Discrepancy and Convex Programming (*) (**).

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Summary. – The pertinence of convexity arguments in the study of discrepancy of sequences is exhibited. The usefulness of this viewpoint can be twofold. Firstly, it allows the interpretation of the problem of estimating the discrepancy as a problem in convex programming in important cases. Secondly, it helps to restrict the family of sets which have to be considered when evaluating the usual (or extreme) discrepancy and the isotrope discrepancy of sequences. In particular, in the latter case it suffices to look at a rather special class of convex polytopes.

1. - Introduction.

In the quantitative theory of uniform distribution modulo one, a central role is played by the notion of discrepancy of a sequence. For a survey of results connected with this notion, we refer to the article of HLAWKA [2]. Finding good estimates for the discrepancy of a given sequence is of particular importance in the theory of numerical integration. Numerous papers have been devoted to the study of this relationship. To provide an access to the literature, we mention HLAWKA [3] and ZAREMBA [7] which have more or less expository character, and the monograph of KOROBOV [4].

It is the purpose of the present note to point out the wide applicability of convexity arguments when investigating discrepancy. A consistent exploitation of the strong links between convexity and discrepancy can shed new light on the notion of discrepancy itself. This is done, for instance, in Section 2 where the problem of finding upper bounds for the discrepancy of a sequence is interpreted as a convex program. This viewpoint has been successfully employed by the present author in the specific problem of estimating the discrepancy of so-called almost-arithmetic progressions (see [5]). As a further application of convexity arguments, we show that they enable us to restrict the family of sets which have to be considered when evaluating either the usual or the isotrope discrepancy of a sequence (see Theorems 2 and 3).

Let us briefly recall the definition of the discrepancy of a finite sequence a_1, \ldots, a_N of elements from the unit interval E = [0, 1]. For a subset M of E, we introduce the counting function $A(M; N) = \sum_{n=1}^{N} c_M(a_n)$ where c_M denotes the characteristic function of M.

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DEFINITION 1. – The discrepancy D_N of the finite sequence $a_1, ..., a_N$ in E is defined to be

$$D_N = \sup_{\mathbf{0} < \alpha \leq 1} \left| \frac{A([0, \alpha); N)}{N} - \alpha \right|.$$

2. - The method.

Let us now assume that the a_i are ordered according to their magnitude. For notational convenience, we set $a_0 = 0$ and $a_{n+1} = 1$. Then $0 = a_0 < a_1 < a_2 < ... < < a_n < a_n < a_{n+1} = 1$.

We note, once and for all, a simple fact which will be used frequently: the convex function g(x) = |x - c|, with some constant $c \in \mathbb{R}$, attains its maximum on the compact interval [a, b] at one of the endpoints.

We have the following simple alternative representation for the discrepancy D_{N} .

THEOREM 1. – Under the above conditions, the discrepancy D_N of the sequence a_1, \ldots, a_N is given by

(1)
$$D_N = \max_{i=1,\dots,N} \max\left(\left|\frac{i}{N} - a_i\right|, \left|\frac{i-1}{N} - a_i\right|\right).$$

PROOF. - We have

$$D_N = \max_{i=0,\ldots,N} \sup_{a_i < lpha \leqslant a_{i+1}} \left| rac{A([0,lpha);N)}{N} - lpha
ight| = \max_{i=0,\ldots,N lpha lpha < lpha \leqslant a_{i+1}} \sup_{a_i < lpha \leqslant a_{i+1}} \left| rac{i}{N} - lpha
ight|.$$

 $\text{But } \sup_{a_i < \alpha \leqslant a_{i+1}} |i/N - \alpha| = \max \left(|i/N - a_i|, \, |i/N - a_{i+1}| \right) \text{ for } a_i < a_{i+1}. \text{ Thus }$

(2)
$$D_N = \max_{\substack{i=0,\dots,N\\a_i < a_{i+1}}} \max\left(\left| \frac{i}{N} - a_i \right|, \left| \frac{i}{N} - a_{i+1} \right| \right).$$

We want to show, first of all, that the right-hand side of (2) is equal to

(3)
$$\max_{i=0,\ldots,N} \max\left(\left|\frac{i}{N}-a_i\right|, \left|\frac{i}{N}-a_{i+1}\right|\right).$$

Suppose we have $a_i < a_{i+1} = a_{i+2} = ... = a_{i+r} < a_{i+r+1}$ with some $r \ge 2$. The indices which are excluded in the first maximum in (2) are the integers i+j with $1 \le j \le < r-1$. We shall prove that the numbers

$$\left| rac{i+j}{N} - a_{i+j}
ight| \qquad ext{and} \qquad \left| rac{i+j}{N} - a_{i+j+1}
ight| \qquad ext{with} \ 1 < j < r-1,$$

which are admitted in (3), are in fact dominated by numbers already occurring in (2). For $1 \le j \le r-1$, we get

$$\begin{aligned} \left|\frac{i+j}{N} - a_{i+j}\right| &= \left|\frac{i+j}{N} - a_{i+1}\right| < \max\left(\left|\frac{i}{N} - a_{i+1}\right|, \left|\frac{i+r}{N} - a_{i+1}\right|\right)\right) = \\ &= \max\left(\left|\frac{i}{N} - a_{i+1}\right|, \left|\frac{i+r}{N} - a_{i+r}\right|\right), \end{aligned}$$

and both numbers in the last maximum occur in (2). Exactly the same argument holds for $|(i+j)/N - a_{i+j+1}|$, $1 \le j \le r-1$. Thus we arrive at

$$D_N = \max_{i=0,\ldots,N} \max\left(\left| \frac{i}{N} - a_i \right|, \left| \frac{i}{N} - a_{i+1} \right| \right) = \max_{i=1,\ldots,N} \max\left(\left| \frac{i}{N} - a_i \right|, \left| \frac{i-1}{N} - a_i \right| \right),$$

since the only terms which are not contained in the last expression are $|0/N - a_0|$ and $|N/N - a_{N+1}|$, both of which are zero.

It will often suffice to work with the following simple consequence of (1):

$$D_N \leq \max_{i=1,\ldots,N} \left| \frac{i}{N} - a_i \right| + \frac{1}{N}.$$

Suppose now that we are given certain linear inequalities for the a_i :

(4)
$$\sum_{i=1}^N \lambda_{ji} a_i \leqslant B_j \qquad \text{for } 1 \leqslant j \leqslant k.$$

We may assume that the inequalities $0 \le a_1 \le a_2 \le ... \le a_N \le 1$ are already included in (4). For $(x_1, ..., x_N) \in \mathbb{R}^N$, put

$$f(x_1,\ldots,x_N) = \max_{i=1,\ldots,N} \max\left(\left| \frac{i}{N} - x_i \right|, \left| \frac{i-1}{N} - x_i \right| \right).$$

Since a function of the form g(x) = |c - x|, $c \in \mathbb{R}$, is convex, and since the maximum of convex functions is convex, the function $f(x_1, \ldots, x_N)$ is a convex function in \mathbb{R}^N . Furthermore, we have $D_N = f(a_1, \ldots, a_N)$ by Theorem 1. Consider the following convex program: maximize the convex function $f(x_1, \ldots, x_N)$ over the bounded convex polytope

$$(5) \qquad P = \left\{ (x_1, \, \dots, \, x_N) \in \mathbb{R}^N \colon \sum_{i=1}^N \lambda_{j_i} x_i \leqslant B_j \text{ for } 1 \leqslant j \leqslant k \text{ and } 0 \leqslant x_i \leqslant 1 \text{ for } 1 \leqslant i \leqslant N \right\}.$$

Since $(a_1, ..., a_N)$ is contained in the polytope (5), a solution of the optimization problem yields an upper bound for D_N . The estimate will become sharper the smaller

we can make the polytope P. When applying this method, one will always use the well-know fact that the maximum of f has to be attained at a vertex of the polytope. Obviously, the method can be generalized by replacing (4) by conditions which restrict (a_1, \ldots, a_N) to a reasonably small bounded convex set in \mathbb{R}^N .

A problem which lends itself to an immediate application of the present method is the following one. P. E. O'NEIL [6] introduced so-called almost-arithmetic progressions- (δ, ε) and proved that sufficiently long initial segments of uniformly distributed sequences mod 1 are essentially obtained by superposition of such almost arithmetic progressions with arbitrarily small δ and ε . Hence good estimates for the discrepancy of uniformly distributed sequences mod 1 can be obtained by having available sharp estimates for the discrepancy of almost-arithmetic progressions. For given $0 \le \delta < 1$ and $\varepsilon > 0$, a sequence $0 \le a_1 < a_2 < ... < a_N \le 1$ is called an *almostarithmetic progression*- (δ, ε) if there exists an η with $0 < \eta < \varepsilon$ such that: (i) $0 < a_1 <$ $< \eta + \delta\eta$; (ii) $\eta - \delta\eta < a_{k+1} - a_k < \eta + \delta\eta$ for $1 \le k < N - 1$; (iii) $1 - \eta - \delta\eta < a_N < 1$. By applying our method, we obtained for the discrepancy D_N of the sequence a_1, \ldots, a_N :

$$D_N \leqslant rac{1}{N} + rac{\delta}{1+\sqrt{1-\delta^2}} \, ,$$

and this upper bound is even best possible (see NIEDERREITER [5]).

3. - Generalization to several dimensions.

A partial analogue to Theorem 1 can be shown for sequences contained in the k-dimensional unit cube $E^k = \{(x_1, ..., x_k) \in \mathbb{R}^k : 0 \le x_i \le 1 \text{ for } 1 \le i \le k\}$ for some $k \ge 2$. We use the following notation. For $\mathbf{0} = (0, ..., 0) \in E^k$ and $\mathbf{x} = (x_1, ..., x_k) \in E^k$, let $[\mathbf{0}, \mathbf{x})$ denote the set $[\mathbf{0}, \mathbf{x}) = \{(y_1, ..., y_k) \in E^k : 0 \le y_i \le x_i \text{ for } 1 \le i \le k\}$. Furthermore, we put $V(\mathbf{x}) = x_1 x_2 \dots x_k$. For a given finite sequence $\mathbf{a}_1, ..., \mathbf{a}_N$ in E^k , we define the counting function A(.; N) in the obvious manner. For the sake of convenience, we write $A([\mathbf{0}, \alpha); N) = A(\alpha; N)$ for $\alpha \in E^k$.

DEFINITION 2. – The *discrepancy* of the finite sequence $a_1, ..., a_N$ in E^k is defined to be

$$D_N = \sup_{\pmb{lpha}\in E^k} \left| rac{A(\pmb{lpha}\,;\,N)}{N} - V(\pmb{lpha})
ight|.$$

Obviously, it suffices to restrict the supremum to those $\alpha \in E^k$ with $V(\alpha) > 0$. Let *B* be the collection of all $\alpha \in E^k$ with $V(\alpha) = 0$. We construct a finite partition of $E^k \setminus B$ in the following manner. For fixed *i*, $1 \le i \le k$, let $0 = \beta_{i0} < \beta_{i1} < ... < < \beta_{is_i} = 1$ be the distinct numbers occurring as *i*-th coordinates of $a_1, ..., a_N$ in ascending order, together with 0 and 1. Now pick an arbitrary *k*-tuple $(\beta_{1j_1}, \beta_{2j_2}, ..., \beta_{kj_k})$ with $0 < j_i < s_i$ for 1 < i < k. With this k-tuple, we define the interval $Q = \{(x_1, \dots, x_k) \in E^k : \beta_{ij_i} < x_i < \beta_{i,j_i+1}$ for $1 < i < k\}$. The finite collection q of all the intervals Q obtained in this way forms then a partition of $E^k \setminus B$. For each $Q \in q$, let $y(Q) = = (\beta_{1,j_1+1}, \dots, \beta_{k,j_k+1})$ be the « upper endpoint » and $z(Q) = (\beta_{1j_1}, \dots, \beta_{kj_k})$ be the « lower endpoint » of Q. We present the following alternative representation for D_x .

THEOREM 2. – With the notation introduced above, the discrepancy of $a_1, ..., a_N$ is given by

(6)
$$D_N = \max_{Q \in \mathfrak{q}} \max\left(\left| \frac{A(\mathbf{y}(Q); N)}{N} - V(\mathbf{y}(Q)) \right|, \left| \frac{A(\mathbf{y}(Q); N)}{N} - V(\mathbf{z}(Q)) \right| \right).$$

PROOF. - We have

$$D_N = \max_{\mathbf{q} \in \mathbf{q}} \sup_{\mathbf{\alpha} \in \mathbf{q}} \left| \frac{A(\mathbf{\alpha}; N)}{N} - V(\mathbf{\alpha}) \right|.$$

By the construction of the intervals Q, it is easy to see that $A(\alpha; N) = A(y(Q); N)$ for all $\alpha \in Q$. But then

$$\sup_{\boldsymbol{\alpha}\in\boldsymbol{Q}} \left| \frac{A(\boldsymbol{\alpha};N)}{N} - V(\boldsymbol{\alpha}) \right| = \sup_{\boldsymbol{\alpha}\in\boldsymbol{Q}} \left| \frac{A(\boldsymbol{y}(Q);N)}{N} - V(\boldsymbol{\alpha}) \right| = \\ = \max\left(\left| \frac{A(\boldsymbol{y}(Q);N)}{N} - V(\boldsymbol{y}(Q)) \right|, \left| \frac{A(\boldsymbol{y}(Q);N)}{N} - V(\boldsymbol{z}(Q)) \right| \right),$$

which already proves (6).

For a point $(z_1, ..., z_k) \in E^k$ which is a $\mathbf{z}(Q)$ for some $Q \in \mathfrak{q}$, let its multiplicity $M(\mathbf{z}(Q))$ be the number of terms of the sequence $\mathbf{a}_1, ..., \mathbf{a}_N$ which lie in the set $\bigcup_{i=1}^k \{(x_1, ..., x_k) \in E^k : x_i = z_i \text{ and } 0 < x_j < z_j \text{ for } 1 < j < k\}$. Let M be an upper bound for all the multiplicities. Let F be the finite set of all points $\mathbf{x} \in E^k$ of the form $\mathbf{x} = (\beta_{1i_1}, ..., \beta_{ki_k})$ with $0 < j_i < s_i$ for 1 < i < k. Then we obtain the following more convenient result.

COROLLARY. - With the above notation, we have

(7)
$$D_N < \max_{\boldsymbol{x} \in F} \left| \frac{A(\boldsymbol{x}; N)}{N} - V(\boldsymbol{x}) \right| + \frac{M}{N}.$$

PROOF. – For $Q \in \mathfrak{q}$, we get the subsequent inequality:

$$\left|\frac{A(\boldsymbol{y}(Q);N)}{N} - V(\boldsymbol{z}(Q))\right| \leqslant \left|\frac{A(\boldsymbol{z}(Q);N)}{N} - V(\boldsymbol{z}(Q))\right| + \frac{A(\boldsymbol{y}(Q);N) - A(\boldsymbol{z}(Q);N)}{N}.$$

By the construction of the intervals Q, the only terms in the sequence $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_N$, which lie in $[0, \boldsymbol{y}(Q))$ but not in $[0, \boldsymbol{z}(Q))$, are those which are counted by $M(\boldsymbol{z}(Q))$.

Therefore,

(8)
$$\left|\frac{A(\mathbf{y}(Q); N)}{N} - V(\mathbf{z}(Q))\right| \leq \left|\frac{A(\mathbf{z}(Q); N)}{N} - V(\mathbf{z}(Q))\right| + \frac{M(\mathbf{z}(Q))}{N} \leq \left|\frac{A(\mathbf{z}(Q); N)}{N} - V(\mathbf{z}(Q))\right| + \frac{M}{N}.$$

We note that the points in E^k which occur as either y(Q) or z(Q) for some $Q \in \mathfrak{q}$ just make up the finite set F. Together with (6) and (8) we get then the desired inequality (7).

4. – Isotrope discrepancy.

Another application of convexity arguments, which is slightly different in nature from the previous ones, emerges in the investigation of the so-called isotrope discrepancy in E^k for $k \ge 2$. Let C denote the family of all convex subsets of E^k . It is well-known that every $C \in \mathbb{C}$ has a measure V(C) in the sense of Jordan. Let a_1, \ldots, a_N again be a finite sequence of points in E^k .

DEFINITION 3. – The isotrope discrepancy J_N of the sequence $a_1, ..., a_N$ is defined to be

(9)
$$J_N = \sup_{C \in \mathcal{C}} \left| \frac{A(C; N)}{N} - V(C) \right|.$$

This notion of discrepancy was proposed by HLAWKA [2], and studied in more detail by ZAREMBA [8]. For a very general viewpoint, see BHATTACHARYA [1, p. 82] and the literature cited there.

We shall show that it suffices to extend the supremum in (9) over a certain restricted class of convex polytopes in E^k . In this section, we adopt the following terminology with respect to convex polytopes. By a closed convex polytope, we mean the convex hull of a finite number of points in \mathbb{R}^k . If a closed convex polytope has a nonvoid interior, then this interior is called an *open convex polytope*. By a *convex polytope* (per se), we mean a convex set which is obtained by deleting an arbitrary number of faces from a closed convex polytope. A face of such a convex polytope is defined to be a face of the corresponding closed convex polytope.

Let $a_1, ..., a_N$ be a given sequence in E^k . We define a family δ of convex polytopes as follows. In δ we collect all closed or open convex polytopes P contained in E^k which satisfy the condition:

(A) each face of P is either lying entirely on the boundary of E^k or contains a point of the sequence.

The following result holds.

THEOREM 3. – For the isotrope discrepancy J_N of the sequence $a_1, ..., a_N$, we have

(10)
$$J_N = \sup_{P \in \mathcal{E}} \left| \frac{A(P; N)}{N} - V(P) \right|.$$

PROOF. - For $C \in \mathbb{C}$, we have $V(\text{int } C) = V(\overline{C}) = V(C)$ and $A(\text{int } C; N) \leq A(C; N) \leq A(\overline{C}; N)$. Thus

$$\left|\frac{A(C; N)}{N} - V(C)\right| \leq \max\left(\left|\frac{A(\operatorname{int} C; N)}{N} - V(\operatorname{int} C)\right|, \left|\frac{A(\overline{C}; N)}{N} - V(\overline{C})\right|\right),$$

and so it suffices to consider closed or open convex sets in E^k . We shall first prove (10) with \mathcal{E} replaced by the larger class \mathcal{T} of all convex polytopes P satisfying (A) which are of the form $P = P_1 \cap E^k$ for some closed or open convex polytope P_1 in \mathbb{R}^k . The argument in the beginning of the proof shows then (10) with \mathcal{E} itself.

It suffices to show that, for each closed or open $C \in \mathbb{C}$, there exist convex polytopes P and Q from \mathfrak{T} with A(P; N) = A(Q; N) = A(C; N) and V(P) < V(C) < V(Q). For then we get

$$\left|\frac{A(C;N)}{N}-V(C)\right| \leq \max\left(\left|\frac{A(P;N)}{N}-V(P)\right|, \left|\frac{A(Q;N)}{N}-V(Q)\right|\right),$$

and we are done.

Let a closed or open $C \in \mathbb{C}$ be given, and suppose that C contains exactly the elements a_{i_1}, \ldots, a_{i_r} of the sequence. Let P be the convex hull of those points (or the empty set, if C contains no elements of the sequence). Then P is a closed convex polytope belonging to \mathcal{F} , furthermore P is a subset of C, and V(P) < V(C) and A(P; N) = A(C; N) follow immediately.

It requires some more work to construct Q. Let a_{j_1}, \ldots, a_{j_s} be the elements of the sequence which are not contained in C. If s = 0, then we put $Q = E^k$. Thus s > 0 in the sequel. If C is not itself open (hence compact), then it is clear that we can enlarge C to a convex set C' (not necessarily contained in E^k) which still does not contain a_{j_1}, \ldots, a_{j_s} , but has a_{i_1}, \ldots, a_{i_r} as interior points. If C is open, we simply put C' = C. Through each point a_{j_m} with $1 \le m \le s$, there is a supporting hyperplane S_m of C' such that C' lies entirely in a closed half-space H_m defined by S_m . Then the set $Q_1 = \bigcap_{m=1}^s H_m$ contains C'. Let H^0_m be the open half-space corresponding to H_m . The convex polytope $Q_2 = H^0_1 \cap H^0_2 \cap \ldots \cap H^0_s \cap E^k$ contains all the points a_{i_1}, \ldots, a_{i_r} , but none of the points a_{j_1}, \ldots, a_{j_s} . Thus $A(Q_2; N) = A(C; N)$; moreover $V(Q_2) = = V(Q_1 \cap E^k) \ge V(C' \cap E^k) \ge V(C)$. Of course, Q_2 need not belong to \mathcal{F} . But note that Q_2 can be written in the form $Q_2 = P_2 \cap E^k$ with an open convex polytope P_2 in \mathbb{R}^k . Thus at least the last part of the definition of \mathcal{F} is satisfied. We also note that $V(Q_2) \ge V(C' \cap E^k) > 0$, and so Q_2 is not contained in a hyperplane.

To complete the proof, we show that for each Q_2 not contained in a hyperplane such that $Q_2 = P_2 \cap E^k$ with an open convex polytope P_2 in \mathbb{R}^k , and which satisfies $A(Q_2; N) = A(C; N)$ and $V(Q_2) > V(C)$, we can find $Q \in \mathfrak{f}$ with $A(Q; N) = A(Q_2; N)$ and $V(Q) > V(Q_2)$. Let the deficiency $d(Q_2)$ of the convex polytope Q_2 be the number of faces of Q_2 which fail to satisfy condition (A). We now proceed by induction on $d(Q_2)$. If $d(Q_2) = 0$, we just take $Q = Q_2$. Suppose we have shown the assertion for all Q_2 of the above type with $d(Q_2) < n$. Let Q_2 be a convex polytope of the above type with $d(Q_2) = n + 1$, and let F be one of the faces of Q_2 which do not satisfy condition (A). Let F_1, \ldots, F_t be the remaining faces of Q_2 , with F_1, \ldots, F_u lying on the boundary of E^k , and F_{u+1}, \ldots, F_t not lying on the boundary of E^k . For $1 , let <math>S_p$ be the hyperplane which contains F_p . The S_p are all distinct since Q_2 is not entirely contained in a hyperplane. For $u + 1 , let <math>H_p^0$ be the open half-space defined by S_p which contains Q_2 . We put $Q_3 = H_{u+1}^0 \cap \ldots \cap H_t^0 \cap E^k$ (with $Q_3 = E^k$ if u = t). Then Q_3 contains Q_2 and $d(Q_3) < d(Q_3)$. If $A(Q_3; N) = A(Q_2; N)$, then an application of the induction hypothesis to Q_3 yields the desired result.

So suppose that points of the given sequence are contained in $Q_3 \setminus Q_2$. Let S be the hyperplane containing F, and let a_j be one of the elements of the sequence in $Q_3 \setminus Q_2$ which has the least orthogonal distance from S. Let T be the hyperplane through a_j parallel to S. Then Q_2 lies entirely in an open half-space H^0 defined by T. The convex polytope $Q_4 = Q_3 \cap H^0$ is certainly of the form $Q_4 = P_4 \cap E^k$ with an open convex polytope P_4 , and Q_4 contains Q_2 . It follows from the definition of Q_4 that $A(Q_4; N) = A(Q_2; N)$. The faces of Q_4 either (i) lie in S_p , $1 , and contain <math>F_p$; or (ii) lie on the boundary of E^k ; or (iii) lie in T. The faces of Q_4 satisfying (i) do not contribute more to $d(Q_4)$ than the faces F_p contribute to $d(Q_2)$. The faces of Q_4 in the second category contribute nothing to $d(Q_4)$. If a face of Q_4 satisfying (iii) exists at all (such a face need not exist if a_j lies in a « corner » of E^k), then it contains a_j , and so contributes nothing to $d(Q_4)$. On the other hand, the face F of Q_2 contributes 1 to $d(Q_2)$. Consequently, we get $d(Q_4) < d(Q_2)$. An application of the induction hypothesis to Q_4 yields the desired result.

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