, $i = 1, \dots, s!$.*

When we denote $R(C) := \{r | r \text{ is an edge of } C\}$, then we can write this Lemma as:

$$\forall C \in \Psi, \forall r \in R(C), \exists S_i : r \subset S_i.$$

Proof. The equipartition Ψ can be written as

$$\Psi := \{[x_{l_1}, x_{l_1+1}] \times \cdots \times [x_{l_s}, x_{l_s+1}] : l_k = 0, \dots, m-1 \ , \ k = 1, \dots, s\}$$

where

$$0 = x_0 < x_1 < \cdots < x_m = 1$$

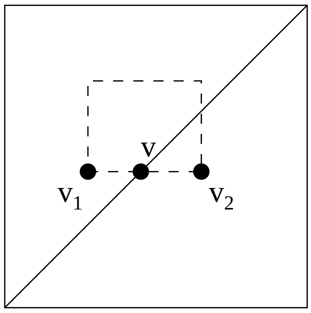
is a partition of the interval $[0, 1]$. Thus, if $C \in \Psi$, then C can be written as

$$C = [x_{l_1}, x_{l_1+1}] \times \cdots \times [x_{l_s}, x_{l_s+1}]$$

and an edge r of C can be written as

$$r = [\mathbf{v}_1, \mathbf{v}_2] = [(x_{l_1}, \dots, x_{l_{i-1}}, x_{l_i}, x_{l_{i+1}}, \dots, x_{l_s}), (x_{l_1}, \dots, x_{l_{i-1}}, x_{l_i+1}, x_{l_{i+1}}, \dots, x_{l_s})]$$

Figure 3: If there is no S_i such that $r \subset S_i$



where $\mathbf{v}_1$ and $\mathbf{v}_2$ are the two vertices the edge connects. Without loss of generality we can assume $i = 1$ to simplify the notation:

$$r = [\mathbf{v}_1, \mathbf{v}_2] = [(x_{l_1}, x_{l_2}, \ldots, x_{l_s}), (x_{l_1+1}, x_{l_2}, \ldots, x_{l_s})].$$

Suppose that there is no S_i such that $r \subset S_i$. Then there exists a point $\mathbf{v}$ on the open edge $(\mathbf{v}_1, \mathbf{v}_2)$ and a simplex S_i such that

$$[\mathbf{v}_1, \mathbf{v}] \subset S_i; \ ; \text{ and } \ (\mathbf{v}, \mathbf{v}_2] \subset I_s \setminus S_i.$$

This is illustrated in Fig. 3.

Without loss of generality we choose S_i equal to T_s. The following reasoning is equivalent for $S_i \neq T_s$ but imposes less stress on the notation. Now, denote

$$\mathbf{v} := (c, x_{l_2}, \ldots, x_{l_s}).$$

Since $\mathbf{v} \in (\mathbf{v}_1, \mathbf{v}_2)$, it follows that

$$x_{l_1} < c < x_{l_1+1}. \tag{3}$$

And since $\mathbf{v}_1$ and $\mathbf{v}$ are elements of T_s, we can deduce that

$$x_{l_1} < c < x_{l_2} \leq \cdots \leq x_{l_s}. \tag{4}$$

We also know that for all strictly positive ϵ with $\epsilon < x_{l_1+1} - c$

$$\mathbf{v}' = (c + \epsilon, x_{l_2}, \ldots, x_{l_s}) \notin T_s$$

and thus

$$c + \epsilon \leq x_{l_2} \leq \cdots \leq x_{l_s}$$

cannot be true. One of these inequalities must be false and since

$$x_{l_2} \leq \cdots \leq x_{l_s},$$

it must hold that

$$c + \epsilon > x_{l_2}$$

for all strictly positive ϵ with $\epsilon < x_{l_1+1} - c$. Thus, together with $c \leq x_{l_2}$ from (4), we find that

$$c = x_{l_2}.$$

But then from (3) it follows that

$$x_{l_1} < x_{l_2} < x_{l_1+1}$$

and this cannot be true because x_{l_1} and x_{l_1+1} are two successive points from

$$0 = x_0 < x_1 < \cdots < x_m = 1$$

and therefore x_{l_2} cannot be strictly in between x_{l_1} and x_{l_1+1}. This means that the assumption that there exists a $C \in \Psi$ with an edge that is not entirely part of one simplex S_i is false and thus the Lemma is proven. $\square$

From here on we denote the s-dimensional volume by vol_s.

Lemma 3.2. *Let S_i be a permutation of T_s and let Ψ be an equipartition of I_s. Let*

$$\begin{aligned} C &= [\mathbf{a}, \mathbf{b}] \\ &= [a_1, b_1] \times \cdots \times [a_s, b_s] \\ &= [x_{l_1}, x_{l_1+1}] \times \cdots \times [x_{l_s}, x_{l_s+1}] \end{aligned}$$

be an element of equipartition Ψ.Then it follows that if $vol_s(S_i \cap C) \neq 0$ then $\mathbf{a} \in S_i$ and $\mathbf{b} \in S_i$.

Proof. If $vol_s(S_i \cap C) \neq 0$, then there exists a $\mathbf{p} = (p_1, \ldots, p_s) \in S_i$ such that $x_{l_i} < p_i < x_{l_i+1}$. We prove that a permutation which sorts $(p_1, \ldots, p_s)$ also sorts $(a_1, \ldots, a_s)$, thereby proving the Lemma, because this means that $\mathbf{p}$ and $\mathbf{a}$ both belong to S_i.

Suppose for i and $j \in \{0, 1, \ldots, m\}$ that $p_i \leq p_j$. We also know that $x_{l_i} < p_i < x_{l_i+1}$ and $x_{l_j} < p_j < x_{l_j+1}$. Since $p_i \leq p_j$, it follows that $x_{l_j+1} > x_{l_i}$ and thus there are two possibilities, namely $x_{l_i} = x_{l_j}$ or $x_{l_i+1} \leq x_{l_j}$. If $x_{l_i} = x_{l_j}$, then also $x_{l_i+1} = x_{l_j+1}$. And if $x_{l_i+1} \leq x_{l_j}$ then

$$x_{l_i} < x_{l_i+1} \leq x_{l_j} < x_{l_j+1}$$

and thus $x_{l_i} < x_{l_j}$ and $x_{l_i+1} < x_{l_j+1}$. Thus in both cases it follows that

$$a_i = x_{l_i} \leq x_{l_j} = a_j \text{ and } b_i = x_{l_i+1} \leq x_{l_j+1} = b_j.$$

Therefore a permutation that sorts $(p_1, \ldots, p_s)$, also sort $(a_1, \ldots, a_s)$ and $(b_1, \ldots, b_s)$. $\square$

The following Lemma proves that the reverse of Lemma 3.2 is also true.

Lemma 3.3. *Let S_i be a permutation of T_s. Let Ψ be an equipartition. Let*

$$\begin{aligned} C &= [\mathbf{a}, \mathbf{b}] \\ &= [a_1, b_1] \times \cdots \times [a_s, b_s] \\ &= [x_{l_1}, x_{l_1+1}] \times \cdots \times [x_{l_s}, x_{l_s+1}] \end{aligned}$$

be an element of equipartition Ψ.Then it follows that if $\mathbf{a} \in S_i$ and $\mathbf{b} \in S_i$ then $vol_s(S_i \cap C) \neq 0$.

Proof. We prove this only for $S_i = T_s$ to simplify the notation. Suppose that $\mathbf{a}$ and $\mathbf{b}$ are both elements of T_s. Let $c = \max_{i=1}^{s} |a_i - b_i|$. Then the simplex with vertices

$$\begin{array}{c} (a_1, a_2, a_3, \ldots, a_s) \\ (b_1, a_2, a_3, \ldots, a_s) \\ (b_1, b_2, a_3, \ldots, a_s) \\ \vdots \\ (b_1, b_2, b_3, \ldots, b_s) \end{array}$$

belongs to C and to S_i. Furthermore, because $c \neq 0$ the volume of this simplex is not zero. $\square$

3.2 Variation in the sense of Vitali on T_s

Now we can define the variation in the sense of Vitali on T_s. Let Ψ be a equipartition of I_s. Let C be an element of Ψ

$$C := [a_1, b_1] \times [a_2, b_2] \times \cdots \times [a_s, b_s].$$

Define $\Delta_\triangle(f; C)$ on T_s as follows:

- If $C \subset T_s$ then $\Delta_\triangle(f; C) := \Delta(f; C)$.
- If $vol_s(T_s \cap C) = 0$ then $\Delta_\triangle(f; C) := 0$.
- Otherwise, $\mathbf{a} = (a_1, \ldots, a_s)$ and $\mathbf{b} = (b_1, \ldots, b_s)$ are both part of a face of at least k simplices S_i, with $k > 1$. In this case, we define

  $$\Delta_\triangle(f; C) := \sum_{\text{all vertices } \mathbf{v} \text{ of C}} \prod_{i=1}^{s} \delta(v_i, a_i) f(\mathbf{v}) / \eta_C(\mathbf{v})$$

  where $\eta_C(\mathbf{v}) := \#\{S_k | \mathbf{v} \in S_k \wedge \mathbf{a}_C \in S_k, k = 1, \ldots, s!\}$.

Define the variation $V_\triangle(f; \Psi)$ of f on T_s with respect to Ψ as

$$V_\triangle(f; \Psi) := \sum_{C \in \Psi} |\Delta_\triangle(f; C)|.$$

We are now ready to define the variation $V_\triangle^{Vitali}(f)$ of f on T_s.

Definition 3.1 (Variation in the sense of Vitali on T_s). *The variation $V_\triangle^{Vitali}(f)$ of a function $f : T_s \to \mathbb{R}$ in the sense of Vitali is defined by*

$$V_\triangle^{Vitali}(f) := \sup_{\Psi} \left(\sum_{C \in \Psi} |\Delta_\triangle(f; C)| \right)$$

where the supremum is extended over all equipartitions Ψ of I_s. If $V_\triangle^{Vitali}(f)$ is finite, f is said to be of bounded variation on T_s in the sense of Vitali.

In two dimensions this definition can be easily explained intuitively. There are two possibilities for C, it is either completely inside one of the simplices $S_1 = T_2$ or S_2 or it is part of both. When it is part of one of the two simplices, the variation on C is calculated as usual for cubes. Otherwise, when C is neither completely inside S_1 nor S_2 then $\mathbf{a}$ and $\mathbf{b}$ must both be on the diagonal (because the diagonal is equal to $S_1 \cap S_2$) and thus C is a square as in Fig. 4. If we put the $+$ and $-$ signs, coming from $|j|$ in this figure, we can see that $C \cap S_1$ and $C \cap S_2$ have one positive and two negative contributions to $\Delta_\triangle(f; C)$ and therefore it seems logical to compare the positive with the average of the negatives. Another reason to divide the negatives by two is that they contribute twice to the variation (once for S_1 and once for S_2). In the next paragraph, we give another motivation for this definition.

3.3 Variation in the sense of Hardy and Krause on T_s

The variation in the Sense of Hardy and Krause on the hypercube I_s can now be generalized to T_s.

Definition 3.2. *Let $V_\triangle^{(k)}(f)$ denote the k-dimensional variation in the sense of Vitali of the restriction of f to the face*

$$T_s^{(k)} := \{\mathbf{x} = (x_1, \ldots, x_s) \in T_s : x_j = 1 \text{ for } j = k+1, \ldots, s\}$$

Figure 4: Why divide by η ?

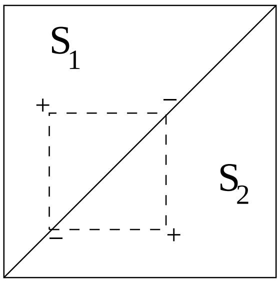
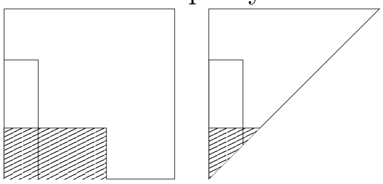


Figure 5: Star Discrepancy on the Simplex



of T_s, then the variation $V_\triangle(f)$ of a function $f : T_s \to \mathbb{R}$ in the sense of Hardy and Krause is defined by

$$V_\triangle(f) := \sum_{k=1}^{s} \frac{1}{(s-k)!} V_\triangle^{(k)}(f).$$

If $V_\triangle(f)$ is finite then f is said to be of bounded variation in the sense of Hardy and Krause.

4 Discrepancy on a simplex

In this section we generalize the definition of the star discrepancy on the hypercube to a star discrepancy on the simplex.

Definition 4.1 (Star Discrepancy on the Simplex). *Let Υ be the set of all hyper-rectangles in I_s containing the origin $\mathbf{o} = (0, 0, \ldots, 0)$*

$$\Upsilon := \left\{ \prod_{i=1}^{s} [0, x_i] : x_i \in (0, 1) \right\}$$

then the star discrepancy on the simplex can be defined as

$$D_\triangle^*(P) := \sup_{U \in \Upsilon} \left| \frac{A(U \cap T_s)}{N} - \frac{vol_s(U \cap T_s)}{vol_s(T_s)} \right|$$

with $A(U)$ the number of points of P inside U.

This definition is very intuitive and is a logical generalization of Definition 1.1. It is the same as the star discrepancy on the hypercube except that for every element U of Υ, we only take the volume of the intersection of U and the simplex T_s (see also Fig. 5). We also need to divide this volume by the volume of the simplex, $vol_s(T_s)$, so that both $\frac{A(U \cap T_s)}{N}$ and $\frac{vol_s(U \cap T_s)}{vol_s(T_s)}$ are between 0 and 1.

5 Koksma-Hlawka inequalities

With the variation in the sense of Hardy and Krause as defined in the previous section, we can derive a Koksma-Hlawka inequality on the simplex. First, we derive a Koksma-Hlawka inequality in a specialized case. Afterwards we generalize this result to obtain a Koksma-Hlawka inequality on a simplex.

5.1 Koksma-Hlawka for transformation *Sort*

Before deriving a general Koksma-Hlawka inequality, we first derive a specific Koksma-Hlawka inequality for point sequences obtained by applying a specific transformation, *Sort*, to point sequences on a cube.

5.1.1 Transformation *Sort*

In [6], we described several transformations amongst which transformation *Sort*. $Sort\colon I_s \to T_s$ transforms point sequences from the hypercube to the simplex by sorting the coordinates of each point such that the coordinates of the lower dimension of each transformed point are smaller than those of the higher dimensions.

$$Sort(P) := \{Sort(x_1, \dots, x_s) : (x_1, \dots, x_s) \in P\}$$

In [6] we proved the following inequality for this transformation.

Lemma 5.1. *Let f be a function on T_s and denote $g = f \ o \ Sort$ then*

$$\left| \int_{T_s} f(\mathbf{x}) \mathsf{d}\mathbf{x} - \frac{1}{s! \ N} \sum_{\mathbf{x}_i \in Sort(P)} f(\mathbf{x}_i) \right| \leq \ D^*(P) \ \frac{V(g)}{s!}$$

where $D^*(P)$ is the discrepancy on I_s of the original point set (before transformation) and $V(g)$ is the variation of g on I_s.

In this section we will replace $\frac{V(g)}{s!}$ with $V_\triangle(f)$, the variation of f on T_s.

5.1.2 Notation

To make this section easier to read, we introduce the following notation:

- Denote with $perm_k$ the permutation which transforms S_1 into S_k.
- Denote with $perm_{kl}$ the permutation $perm_l \ o \ perm_k^{-1}$ which transforms S_k into S_l.
- Denote with $C_{\mathbf{ab}}$ an element of equipartition Ψ with vertices $\mathbf{a}$ and $\mathbf{b}$ such that $a_i < b_i$ for $i = 1, \dots, s$.
- Denote $g = f \ o \ Sort$.
- Let g_k be the restriction of g to S_k, thus $g_k(x) := g(x)$ if $x \in S_k$ and $g_k(x) := 0$ elsewhere.
- Denote by $\sum_{\mathbf{v}(C)}$ the sum over all vertices $\mathbf{v}$ of C.
- Define $\mathbf{a}_C$ the vertex of C that lies closest to the origin o.

5.1.3 Variation in the new notation

Using the newly introduced notation, the variation in the sense of Vitali on a simplex can be written as follows:

$$\Delta_{\triangle}(g;C) = \sum_{\mathbf{v}(C)} \frac{g_1(\mathbf{v})}{\eta_C(\mathbf{v})} \prod_{i=1}^{s} \delta(v_i, (\mathbf{a}_C)_i)$$

$$V_{\triangle}^{Vitali}(g) = \sup_{\Psi} \sum_{C \in \Psi} |\Delta_{\triangle}(g;C)|$$

We can generalize this definition to all simplices S_k:

$$\Delta_{\triangle}(g;C;S_k) = \sum_{\mathbf{v}(C)} \frac{g_k(\mathbf{v})}{\eta_C(\mathbf{v})} \prod_{i=1}^{s} \delta(v_i, (\mathbf{a}_C)_i)$$

$$V_{\triangle}^{Vitali}(g;S_k) = \sup_{\Psi} \sum_{C \in \Psi} |\Delta_{\triangle}(g;C)|$$

5.1.4 Permutations and simplices

First, we prove some properties which will be used during the proof in the following paragraph.

Property 5.1. *If $\mathbf{x} \in S_k$ and $\mathbf{x} \in S_l$ then $perm_{kl}(\mathbf{x}) = \mathbf{x}$.*

Proof. From $\mathbf{x} \in S_l$ we can deduce that $perm_l^{-1}(\mathbf{x}) = Sort(\mathbf{x})$ and thus that

$$\mathbf{x} = perm_l(Sort(\mathbf{x})).$$

But we also know that $\mathbf{x} \in S_k$ and thus $perm_{kl}(\mathbf{x}) \in S_l$ which leads to

$$\begin{aligned} perm_{kl}(\mathbf{x}) &= perm_l(Sort(perm_{kl}(\mathbf{x}))) \\ &= perm_l(Sort(\mathbf{x})) = \mathbf{x}. \end{aligned}$$

□

Property 5.2. *Suppose $\{\mathbf{a}, \mathbf{b}\} \in S_k \cap S_l$ and $\mathbf{v}$ a vertex of $C_{\mathbf{ab}}$, then*

$$\mathbf{v} \in (C_{\mathbf{ab}} \cap S_k) \Leftrightarrow perm_{kl}(\mathbf{v}) \in (C_{\mathbf{ab}} \cap S_l)$$

and

$$\prod \delta(v_i, a_i) = \prod \delta(perm_{kl}(\mathbf{v})_i, a_i).$$

Proof. This follows immediately from $perm_{kl}(\mathbf{a}) = \mathbf{a}$.

□

Property 5.3. $perm_k(C_{\mathbf{ab}}) = C_{perm_k(\mathbf{a}), perm_k(\mathbf{b})}$

Proof. Since

$$a_i < b_i \ , \ i = 1, \ldots, s$$

it obviously follows that

$$perm_k(\mathbf{a})_i < perm_k(\mathbf{b})_i \ , \ i = 1, \ldots, s.$$

□

Property 5.4. $\eta_C(\mathbf{v}) = \eta_{perm_l(C)}(perm_l(\mathbf{v}))$

Proof. From Property 5.3 follows that $\mathbf{a}_{perm_l(C)} = perm_l(\mathbf{a}_C)$, which leads to

$$\eta_{perm_l(C)}(perm_l(\mathbf{v})) = \#\{S_k|perm_l(\mathbf{a}_C) \in S_k \wedge perm_l(\mathbf{v}) \in S_k\}.$$

Denote by

$$\{S_{k_1}, \ldots, S_{k_{\eta_C(\mathbf{v})}}\} := \{S_k|\mathbf{a} \in S_k \wedge \mathbf{v} \in S_k\},$$

then

$$\{perm_l(S_{k_1}), \ldots, perm_l(S_{k_{\eta_C(\mathbf{v})}})\} \subset \{S_k|perm_l(\mathbf{a}) \in S_k \wedge perm_l(\mathbf{v}) \in S_k\}$$

and, because $perm_l$ is a one-to-one mapping of the collection of all simplices $S_k \subset I_s$, we may conclude that $\eta_C(\mathbf{v}) \leq \eta_{perm_l(C)}(perm_l(\mathbf{v}))$.

The same reasoning with $(perm_l)^{-1}$ leads to $\eta_{perm_l(C)}(perm_l(\mathbf{v})) \leq \eta_C(\mathbf{v})$. Combining both inequalities leads to the desired result. □

Property 5.5. *$g(perm_k(\mathbf{v})) = g(\mathbf{v})$ and $g_k(\mathbf{v}) = g_l(perm_{kl}(\mathbf{v}))$*

Proof. This follows immediately from $g = f \ o \ Sort$ and $v \in S_k \Leftrightarrow perm_{kl}(\mathbf{v}) \in S_l$. □

5.1.5 A formula for the variation on a simplex

With the properties given above, we can deduce that

Lemma 5.2. *For every hyper-rectangle C belonging to an equipartition Ψ,*

$$\Delta_\triangle(g; C; S_k) = \Delta_\triangle(g; perm_{kl}(C); S_l). \tag{5}$$

Proof. By first using Properties 5.4 and 5.5 and then applying Property 5.3, we get

$$\begin{aligned}
\Delta_\triangle(g; C; S_k) &= \sum_{\mathbf{v}(C)} \frac{g_k(\mathbf{v})}{\eta_C(\mathbf{v})} \prod_{i=1}^{s} \delta(v_i, (\mathbf{a}_C)_i) \\
&= \sum_{\mathbf{v}(C)} \frac{g_l(perm_{kl}(\mathbf{v}))}{\eta_{perm_{kl}(C)}(perm_{kl}(\mathbf{v}))} \prod_{i=1}^{s} \delta(perm_{kl}(\mathbf{v})_i, (perm_{kl}(\mathbf{a}_C))_i) \\
&= \sum_{\mathbf{v}(C)} \frac{g_l(perm_{kl}(\mathbf{v}))}{\eta_{perm_{kl}(C)}(perm_{kl}(\mathbf{v}))} \prod_{i=1}^{s} \delta(perm_{kl}(\mathbf{v})_i, ((\mathbf{a}_{perm_{kl}(C)})_i) \\
&= \sum_{\mathbf{v}(perm_{kl}(C))} \frac{g_l(\mathbf{v})}{\eta_C(\mathbf{v})} \prod_{i=1}^{s} \delta(\mathbf{v}_i, (\mathbf{a}_C)_i) \\
&= \Delta_\triangle(g; perm_{kl}(C); S_l)
\end{aligned}$$

□

If $vol_s(C \cap S_k) \neq 0$ and $vol_s(C \cap S_l) \neq 0$ than, by Property 5.1 and Lemma 3.2, $perm_{kl}(C) = C$ and

$$\Delta_\triangle(g; C; S_k) = \Delta_\triangle(g; C; S_l). \tag{6}$$

From the previous we can prove that

Lemma 5.3.

$$\sum_{S_k} \Delta_\triangle(g; C; S_k) = \Delta(g; C)$$

Proof.

$$\begin{aligned}
\sum_{S_k} \Delta_{\triangle}(g;C;S_k) &= \sum_{S_k, vol_s(S_k \cap C) \neq 0} \Delta_{\triangle}(g;C;S_k) \\
&= \sum_{S_k, vol_s(S_k \cap C) \neq 0} \sum_{\mathbf{v}(C)} \frac{g_k(\mathbf{v})}{\eta_C(\mathbf{v})} \prod_{i=1}^{s} \delta(v_i, (\mathbf{a}_C)_i) \\
&= \sum_{S_k, vol_s(S_k \cap C) \neq 0} \sum_{\mathbf{v}(C)} \frac{g(\mathbf{v})}{\eta_C(\mathbf{v})} \prod_{i=1}^{s} \delta(v_i, (\mathbf{a}_C)_i) \\
&= \sum_{\mathbf{v}(C)} \frac{\eta_C(\mathbf{v}) g(\mathbf{v})}{\eta_C(\mathbf{v})} \prod_{i=1}^{s} \delta(v_i, (\mathbf{a}_C)_i) \\
&= \sum_{\mathbf{v}(C)} g(\mathbf{v}) \prod_{i=1}^{s} \delta(v_i, (\mathbf{a}_C)_i) \\
&= \Delta(g;C)
\end{aligned}$$

□

This lemma is valid for every cube $C \subset I_s$ and can be generalized to every equipartition Ψ. From (6) we can conclude that for every C, all non-zero $\Delta_{\triangle}(g;C;S_k)$ have the same sign and therefore

$$\begin{aligned}
\sum_{S_k} V_{\triangle}^{Vitali}(g;\Psi;S_k) &= \sum_{S_k} \sum_{C \in \Psi} |\Delta_{\triangle}(g;C;S_k)| \\
&= \sum_{C \in \Psi} \left| \sum_{S_k} \Delta_{\triangle}(g;C;S_k) \right| \\
&= \sum_{C \in \Psi} |\Delta(g;C)| \\
&= V^{Vitali}(g;\Psi).
\end{aligned}$$

Since Ψ is based on the same partition in every dimension, $perm_k(\Psi) = \Psi$. We can therefore deduce that

$$V_{\triangle}^{Vitali}(g;\Psi;T_s) = V_{\triangle}^{Vitali}(perm_k(g); perm_k(\Psi); perm_k(T_s)) = V_{\triangle}^{Vitali}(g;\Psi;S_k),$$

for every $k \in 1, \ldots, s!$. Combining the last two equalities leads to

$$\begin{aligned}
V^{Vitali}(g;\Psi) &= \sum_{S_k} V_{\triangle}^{Vitali}(g;\Psi;S_k) = \sum_{S_k} V_{\triangle}^{Vitali}(g;\Psi;T_s) \\
&= s!\ V_{\triangle}^{Vitali}(g;\Psi;T_s).
\end{aligned}$$

And since this is valid for every equipartition Ψ, it is also valid for the supremum over all equipartitions Ψ. We may conclude that for $g = f \ o \ Sort$

$$s!\ V_{\triangle}^{Vitali}(f) = s!\ V_{\triangle}^{Vitali}(g;T_s) = V^{Vitali}(g).$$

Thereby proving

Lemma 5.4. *Let f be a function on T_s and denote $g := f \ o \ Sort$. Then*

f is of bounded variation in the sense of Vitali on T_s

$$\Longleftrightarrow$$

g is of bounded variation in the sense of Vitali on I_s

and if both are of bounded variation then

$$V_{\triangle}^{Vitali}(f) = \frac{V^{Vitali}(g)}{s!}$$

5.1.6 Variation of a sorted function

Next, we will prove that

Lemma 5.5. *Let f be a function on T_s and denote $g := f$ o Sort. Then*

$$f \text{ is of bounded variation in the sense of Hardy and Krause on } T_s$$
$$\Longleftrightarrow$$
$$g \text{ is of bounded variation in the sense of Hardy and Krause on } I_s$$

and if both are of bounded variation then

$$V_{\triangle}(f) = \frac{V(g)}{s!}.$$

Proof. Let $f : T_s \to \mathbb{R}$ and $g = f$ *o Sort*. We prove this lemma in four steps:

1. $V^{(k)}(g; i_1, \ldots, i_k) = V^{(k)}(g; 1, \ldots, k)$.
   Since $g = f$ *o Sort* and $I_s^{i_1,\ldots,i_k}$ is a permutation of $I_s^{1,\ldots,k}$, $V^{(k)}(g; i_1, \ldots, i_k)$ calculates the variation in the sense of Vitali of a permutated function over the permutated domain.
2. $V_{\triangle}^{(k)}(f) = \frac{1}{k!} V^{(k)}(g; 1, \ldots, k)$.
   $V_{\triangle}^{(k)}(f)$ is the variation in the sense of Vitali over the k-dimensional simplex T_k of the function $f(x_1, \ldots, x_k, 1, 1, 1, \ldots) : T_k \to \mathbb{R}$ and $V^{(k)}(g; 1, \ldots, k)$ is the variation in the sense of Vitali over the k-dimensional unit cube I_k of the function $g(x_1, \ldots, x_k, 1, 1, 1, \ldots) : I_k \to \mathbb{R}$ and $g(x_1, \ldots, x_k, 1, 1, 1, \ldots) = f(x_1, \ldots, x_k, 1, 1, 1, \ldots)$ *o Sort*. And thus the result can be deducted from Lemma 5.4.
3. $V_{\triangle}^{(k)}(f) = \frac{(s-k)!}{s!} \sum_{1 \le i_1 \le \cdots \le i_k \le s} V^{(k)}(g; i_1, \ldots, i_k)$.

$$\begin{aligned}
\sum_{1 \le i_1 \le \cdots \le i_k \le s} V^{(k)}(g; i_1, \ldots, i_k) &= \sum_{1 \le i_1 \le \cdots \le i_k \le s} V^{(k)}(g; 1, \ldots, k) \\
&= \binom{s}{k} V^{(k)}(g; 1, \ldots, k) \\
&= \binom{s}{k} k! V_{\triangle}^{(k)}(f) \\
&= \frac{s!}{(s-k)!} V_{\triangle}^{(k)}(f)
\end{aligned}$$

4. $V_{\triangle}(f) = \frac{V(g)}{s!}$

$$\begin{aligned}
V_{\triangle}(f) &= \sum_{k=1}^{s} \frac{1}{(s-k)!} V_{\triangle}^{(k)}(f) \\
&= \sum_{k=1}^{s} \frac{1}{(s-k)!} \frac{(s-k)!}{s!} \sum_{1 \le i_1 \le \cdots \le i_k \le s} V^{(k)}(g; i_1, \ldots, i_k) \\
&= \frac{1}{s!} \sum_{k=1}^{s} \sum_{1 \le i_1 \le \cdots \le i_k \le s} V^{(k)}(g; i_1, \ldots, i_k) \\
&= \frac{V(g)}{s!}
\end{aligned}$$

□

5.1.7 Conclusion

Using Lemma 5.5 and 5.1 we can conclude that for transformation *Sort*:

$$\left| \int_{T_s} f(\mathbf{x}) \mathrm{d}\mathbf{x} - \frac{1}{s!\ N} \sum_{\mathbf{x}_i \in Sort(P)} f(\mathbf{x}_i) \right| \leq D^*(P)\ V_{\triangle}(f) \tag{7}$$

where $V(f)$ is the variation of the function f on T_s as defined in Definition 3.2 and $D^*(P)$ is the discrepancy on I_s of the original point set before transformation.

5.2 Koksma-Hlawka with simplex discrepancy

With the star discrepancy and the variation on the simplex (Definition 4.1 and 3.2), we can derive a Koksma-Hlawka inequality. To do so, we need the following result:

Lemma 5.6. *For a point set $P \in T_s$, denote $Sort^{-1}(P) := \bigcup_{i=1}^{s!} \{perm_i(P)\}$. Then*

$$D^*_{\triangle}(P) \geq D^*(Sort^{-1}(P)). \tag{8}$$

Observe that, just as P, $Sort^{-1}(P)$ is a point set and thus may include the same point more than once.

Proof. Let $A_P(U) := \#(P \cap U)$ for any point set P and any $U \in \Upsilon$.

Since $\#Sort^{-1}(P) = s!\#P$ it holds that for every $U \in \Upsilon$

$$\begin{aligned}
D^*(Sort^{-1}(P))(U) &= \left| \frac{A_{Sort^{-1}(P)}(U)}{s!\ N} - vol_s(U) \right| \\
&= \left| \sum_{S_i} \left(\frac{A_{perm_i(P)}(U)}{s!\ N} - vol_s(U \cap S_i) \right) \right| \\
&= \left| \sum_{S_i} \left(\frac{A_{perm_i(P)}(U \cap S_i)}{s!\ N} - vol_s(U \cap S_i) \right) \right| \\
&\leq \sum_{S_i} \left| \frac{A_{perm_i(P)}(U \cap S_i)}{s!\ N} - vol_s(U \cap S_i) \right| \\
&= \sum_{perm_i} \left| \frac{A(perm_i(U) \cap T_s)}{s!\ N} - vol_s(perm_i(U) \cap T_s) \right| \\
&\leq \frac{1}{s!} \sum_{perm_i} \left| \frac{A(perm_i(U) \cap T_s)}{N} - \frac{vol_s(perm_i(U) \cap T_s)}{vol_s(T_s)} \right| \\
&\leq \frac{1}{s!} \sum_{perm_i} D^*_{\triangle}(P) \\
&= D^*_{\triangle}(P)
\end{aligned}$$

where

$$\left| \frac{A(perm_i(U) \cap T_s)}{N} - \frac{vol_s(perm_i(U) \cap T_s)}{vol_s(T_s)} \right| \leq D^*_{\triangle}(P)$$

holds because $perm_i(U) \in \Upsilon$. From this follows that

$$D^*(Sort^{-1}(P)) = \sup_{U \in \Upsilon} D^*(Sort^{-1}(P))(U) \leq D^*_{\triangle}(P).$$

□

Theorem 5.1 (Koksma-Hlawka on the Simplex). *For every point set P on T_s with $\#P = N$ and every function $f : T_s \to \mathbb{R}$ with bounded variation on T_s*

$$|Q[f] - I[f]| = \left| \frac{\sum_{\mathbf{x}_i \in P} f(\mathbf{x}_i)}{N} vol_s(T_s) - \int_{T_s} f(\mathbf{x}) \mathsf{d}\mathbf{x} \right| \leq D^*_{\triangle}(P) V_{\triangle}(f).$$

Proof. Since $Sort^{-1}(P)$ is a point set on I_s, we can apply (7)

$$\left| \frac{vol_s(T_s)}{\#(Sort^{-1}(P))} \sum_{\mathbf{x}_i \in Sort^{-1}(Sort^{-1}(P))} f(\mathbf{x}_i) - \int_{T_s} f(\mathbf{x}) \mathsf{d}\mathbf{x} \right| \leq D^*(Sort^{-1}(P)) V_{\triangle}(f). \quad (9)$$

And from $Sort(Sort^{-1}(P)) = s!$ times P we can deduce that

$$\frac{\sum_{\mathbf{x}_i \in Sort(Sort^{-1}(P))} f(\mathbf{x}_i)}{\#(Sort^{-1}(P))} = \frac{s! \sum_{\mathbf{x}_i \in P} f(\mathbf{x}_i)}{s!\ \#P} = \frac{\sum_{\mathbf{x}_i \in P} f(\mathbf{x}_i)}{\#P}$$

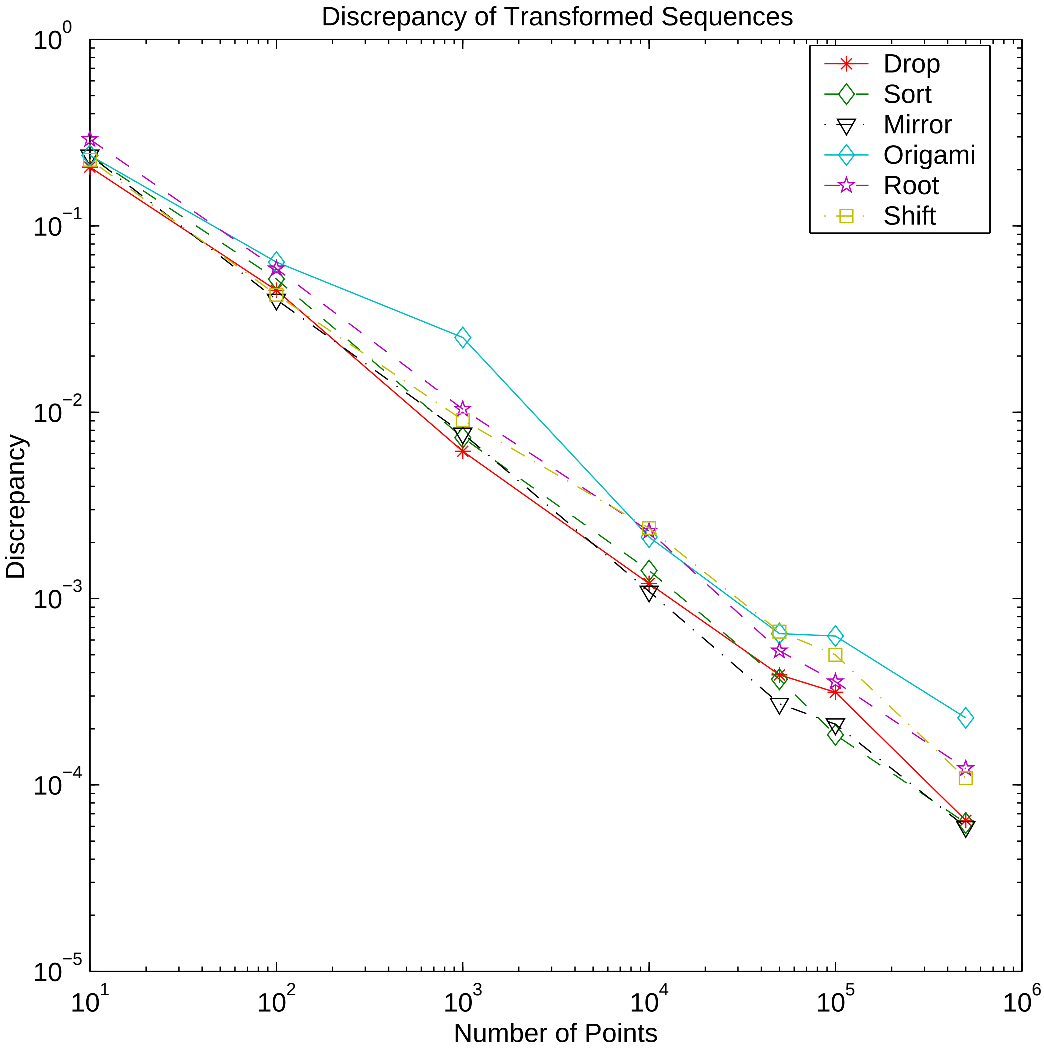
which, together with (8) and (9) proves this theorem. □

6 Numerically calculated discrepancy

We used a program written by E. Thiémard, [4] and adjusted it for the simplex star discrepancy from Definition 4.1 to calculate the discrepancy of sequences created by the transformations introduced in [6]. We calculated the discrepancy in two dimensions (for higher dimensions this algorithm is impractical) of the sequences created by transformations *Sort*, *Root*, *Shift*, *Origami*, *Drop*, and *Mirror*. As original sequences on I_s, we used a Sobol sequence. Figure 6 shows a log-log plot of the number of points (up to $5 \cdot 10^5$) on the horizontal axis versus the discrepancy on the vertical axis. The program returns an upper and a lower bound for the discrepancy. The obtained results can be seen in the table below. The calculated results seem to suggest that transformations *Sort* and *Mirror* have a better discrepancy than the others. Especially *Origami* performs worse than the other transformations. Together with the results in [6] we are inclined to conclude that *Sort* seems better and *Origami* seems worse than the others. Theoretical results and generalization to higher dimensions must still be investigated.

N	10	100	1000	10000	50000	100000	500000
Drop	0.2065	0.0444	0.00612	0.00112	0.000357	0.000291	0.000039
	0.2069	0.0458	0.00623	0.00129	0.000423	0.000337	0.000090
Sort	0.2382	0.0512	0.00725	0.00135	0.000331	0.000169	0.000036
	0.2391	0.0524	0.00737	0.00148	0.000408	0.000203	0.000089
Mirror	0.2382	0.0395	0.00762	0.00104	0.000230	0.000187	0.000033
	0.2391	0.0409	0.00777	0.00114	0.000315	0.000236	0.000086
Origami	0.2382	0.0635	0.0251	0.00207	0.000606	0.000611	0.000209
	0.2391	0.0645	0.0253	0.00221	0.000692	0.000649	0.000249
Root	0.2911	0.0583	0.01032	0.00224	0.000485	0.000332	0.000094
	0.2921	0.0596	0.01043	0.00237	0.000565	0.000385	0.000151
Shift	0.2257	0.0422	0.00902	0.00236	0.000636	0.000478	0.000088
	0.2270	0.0431	0.00917	0.00241	0.000692	0.000522	0.000129

Figure 6: Star Discrepancy on the Simplex



7 Conclusion and future research

We introduced a star discrepancy for the simplex, a way to measure the uniformity of a point set on the simplex. With this discrepancy it will be possible to evaluate different point sets on the simplex (not only those that are created by a transformation) and determine which one is best. Further investigation is needed to derive theoretical results for the transformations given in [6] to generalize the current work to other simplices then T_s and to grids of simplices (e.g. triangularization).

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