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Finding optimal volume subintervals with k points and calculating the star discrepancy are NP-hard problems

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ABSTRACT

The well-known star discrepancy is a common measure for the uniformity of point distributions. It is used, e.g., in multivariate integration, pseudo random number generation, experimental design, statistics, or computer graphics.

We study here the complexity of calculating the star discrepancy of point sets in the d-dimensional unit cube and show that this is an NP-hard problem.

To establish this complexity result, we first prove NP-hardness of the following related problems in computational geometry: Given n points in the d-dimensional unit cube, find a subinterval of minimum or maximum volume that contains k of the n points.

Our results for the complexity of the subinterval problems settle a conjecture of E. Thiémard [E. Thiémard, Optimal volume subintervals with k points and star discrepancy via integer programming, Math. Meth. Oper. Res. 54 (2001) 21–45].

1. Introduction

Geometric discrepancy theory studies the irregularity of distributions of point sets and has considerable theoretical and practical importance. There are many notions of discrepancy known which have a wide range of applications as in optimization, combinatorics, pseudo random number generation, option pricing, experimental design, computer graphics, and other areas, see, e.g., [1,2,7,8,19,20,22].

In particular for the ubiquitous task of multivariate numerical integration (arising in numerous applications such as mathematical finance, econometrics, physics or quantum chemistry)

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quasi-Monte Carlo algorithms, based on low-discrepancy samples, have attracted a lot of research interest in the last decades. Here the error of the quasi-Monte Carlo approximation for certain classes of integrands can be expressed in terms of the discrepancy of the set of sample points via inequalities of Koksma–Hlawka or Zaremba-type, see, e.g., [7,15,16,22,24,31]. The essence is that sample points with small discrepancy lead to small integration errors.

The most prominent discrepancy measure is the so-called star discrepancy, which is defined as follows: Let $X = (x^i)_{i=1}^n$ be a finite sequence in the d-dimensional (half-open) unit cube $[0, 1)^d$. For $y = (y_1, \dots, y_d) \in [0, 1]^d$ let $A(y, X)$ be the number of points of X lying in the d-dimensional half-open subinterval $[0, y) := [0, y_1) \times \cdots \times [0, y_d)$, and let V_y be the d-dimensional (Lebesgue) volume of $[0, y)$. We call

$$\mathrm{d}^*_\infty(X) = \sup_{y \in (0,1]^d} \left| V_y - \frac{1}{n} A(y, X) \right|$$

the L^∞*-star discrepancy*, or simply the *star discrepancy* of X. Other important discrepancy measures are, e.g., the L^p*-star discrepancies*

$$\mathrm{d}^*_p(X) = \left(\int_{[0,1]^d} \left| V_y - \frac{1}{n} A(y, X) \right|^p \mathrm{d}y \right)^{1/p}, \quad 1 \le p < \infty.$$

In many applications it is of interest to measure the quality of certain sets by calculating their star discrepancy, e.g., to test whether successive pseudo random numbers are statistically independent [22], or whether certain sample sets are suitable for multivariate numerical integration of certain classes of integrands. Apart from that, we find particularly interesting that the fast calculation or approximation of the star discrepancy would allow practicable semi-constructions of low-discrepancy samples of moderate size as described in [4,12]. (Here "moderate size" means that the number of sample points should be at most polynomial in the dimension d.) The underlying simple idea is the following: Let $\mathcal{X}$ be a set of point configurations endowed with some probability measure. Let us assume that the mean value of the star discrepancy taken over all elements of $\mathcal{X}$ (i.e., all point configurations in $\mathcal{X}$) is small, and that there exists a large deviation bound ensuring that the star discrepancy is concentrated around its mean (examples of such settings are discussed in [3–5,11,14]). Then one may choose a point set from $\mathcal{X}$ randomly and calculate its actual star discrepancy. If it is sufficiently close to the mean, we accept the set, otherwise we choose another set randomly from $\mathcal{X}$. The large deviation bound guarantees us that with high probability we only have to perform a small number of random choices to receive the low-discrepancy set we are seeking for.

Actually there are derandomized algorithms known to construct such samples deterministically [3–5], but these exhibit high running times. Therefore efficient semi-constructions would be appreciated to avoid the costly derandomization procedures. The *critical step* of the semi-construction described above is clearly the efficient calculation (or approximation) of the star discrepancy of a chosen set.

It is known that the L^2-star discrepancy of a given n-point set in dimension d can be calculated via Warnock's formula [29] with $O(dn^2)$ arithmetic operations. Heinrich and Frank developed an asymptotically even faster algorithm using $O(n(\log n)^{d-1})$ operations for fixed d [9,13]. (As indicated by the exponent of the log-term, the algorithm is unfortunately not beneficial in high dimensions.) But, as pointed out by Matoušek in [20], no similarly efficient algorithms are known for the L^p-star discrepancy if $p \neq 2$.

In particular, all known algorithms for calculating the star discrepancy or approximating it up to a user-specified error, have running times exponential in d, see [6,11,26,27]. Let us have a closer look at the problem: If we define for a finite sequence $X = (x^i)_{i=1}^n$ in $[0, 1)^d$ and for $j \in \{1, \dots, d\}$

$$\Gamma_j(X) = \{x^i_j\,;\ i \in \{1, \dots, n\}\} \quad \text{and} \quad \bar{\Gamma}_j(X) = \Gamma_j(X) \cup \{1\},$$

and put

$$\Gamma(X) = \Gamma_1(X) \times \cdots \times \Gamma_d(X) \quad \text{and} \quad \bar{\Gamma} = \bar{\Gamma}_1(X) \times \cdots \times \bar{\Gamma}_d(X),$$

it is not hard to see that

$$d_{\infty}^{*}(X) = \max\left\{ \max_{y\in\bar{\Gamma}(X)}\left(V_y - \frac{1}{n}A(y,X)\right), \max_{y\in\Gamma(X)}\left(\frac{1}{n}\bar{A}(y,X) - V_y\right)\right\}, \tag{1}$$

where $\bar{A}(y, X)$ denotes the number of points of X lying in the closed d-dimensional subinterval $[0, y]$. Indeed, consider an arbitrary test box $[0, y)$, $y \in (0, 1]^d$. Then for every $j \in \{1, \ldots, d\}$ we find a maximal $x_j \in \Gamma_j(X) \cup \{0\}$ and a minimal $z_j \in \bar{\Gamma}(X)$ satisfying $x_j < y_j \le z_j$. Put $x = (x_1, \ldots, x_d)$ and $z = (z_1, \ldots, z_d)$. We get the inequalities

$$V_y - \frac{1}{n}A(y,X) = V_y - \frac{1}{n}A(z,X) \le V_z - \frac{1}{n}A(z,X),$$

and

$$\frac{1}{n}A(y,X) - V_y = \frac{1}{n}\bar{A}(x,X) - V_y \le \frac{1}{n}\bar{A}(x,X) - V_x,$$

showing that the right-hand side of (1) is at least as big as $d_{\infty}^{*}(X)$. If, on the other hand, we have some $y \in \Gamma(X)$, then we may consider for a small $\varepsilon > 0$ the vector $y(\varepsilon)$, defined by $y(\varepsilon)_j = \min\{y_j + \varepsilon, 1\}$ for $j = 1, \ldots, d$. Obviously, $y(\varepsilon) \in (0, 1]^d$ and

$$\lim_{\varepsilon\to 0}\left(\frac{1}{n}A(y(\varepsilon),X) - V_{y(\varepsilon)}\right) = \frac{1}{n}\bar{A}(y,X) - V_y.$$

These arguments show that (1) is valid. (Formulas similar to (1) can be found in several places in the literature—the first reference we are aware of is [21, Thm. 2].) Thus an enumeration algorithm would provide us with the exact value of $d_{\infty}^{*}(X)$. But since the cardinality of $\Gamma(X)$ for almost all X is n^d, such an algorithm would be infeasible for n and d large.

Since no efficient algorithm for the exact calculation or tight approximation of the star discrepancy is known, other authors tried to deal with this large scale integer programming problem by using optimization heuristics. In [30] Winker and Fang used threshold accepting, a refined (randomized) local search algorithm based on a similar idea as the simulated annealing algorithm, to find lower bounds for the star discrepancy. The algorithm performed well in numerical tests on rank-1 integration lattices, but in general no approximation quality can be guaranteed. The authors expressed their hope that future research might give new insights into the real computational complexity of calculating the star discrepancy.

In [28] Thiémard gave an integer linear programming formulation for the problem and used techniques as cutting plane generation and branch and bound to tackle it. With the resulting algorithm he was able to perform non-trivial star discrepancy comparisons between low-discrepancy sequences. The key observation to approach a highly non-linear expression as (1) via linear programming is that one can divide it into at most $2n$ subproblems of the type "optimal volume subintervals with k points" (for the precise definition see the next section). However, Thiémard conjectured these subproblems to be NP-hard.

In this paper we prove the conjecture of Thiémard by establishing the NP-hardness of these optimal volume subinterval problems. (Notice by the way that another conjecture of Thiémard, made in [27], was proved to be wrong by Pillards and Cools in [25].) Moreover, we use these results to show that indeed the problem of calculating the star discrepancy is also NP-hard. Recall that NP-hardness of an optimization problem U is proved by verifying that deciding the so-called threshold language of U is an NP-hard problem (see, e.g., [17, Sect. 2.3.3] or, for a less formal explanation, [10, Sect. 2.1]). Thus we actually prove the NP-completeness of decision problems corresponding to the optimization problems mentioned above.

Furthermore, we state some errors occurring in [28] which may lead to incorrect solutions of Thiémard's algorithm for certain instances. We show how to avoid the undesired consequences of these errors.

2. Optimal volume subintervals with k points

In addition to the notation introduced in the previous section, we will use the following conventions: For $\nu \in \mathbb{N}$ let $[\nu] = \{1, \dots, \nu\}$. For $x = (x_1, \dots, x_d) \in [0, 1]^d$ we denote the d-dimensional subinterval $[0, x_1] \times \cdots \times [0, x_d]$ by $[0, x]$. (For convenience, we will often use the shorter term "box" instead of "subinterval".) If A is a set, 1_A denotes its characteristic function and $|A|$ its cardinality.

For a given n-point sequence $X = (x^i)_{i=1}^n$ in $[0, 1)^d$ and some given integer $0 \le k \le n$, Eric Thiémard considered in [28] the problems of finding the minimum volumes of closed subintervals containing exactly k points of X

$$\tilde{V}^k_{\min} = \min\{V_y;\, y \in \Gamma(X), \bar{A}(y, X) = k\}$$

and the maximal volume of half-open subintervals containing k points

$$\tilde{V}^k_{\max} = \max\{V_y;\, y \in \bar{\Gamma}(X), A(y, X) = k\}.$$

Remark 2.1. It is easy to see that we have

$$\tilde{V}^k_{\min} = \inf\{V_y;\, y \in [0, 1]^d, A(y, X) = k\}$$

and

$$\tilde{V}^k_{\max} = \sup\{V_y;\, y \in [0, 1]^d, A(y, X) = k\}.$$

From identity (1) we get

$$\mathrm{d}^*_\infty(X) = \max\left\{ \max_{k=0,\dots,n-1} \left(\tilde{V}^k_{\max} - \frac{k}{n} \right), \max_{k=1,\dots,n} \left(\frac{k}{n} - \tilde{V}^k_{\min} \right) \right\}. \tag{2}$$

Thus solving the optimal volume subinterval problems $\tilde{V}^k_{\max}$, $k = 0, \dots, n-1$, and $\tilde{V}^k_{\min}$, $k = 1, \dots, n$, would give us the exact star discrepancy of X. In [28] Thiémard formulated the optimal volume subinterval problems as integer linear programs and proposed a strategy (using cutting plane generation and branch and bound) to calculate $d^*_\infty(X)$ in a way that most of these integer programs do not have to be solved to optimality.

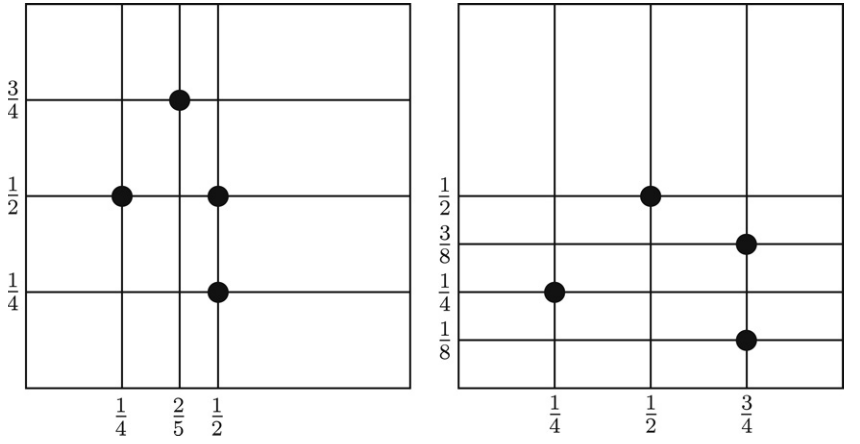
A drawback of the problem formulation of Thiémard is that for some choices of k and X the $\tilde{V}^k_{\min}$- and $\tilde{V}^k_{\max}$-problem do not have a solution (more precisely, there exists no subinterval containing exactly k points). In [28, Remark 1] it is stated that this could not happen if X consists of n distinct points. The following simple example shows that this statement is false:

Let $d = 2$ and $n = 3$. Put $x^1 = (0.3; 0.5)$, $x^2 = (0.5; 0.5)$, and $x^3 = (0.5; 0.3)$. In this situation we do neither find a half-open nor a closed box containing exactly 2 of the 3 points of the sequence $X = (x^1, x^2, x^3)$. But if we require $|\Gamma_j(X)| = n$ for at least one index $j \in [d]$, then the $\tilde{V}^k_{\min}$- and $\tilde{V}^k_{\max}$-problems always have a solution.

The concrete strategy of Thiémard to calculate the star discrepancy made strong use of the inequalities

$$\tilde{V}^1_{\min} \le \cdots \le \tilde{V}^n_{\min} \quad \text{and} \quad \tilde{V}^0_{\max} \le \cdots \le \tilde{V}^{n-1}_{\max} \tag{3}$$

under the assumption that X consists of n distinct points. But as the following examples reveal, this assumption is not sufficient to guarantee that these inequalities hold (even if all of the subinterval problems have a solution):



For the sample on the left we get

$$\tilde{V}^3_{\min} = \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{4} < \frac{3}{10} = \frac{2}{5} \cdot \frac{3}{4} = \tilde{V}^2_{\min}.$$

Such a counterexample can again not occur if $|\Gamma_j(X)| = n$ for at least one index $j \in [d]$. For the sequence in the right figure we actually have $|\Gamma_2(X)| = n = 4$, but still we obtain

$$\tilde{V}^3_{\max} = \frac{1}{2} < \frac{3}{4} = \tilde{V}^2_{\max}.$$

To avoid counterexamples of this type, it is sufficient to require $|\Gamma_j(X)| = n$ for all indices $j \in [d]$. Thus the condition that all projections of X to a single coordinate axis consist of n distinct values implies the inequalities (3).

Since we do not want to restrict ourselves to those sequences with pairwise distinct coordinates, let us introduce modified subinterval problems which will help us to overcome the undesirable properties of the problem formulation of Thiémard.

For a given n-point sequence $X = (x^i)_{i=1}^n$ in $[0, 1)^d$ and some given integer $0 \leq k \leq n$ we consider the problems of finding the minimum volume of all closed subintervals containing at least k points

$$V^k_{\min} = \min\{V_y;\, y \in \Gamma(X),\ \bar{A}(y, X) \geq k\}$$

and of finding the maximum volume of all open subintervals containing at most k points

$$V^k_{\max} = \max\{V_y;\, y \in \bar{\Gamma}(X),\ A(y, X) \leq k\}.$$

Evidently, for all $0 \leq k \leq n$, the $V^k_{\min}$- and $V^k_{\max}$-problems always have a solution, and we get

$$V^0_{\min} \leq V^1_{\min} \leq \cdots \leq V^n_{\min} \qquad \text{and} \qquad V^0_{\max} \leq V^1_{\max} \leq \cdots \leq V^n_{\max}.$$

What is most important, an analogue of identity (2) holds:

$$d^*_\infty(X) = \max\left\{ \max_{k=0,\ldots,n-1} \left(V^k_{\max} - \frac{k}{n} \right),\ \max_{k=1,\ldots,n} \left(\frac{k}{n} - V^k_{\min} \right) \right\}. \tag{4}$$

Furthermore, it is easy to see from the discussion above that the $V^k_{\min}$- and $\tilde{V}^k_{\min}$-problems have the same solution if $|\Gamma_j(X)| = n$ for some $j \in [d]$, and that the $V^k_{\max}$- and $\tilde{V}^k_{\max}$-problems have the same solution if $|\Gamma_j(X)| = n$ for all $j \in [d]$.

In [28] Eric Thiémard conjectured that the $\tilde{V}^k_{\min}$- and $\tilde{V}^k_{\max}$-problems are NP-hard, but stated that he was not able to prove it.

We will formulate the decision problems corresponding to the $V^k_{\min}$- and $V^k_{\max}$-problems and prove that they are NP-complete, and that the same holds for the decision problems corresponding to the $\tilde{V}^k_{\min}$- and $\tilde{V}^k_{\max}$-problems.

Let us previously define the *coding length* of a real number from the interval $[0, 1)$ to be the number of digits in its binary expansion.

We will state the decision problems in a quite general form. But since in practice only inputs with finite coding length are of interest, the reader may think of rational numbers with finite binary expansion instead of general real numbers as in our formulation. Notice that to prove the hardness of a decision problem it is obviously sufficient to find some subproblem which is already a hard problem. In the subproblems, which we actually prove to be NP-hard, we indeed only consider rational numbers with finite binary expansion.

Let us now define the (k^+, ε^-)-box problem.

Definition 2.2. Let $X = (x^i)_{i=1}^n$ be a finite sequence in $[0, 1)^d$ and let $\varepsilon \in (0, 1]$. For $y \in \Gamma(X)$ the closed box $[0, y]$ is called (k^+, ε^-)-*box for* X if $\bar{A}(y, X) \geq k$ and $V_y \leq \varepsilon$.

Decision Problem (k^+, ϵ^-)-Box
Instance: Natural numbers $n, d \in \mathbb{N}$, $k \in [n]$, sequence $X = (x^i)_{i=1}^n$ in $[0, 1)^d$, $\varepsilon \in (0, 1]$
Question: Is there a (k^+, ϵ^-)-box for X?

Theorem 2.3. *The decision problem* (k^+, ε^-)-Box *is NP-complete.*

The problem is obviously in NP. We will prove NP-hardness for the subproblem where $n = d$, and where the coding length of x_j^i is of order $O(1)$ for all i, j and the coding length of ε of order $O(n)$. To do so, we need some further definitions.

Definition 2.4. Given some undirected finite graph $G = (V, E)$, some $k \in [|V|]$ and two disjoint subsets I, J of V, each of cardinality k, we call the pair (I, J) a *balanced subgraph of size* k if $\{i, j\} \in E$ for each $i \in I$ and $j \in J$.

Decision Problem Balanced Subgraph
Instance: Graph $G = (V, E)$, $k \in \mathbb{N}$
Question: Is there a balanced subgraph of G of size k?

The subproblem of Balanced Subgraph, where we only consider bipartite graphs G as part of the input, is called Balanced Complete Bipartite Subgraph. It was proved by David Johnson in [18] to be NP-complete by reduction of the problem Clique. For our purpose it thus suffices to reduce Balanced Subgraph to the problem (k^+, ε^-)-Box.

Proof of Theorem 2.3. Let $G = (V, E)$, $k \in [n]$ with $n = |V|$ be an instance of the problem Balanced Subgraph. For convenience we assume $V = [n]$.

Let $\alpha < \beta \in (0, 1)$ (e.g., we may choose $\beta = 1/2, \alpha = 1/4$). Put

$$x_j^i = \begin{cases} \alpha, & \text{if } \{i, j\} \in E \\ \beta, & \text{else} \end{cases}$$

and

$$x^i = (x_j^i)_{j=1}^n, \quad i = 1, \ldots, n.$$

We will prove that there exists a balanced subgraph of size k for G if and only if there is a $(k^+, (\alpha^k \beta^{n-k})^-)$-box for $X := (x^i)_{i=1}^n$.

First, assume the existence of $I, J \subseteq V$ such that $|I| = |J| = k, I \cap J = \emptyset$, and $\{i, j\} \in E$ for all $i \in I, j \in J$. Put

$$y_j = \alpha \cdot 1_J(j) + \beta \cdot 1_{V \setminus J}(j), \quad j = 1, \ldots, n \quad \text{and} \quad y = (y_j)_{j=1}^n$$

and obtain $V_y = \alpha^k \beta^{n-k}$ as well as $\bar{A}(y, X) = \sum_{i=1}^n 1_{[0,y]}(x^i) \geq \sum_{i \in I} 1_{[0,y]}(x^i) = k$. Therefore, $[0, y]$ is a $(k^+, (\alpha^k \beta^{n-k})^-)$-box for X.

Conversely, assume the existence of a point $y \in \Gamma(X)$ such that $V_y \leq \alpha^k \beta^{n-k}$ and $\bar{A}(y, X) \geq k$. Then, $y_j \geq \alpha$ for all $j \in [n]$, since otherwise $1_{[0,y]}(x^i) = 0$ for each i. Since $V_y \leq \alpha^k \beta^{n-k}$ we also get

$y_j < \beta$ for at least k coordinates $j_1, \dots, j_k$. By assumption there are pairwise distinct indices $i_1, \dots, i_k$ such that $x^{i_1}, \dots, x^{i_k} \in [0, y]$. This yields $\{i, j\} \in E$ for all $i \in \{i_1, \dots, i_k\}$ and $j \in \{j_1, \dots, j_k\}$. The sets $\{i_1, \dots, i_k\}$ and $\{j_1, \dots, j_k\}$ are necessarily disjoint, since $\{j, j\} \notin E$ for any $j \in [n]$. $\square$

Remark 2.5. Let us mention that we can also prove NP-hardness for the subproblem where the finite sequences consist of points with pairwise distinct coordinates. For this purpose, let G be as in the proof stated above and let $\varphi : [n] \times [n] \to [n^2]$ be bijective. Now put, e.g.,

$$x_j^i = \begin{cases} \dfrac{\varphi(i,j)}{2^{2nk}}, & \text{if } \{i,j\} \in E \\ 1 - \dfrac{\varphi(i,j)}{2^{2n}}, & \text{else.} \end{cases}$$

Some calculations show that for $n \geq 4$ there is a balanced subgraph of size k for G if and only if there exists a $(k^+, ((\frac{n^2}{2^{2nk}})^k(1 - \frac{1}{2^{2n}})^{n-k})^-)$-box for $X = ((x_j^i)_{j=1}^d)_{i=1}^n$. (The detailed calculations can be found in the appendix of this article.)

In the situation of pairwise distinct coordinates there exists a (k^+, ε^-)-box if and only if there exists a (k, ε^-)-box, i.e., a box $[0, y)$, $y \in \Gamma(X)$, such that $V_y \leq \varepsilon$ and $\bar{A}(y, X) = k$. Thus our argument above shows that the decision problem (k, ε^-)-Box, which corresponds to the $\tilde{V}^k_{\min}$-problems, is also NP-hard, proving the first part of the conjecture of Thiémard.

We now turn to the (k^-, ε^+)-box-problem and start with the definition of (k^-, ε^+)-boxes.

Definition 2.6. According to Definition 2.2, for a given sequence $X = (x^i)_{i=1}^n$ in $[0, 1)^d$ and a given $\varepsilon \in (0, 1]$ we define a (k^-, ε^+)-*box for* X to be a half-open box $[0, y)$ where $y \in \bar{\Gamma}(X)$, $A(y, X) \leq k$, and $V_y \geq \varepsilon$.

Decision Problem (k^-, ϵ^+)-Box
Instance: Integers $n, d \in \mathbb{N}$, $0 \leq k \leq n$, sequence $X = (x^i)_{i=1}^n$ in $[0, 1)^d$, $\varepsilon \in (0, 1]$
Question: Is there a (k^-, ϵ^+)-box for X?

The (k^-, ε^+)-box problem slightly differs from the problem we have just examined, since for the (k^-, ε^+)-box problem we can even prove NP-hardness for a fixed k. In particular, it will be demonstrated that it is NP-hard to decide whether for instances $n, d \in \mathbb{N}$, $X = (x^i)_{i=1}^n \in [0, 1)^{dn}$, $\varepsilon \in (0, 1]$, there exists a $(0^-, \varepsilon^+)$-box (we will use this fact in the next section to prove NP-hardness of the problem of calculating the star discrepancy).

As long as P≠NP, this cannot be shown for the (k^+, ε^-)-box problem since for a given sequence $X = (x^1, \dots, x^n) \in [0, 1)^d$ we may enumerate the $\binom{n}{k}$ subsets $S \subseteq [n]$ of cardinality $|S| = k$ and put $B_S = \prod_{j=1}^d [0, \max\{x_j^s; s \in S\}]$. Obviously, all these boxes B_S contain at least k points and it is easily verified that $V^k_{\min} = \min \{\mathrm{vol}(B_S); S \subseteq [n],\ |S| = k\}$. Hence for fixed k we can solve the (k^+, ε^-)-box problem in polynomial time.

Theorem 2.7. *The decision problem* (k^-, ε^+)-Box *is NP-complete. Moreover, the subproblem where k is a fixed non-negative integer (and not part of the input anymore) is also NP-complete, regardless of the choice of k.*

The problem (k^-, ε^+)-Box is obviously in NP. For a fixed k we will actually prove NP-hardness for the subproblem where $n = d$, $x_j^i \in \{0, \frac{1}{2}\}$ for all i, j and the coding length of ε is $\leq n$. For the proof, we need a further definition.

Definition 2.8. Let $G = (V, E)$ be a graph and T a subset of V. Then T is a *dominating set of* G if for all $v \in V \setminus T$ there exists a $t \in T$ such that $\{v, t\}$ is contained in the edge set E.

Decision Problem Dominating Set
Instance: Graph $G = (V, E)$, $m \in [|V|]$
Question: Is there a dominating set $T \subseteq V$ of cardinality at most m?

It is well known that the decision problem Dominating Set is NP-complete, see, e.g., [10].

Proof of Theorem 2.7. We first prove the NP-hardness result for $k = 0$. We do so by reducing DOMINATING SET to the problem $(0^-, \varepsilon^+)$-Box. Therefore, let $G = (V, E)$, $c \in [|V|]$ be an instance of DOMINATING SET. Without loss of generality we may assume that $V = [n]$ for $n = |V|$. Now, let α and $\beta \in [0, 1)$ such that $\beta < \alpha^n$. In particular, we may choose $\alpha = 1/2$ and $\beta = 0$. For $i, j \in [n]$ put

$$x^i_j = \begin{cases} \alpha, & \text{if } \{i, j\} \in E \text{ or } i = j \\ \beta, & \text{else.} \end{cases}$$

and let

$$x^i = (x^i_j)_{j=1}^n \quad \text{and} \quad X = (x^i)_{i=1}^n.$$

We will show that there exists a dominating set $C \subseteq V$ of cardinality $\le c$ if and only if there is a $y \in \bar{\Gamma}(X)$ such that $V_y \ge \alpha^c$ and $A(y, X) = 0$.

Let us first assume that there exists a dominating set $C \subseteq V$ of G of cardinality at most c. Put

$$y_j = \alpha \cdot 1_C(j) + 1_{[n]\setminus C}(j)\ ,\ j = 1, \dots, n \quad \text{and} \quad y = (y_j)_{j=1}^n.$$

Obviously, $y \in \bar{\Gamma}(X)$ and $V_y = \prod_{j\in C} \alpha = \alpha^{|C|} \ge \alpha^c$. Thus, it suffices to prove that the half-open anchored box $[0, y)$ does not contain any point of X. Now for each $i \in C$ we have $x^i_i = \alpha$, i.e., $x^i \notin [0, y)$. For every $i \in V \setminus C$ there is a $\nu \in C$ such that $\{i, \nu\} \in E$ (by definition of a dominating set) yielding $x^i_\nu = \alpha$, implying again $x^i \notin [0, y)$. Therefore $A(y, X) = 0$.

Assume now the existence of a $y \in \bar{\Gamma}(X)$ such that $V_y \ge \alpha^c$ and $A(y, X) = 0$. Since $\beta < \alpha^n \le V_y$, we get

$$\left|\left\{j \in [n]; y_j \ge \alpha\right\}\right| = n.$$

On the other hand, putting $C = \{i \in [n]\ ;\ y_i = \alpha\}$, we obtain $|C| \le c$. But since $A(y, X) = 0$ we get $|C| \ge 1$ and for each $i \in [n]$ there exists a $\nu \in C$ such that $\{i, \nu\} \in E$ or $i \in C$. Therefore, C is a dominating set of G of cardinality $\le c$.

Now let $k \in \mathbb{N}$ be arbitrary and let $n, d \in \mathbb{N}$, a finite sequence $X = (x^1, \dots, x^n)$ in $[0, 1)^d$ and $\varepsilon > 0$ be given. Put $\tilde{X} = (x^i)_{i=1}^{n+k}$, where $x^{n+i} = (0)_{j=1}^d$ for $i \in [k]$. Obviously, there exists a $y \in \bar{\Gamma}(X)$ such that $V_y \ge \varepsilon$ and $A(y, X) = 0$ if and only if there is a $\tilde{y} \in \bar{\Gamma}(\tilde{X})$ such that $V_{\tilde{y}} \ge \varepsilon$ and $A(\tilde{y}, \tilde{X}) = k$. This proves the general case. □

Remark 2.9. We can also prove NP-hardness of (k^-, ε^+)-Box for fixed k if we restrict ourselves to sequences X whose points have pairwise distinct coordinates. Let G and c be as in the previous proof and let $\varphi : [n] \times [n] \to [n^2]$ be some bijection. Now put, e.g.,

$$x^i_j = \begin{cases} \dfrac{1}{2}\left(1 + \dfrac{\varphi(i,j)}{2^{3n}}\right), & \text{if } \{i, j\} \in E \text{ or } i = j \\ \dfrac{\varphi(i,j)}{2^{3n}}, & \text{else.} \end{cases}$$

It can be verified that there exists a dominating set $C \subseteq V$ of cardinality $\le c$ if and only if there is a $(0^-, ((1/2)^c)^+)$-box for $X = ((x^i_j)_{j=1}^d)_{i=1}^n$. (The full argument can be found in the appendix.)

To prove the NP-hardness for the subproblem with $k \in \mathbb{N}$ fixed, we may use the same argument as at the end of the proof of Theorem 2.7, but put $x^{n+i}_j = \psi(i, j)\varepsilon/2^{k+d}$ for some bijection $\psi : [k] \times [d] \to [kd]$ and all $i \in [k], j \in [d]$.

Thus altogether we showed that for each non-negative integer k the $\tilde{V}^k_{\max}$-problem is NP-hard, and that solving the $\tilde{V}^k_{\min}$-problems for all $k \in [n]$ is also NP-hard. In this sense we proved the conjecture of Thiémard.

3. Calculating the star discrepancy is NP-hard

In this section we prove that the calculation of the star discrepancy for a given n-point sequence is an NP-hard problem. Let us first introduce the corresponding decision problem.

Decision Problem STAR DISCREPANCY
Instance: Natural numbers $n, d \in \mathbb{N}$, sequence $X = (x^i)_{i=1}^n$ in $[0, 1)^d$, $\varepsilon \in (0, 1]$
Question: Is $d_\infty^*(X) \geq \varepsilon$?

We will prove NP-hardness for the subproblem where $n = d$, the coding length of each x_j^i is bounded by $O(n)$ for all i, j, and the coding length of ε is bounded by $O(n^2)$. (Note that for well-distributed sequences of points the star discrepancy tends to 0 if n approaches infinity, thus it is natural to allow the coding length of ε to increase with n.)

Theorem 3.1. STAR DISCREPANCY *is NP-complete.*

Proof. Let us pose the question of the decision problem STAR DISCREPANCY in a different but (due to identity (1)) equivalent way: Is there a $y \in \bar{\Gamma}(X)$ such that $V_y - \frac{1}{n}A(y, X) \geq \varepsilon$ or $\frac{1}{n}\bar{A}(y, X) - V_y \geq \varepsilon$? From this formulation it is easy to see that STAR DISCREPANCY is in NP.

As in the proof of Theorem 2.7, we will establish the NP-hardness of STAR DISCREPANCY by reduction of DOMINATING SET. For this purpose, let $G = (V, E)$, $k \in [|V|]$ be an instance of DOMINATING SET. Again, we may assume $V = [n]$ for $n = |V|$. We may further assume without loss of generality $n \geq 2$ and $k < n$. Put

$$x_j^i = \begin{cases} 1 - \dfrac{1}{2^{n+1}}. & \text{if } \{i, j\} \in E \text{ or } i = j \\ 0, & \text{else.} \end{cases}$$

We will prove for $X = (x^i)_{i=1}^n$ that we have $d_\infty^*(X) \geq (1 - \frac{1}{2^{n+1}})^k$ if and only if there exists a dominating set $C \subset V$ for G with $|C| \leq k$.

From the proof of Theorem 2.7 we know that the existence of such a dominating set C is equivalent to the existence of a $y \in \bar{\Gamma}(X)$ satisfying $V_y \geq (1 - \frac{1}{2^{n+1}})^k$ and $A(y, X) = 0$. Since the existence of such a y implies $d_\infty^*(X) \geq V_{\max}^0 \geq (1 - \frac{1}{2^{n+1}})^k$, it remains only to show that $d_\infty^*(X) \geq (1 - \frac{1}{2^{n+1}})^k$ implies $d_\infty^*(X) = V_{\max}^0$.

In view of identity (4) we verify first $\frac{l}{n} - V_{\min}^l < \left(1 - \frac{1}{2^{n+1}}\right)^k$ for all $l \in [n]$: Whenever $l \in [n-1]$, we get with Bernoulli's inequality $1 + \nu a \leq (1 + a)^\nu$ for all $a \in [-1, \infty)$, $\nu \in \mathbb{N}$, the estimates

$$\frac{l}{n} - V_{\min}^l \leq \frac{n-1}{n} < 1 - \frac{k}{2^{n+1}} \leq \left(1 - \frac{1}{2^{n+1}}\right)^k.$$

For the volume $V_{\min}^n$ of the smallest box containing all n points of the sequence X we have

$$V_{\min}^n = \left(1 - \frac{1}{2^{n+1}}\right)^n.$$

Bernoulli's inequality gives us

$$1 < \left(1 - \frac{n}{2^{n+1}}\right) + \left(1 - \frac{k}{2^{n+1}}\right) \leq \left(1 - \frac{1}{2^{n+1}}\right)^n + \left(1 - \frac{1}{2^{n+1}}\right)^k.$$

Hence,

$$1 - V_{\min}^n = 1 - \left(1 - \frac{1}{2^{n+1}}\right)^n < \left(1 - \frac{1}{2^{n+1}}\right)^k.$$

Now we verify $V_{max}^l - \frac{l}{n} < \left(1 - \frac{1}{2^{n+1}}\right)^k$ for all $l \in [n-1]$: Let $l \in [n-1]$. Each half-open box $[0, y)$ containing no more than $n - 1$ points satisfies

$$V_y \leq 1 - \frac{1}{2^{n+1}}.$$

Since we assumed $n \geq 2$, we have therefore

$$V_{\max}^{l} - \frac{l}{n} \leq \left(1 - \frac{1}{2^{n+1}}\right) - \frac{1}{n}.$$

From

$$\left(1 - \frac{1}{2^{n+1}}\right) - \frac{1}{n} < \left(1 - \frac{1}{2^{n+1}}\right) - \frac{n-1}{2^{n+1}} \leq 1 - \frac{k}{2^{n+1}}$$

we obtain with the help of Bernoulli's inequality

$$V_{\max}^{l} - \frac{l}{n} < \left(1 - \frac{1}{2^{n+1}}\right)^{k}.$$

Thus, due to (4), we have $d_\infty^*(X) = V_{\max}^0$. This completes the proof. □

4. Discussion

We proved in the previous section that calculating the star discrepancy is an NP-hard problem. To what extent does this affect applications for which estimating the discrepancy is essential?

Recall first that the bad instances we used to establish the NP-hardness of Star Discrepancy displayed in fact a huge discrepancy—for n approaching infinity their star discrepancy tends to the worst possible value 1. It is easily seen that these point sets are, e.g., no serious candidates for well-distributed integration samples and that their components are not suited to serve as good pseudo random numbers. Hence for multivariate integration or pseudo random number generation it is not necessary to test the discrepancy of such pathological point configurations.

So it would be interesting to learn about the complexity of calculating the discrepancy of more interesting point sets.

A first step may be the study of the following relaxed decision problem: Let $\alpha \in (0, 1)$. We consider instances consisting of natural numbers n, d, a sequence $X = (x^i)_{i=1}^n$ in $[0, 1)^d$, and an $\varepsilon \in (0, 1]$. We ask if $d_\infty^*(X) \geq \varepsilon$ holds, but do not demand the true answer in the case that $\varepsilon \leq d_\infty^*(X) \leq (1+\alpha)\varepsilon$. That is the answer "Yes" tells us that in fact $d_\infty^*(X) \geq \varepsilon$, but the answer "No" gives us only the secure information that $d_\infty^*(X) \leq (1+\alpha)\varepsilon$. If $\varepsilon > (1+\alpha)^{-1}$ (as it is the case for the bad instances in the proof of Theorem 2.7 for large n), an algorithm could always provide an acceptable answer by saying "No". (The definition of the relaxed decision problem is inspired by the concept of relaxed verification for continuous problems proposed by Novak and Woźniakowski in [23].)

Studying a relaxed decision problem of this form seems to be of more practical interest than the more rigid decision problem Star Discrepancy, since pathological sequences whose discrepancy of the first n points tends to one as n approaches infinity can be easily handled, and in the applications one is in general not interested in the exact value of the discrepancy of a given point set but only wants to have relatively good upper and lower bounds for it. We think that complexity results for such a relaxed decision problem would be interesting. (Other kinds of complexity results may of course be interesting, too.)

But even if the relaxed decision problem turns out to be infeasible, one may still find distinguished classes of point configurations being good candidates for the samples one is looking for in the applications and which allow for a fast evaluation or approximation of the star discrepancy. A simple example of a class of sets whose star discrepancy can be efficiently evaluated via (1) are tensor product sets ("grids") X—here we obviously have that the cardinality of $\Gamma(X)$ and $\bar{\Gamma}(X)$ are of order $O(n)$. Unfortunately, the discrepancy of these sets is at least of order $\Omega(n^{-1/d})$ in dimension d, which is rather bad.

Finding more suitable classes would be helpful for many applications. For the semi-construction of low-discrepancy sets of moderate size mentioned in the introduction maybe certain classes of lattice rules or of subsets of distinguished tensor product sets (see [4]) could be interesting candidates.

Appendix

For the sake of completeness we verify in this appendix the unproven statements from Remarks 2.5 and 2.9.

Lemma A.1. *Let $G = (V, E)$, $k \in [n]$ with $n = |V|$ be an instance of the problem* Balanced Subgraph. *We assume $V = [n]$ and put $d = n$. Let $\varphi : [n] \times [n] \to [n^2]$ be bijective. Put*

$$x_j^i = \begin{cases} \dfrac{\varphi(i,j)}{2^{2nk}}, & \text{if } \{i,j\} \in E \\ 1 - \dfrac{\varphi(i,j)}{2^{2n}}, & \text{else}. \end{cases}$$

For $n \geq 4$ there is a balanced subgraph of size k for G if and only if there exists a (k^+, ε^-)-box for $X = ((x_j^i)_{j=1}^d)_{i=1}^n$, where $\varepsilon = (\frac{n^2}{2^{2nk}})^k (1 - \frac{1}{2^{2n}})^{n-k}$.

Proof. First, assume the existence of $I, J \subseteq V$ such that $|I| = |J| = k$, $I \cap J = \emptyset$, and $\{i, j\} \in E$ for all $i \in I, j \in J$. Put

$$y_j = \frac{n^2}{2^{2nk}} \cdot 1_J(j) + \left(1 - \frac{1}{2^{2n}}\right) \cdot 1_{V \setminus J}(j), \quad j = 1, \ldots, n.$$

Then $V_y = \varepsilon$ and $\bar{A}(y, X) \geq \sum_{i \in I} 1_{[0,y]}(x^i) = k$.

Now let us assume that there exists a $y \in \Gamma(X)$ such that $V_y \leq \varepsilon$ and $\bar{A}(y, X) \geq k$. There must be at least k coordinates $j_1, \ldots, j_k$ satisfying

$$y_j \leq \frac{n^2}{2^{2nk}},$$

since otherwise

$$V_y > \left(\frac{1}{2^{2nk}}\right)^{k-1} \left(1 - \frac{n^2}{2^{2n}}\right)^{n-k+1} > \left(\frac{n^2}{2^{2nk}}\right)^k \left(1 - \frac{1}{2^{2n}}\right)^{n-k} = \varepsilon.$$

Here the second inequality can be easily seen by using the inequality of Bernoulli $1 + \nu a \leq (1 + a)^\nu$ for all $a \in [-1, \infty)$, $\nu \in \mathbb{N}$:

$$\begin{aligned} \left(1 - \frac{n^2}{2^{2n}}\right)^{n-k+1} &= \left(1 - \frac{n^2}{2^n \cdot 2^n}\right)^{n-k+1} \geq \left(1 - \frac{1}{2^n}\right)^{n-k+1} \geq \left(1 - \frac{1}{2^n}\right)^n \\ &\geq 1 - \frac{n}{2^n} \geq \frac{n}{2^n} > \left(\frac{n}{2^n}\right)^{2k} = \frac{1}{2^{2nk}} \cdot n^{2k}, \end{aligned}$$

which leads to

$$\left(\frac{1}{2^{2nk}}\right)^{k-1} \left(1 - \frac{n^2}{2^{2n}}\right)^{n-k+1} > \left(\frac{1}{2^{2nk}}\right)^{k-1} \cdot \frac{1}{2^{2nk}} \cdot n^{2k} = \left(\frac{1}{2^{2nk}}\right)^k \cdot n^{2k} = \left(\frac{n^2}{2^{2nk}}\right)^k.$$

Now finish the proof the same way as the proof of Theorem 2.3. □

Lemma A.2. *Let $G = (V, E)$, $c \in [n]$ with $n = |V|$ be an instance of* Dominating Set. *We may assume $V = [n]$ and put $d = n$. Let $\varphi : [n] \times [n] \to [n^2]$ be some bijection, and put*

$$x_j^i = \begin{cases} \dfrac{1}{2}\left(1 + \dfrac{\varphi(i,j)}{2^{3n}}\right), & \text{if } \{i,j\} \in E \text{ or } i = j \\ \dfrac{\varphi(i,j)}{2^{3n}}, & \text{else}. \end{cases}$$

Then there exists a dominating set $C \subseteq V$ of cardinality $\leq c$ if and only if there is a $(0^-, \varepsilon^+)$-box for $X = ((x_j^i)_{j=1}^d)_{i=1}^n$, where $\varepsilon = (1/2)^c$.

Proof. Let us first assume that there exists a dominating set $C \subseteq [n]$ of cardinality $\leq c$. Put

$$y_j = \frac{1}{2} \cdot 1_C(j) + 1_{[n]\setminus C}(j), \quad j = 1, \dots, d = n.$$

Then $V_y = (1/2)^{|C|} \geq (1/2)^c$. Furthermore, we have for $i \in C$: $x_i^i > 1/2$ and $y_i = 1/2$, i.e., $x^i \notin [0, y)$. For $i \in [n] \setminus C$ there exists a $\nu \in C$ such that $\{i, \nu\} \in E$. Hence $x_\nu^i > 1/2$ and $y_\nu = 1/2$, implying $x^i \notin [0, y)$. Thus $A(y, X) = 0$. It is easy to see that now there exists a $y' \in \bar{\Gamma}(X)$ such that $y' \geq y$, i.e., $V_{y'} \geq V_y$, and $A(y', X) = A(y, X) = 0$.

Let us now assume that there exists a $y \in \bar{\Gamma}(X)$ such that $V_y \geq (1/2)^c$ and $A(y, X) = 0$. Then $|\{j \in [n]; y_j \geq 1/2\}| = n$. Put $C = \{i \in [n]; y_i \neq 1\}$. We show $|C| \leq c$: If $c = n$, there is nothing to prove. If $c < n$, then

$$V_y = \prod_{\nu \in C} y_\nu \leq \left(\frac{1}{2}\left(1 + \frac{n^2}{2^{3n}}\right)\right)^{|C|},$$

and from

$$\left(\frac{1}{2}\left(1 + \frac{n^2}{2^{3n}}\right)\right)^{c+1} \leq \left(\frac{1}{2}\right)^{c+1}\left(1 + \frac{1}{2^n}\right)^n < \left(\frac{1}{2}\right)^c$$

follows $|C| \leq c$. Let $i \in [n] \setminus C$. Since $x^i \notin [0, y)$, there exists a $\nu \in C$ such that $x_\nu^i \geq y_\nu \geq 1/2$. Thus $\{i, \nu\} \in E$. This shows that C is a dominating set of G. □

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