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Construction of Quasi-DOE on Sobol's Sequences with Better Uniformity 2D Projections

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***Abstract* – In order to establish the projection properties of computer uniform designs of experiments on Sobol's sequences, an empirical comparative statistical analysis of the homogeneity of 2D projections of the best known improved designs of experiments was carried out using the novel objective indicators of discrepancies. These designs show an incomplete solution to the problem of clustering points in low-dimensional projections graphically and numerically, which requires further research for new Sobol's sequences without the drawback mentioned above. In the article, using the example of the first 20 improved Sobol's sequences, a methodology for creating refined designs is proposed, which is based on the unconventional use of these already found sequences. It involves the creation of the next dimensional design based on the best homogeneity and projection properties of the previous one. The selection of sequences for creating an initial design is based on the analysis of numerical indicators of the weighted symmetrized centered discrepancy for two-dimensional projections. According to the algorithm, the combination of sequences is fixed for the found variant and a complete search of the added one-dimensional sequences is performed until the best one is detected. According to the proposed methodology, as an example, a search for more perfect variants of designs for factor spaces from two to nine dimensions was carried out. New combinations of Sobol's sequences with better projection properties than those already known are given. Their effectiveness is confirmed by statistical calculations and graphically demonstrated box plots and histograms of the projection indicators distribution of the weighted symmetrized centred discrepancy. In addition, the numerical results of calculating the volumetric indicators of discrepancies for the created designs with different number of points are given.**

***Keywords* – Computer design of the experiment, discrepancy, direction numbers, projection properties, Sobol's quasi-sequence, uniform distribution.**

I. Introduction

The process of collecting data for scientific and engineering research is a rather complex problem due to the difficulties of their obtaining in large quantities, which, however, can be solved using the design of experiments. An effective design of the experiment is of decisive importance in the study of scientific problems. In the modern designing of experiments, significant attention is paid to their computer variants [1]. The scope of their use is rather vast: from technical applications [2]–[5] to financial engineering [6], which is explained by the comprehensive implementation of computer modelling in the practice of scientific research, for example, surrogate optimization, quasi-Monte Carlo simulation, stochastic global optimization, Pareto set approximation in multi-criteria optimization, and some computer graphics applications. Among the computer designs of experiments (DOE), we will focus on the space filling design, namely uniform designs of experiments [7], which are among the most widely used in modelling in various tasks. To create appropriate designs with a uniform distribution in a unit hypercube, the quasi-Monte Carlo method is used, involving one-dimensional sequences with low discrepancies to obtain a set of deterministic points. Plans on such sequences are called quasi-DOEs. In general, the best results are believed to be achieved by plotting on quasi-random Sobol's LPτ-sequences [8]. A design is considered effective if it demonstrates uniformity not only in hyperspace, but also for specific low-dimensional projections [9]. However, the creation of designs with improved uniformity of low-dimensional projections is a non-trivial task, and many scientific studies have been devoted to this problem. Although quasi-random designs based on Sobol's sequences provide the best properties of filling hyperspace points, researchers have determined that in certain cases the tendency of distribution points to group into clusters in 2D projections, violating their uniformity. The established cause of such a problem is an unsuccessful selection of sets of direction numbers to calculate the points of the Sobol's sequences, which make up the overall experimental design for each specific case. That is, it is the rational choice of sets of quasi-sequences that ensures the necessary homogeneous properties of designs and the absence of bad two-dimensional projections and the collapse effect [6]. Attention to maintaining noncollapsing designs is important, since the space filling criterion is always aimed only at the entire project space, that is, it is essentially volumetric. In fact, low-dimensional projections characterise the property of the design for placing samples of the sampling to obtain information in accordance with the maximum possible number of factors, even if some of them do not affect the response. As a result, a guaranteed coverage of all subsets of the design with samples is observed [10], [11].

The first significant steps in improving the projection properties of experimental designs on uniformly distributed sequences of binary-rational Sobol's quasi-random numbers

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were made in paper [12], where the authors proposed the introduction of additional conditions of uniformity, known as Property A and Property A′. Formulated properties and conditions for achieving homogeneity when implementing one or both of them as a result of following certain rules for choosing direction numbers provided advantages for using this type of created Sobol’s sequences over known others. However, it turned out that matching properties, especially Property A, which is of greater practical interest, is not enough to ensure the absence of bad correlations between pairs of measurements [13], [14].

Hereinafter, the improvement of quasi-sequences was carried out using optimization techniques in order to avoid problems caused by an unsuccessful choice of direction numbers. In the study [15], a computer search is performed for new sets of direction numbers that are subject to Property A and are found as a result of optimization with a criterion based on t-values in the range of values for m, that is, minimization in a certain sense of t-values of two-dimensional projections of point sets. The authors themselves note the existence of a problem regarding the correctness of the selection of appropriate search criteria, which does not allow us to consider the task of finding Sobol’s sequences with more perfect low-dimensional projections as finally solved. In [16], certain shortcomings of the results obtained in [15] are given, in particular, it is stated that despite the potentially attractive theoretical advantages of the defined directions of numbers, they are not confirmed in practice, and in some cases even demonstrate unacceptable quality of 2D projections. At the same time, in [6] the opposite is stated about the positive results of the studies [15], which is confirmed by a comparative analysis of numerical calculations on test models. The same authors [15] note that the new Sobol’s sequences obtained by them on the basis of “optimal” sets of direction numbers are, in the worst cases, at least comparable to the old ones.

The next important stage of the research in the direction of correcting bad 2D projections was the paper [17], demonstrating the effect of imposing additional homogeneity properties on low-dimensional sequence projections in addition to the uniformity properties of the multidimensional sequence itself, which made it possible to achieve positive results in comparison with other known Sobol’s sequence generators when calculating multidimensional integrals.

In the paper [18], in the context of considering the problem of calculating multidimensional integrals by the quasi-Monte Carlo method, a fully deterministic algorithm for optimizing the direction numbers of Sobol’s sequences is proposed. In [19], the authors try to find a solution to this very problem as a result of optimizing the free parameters available in the definition of the Matousek scrambling and the Owen scrambling in order to obtain the best distribution. The authors of [18], [19] propose a continuation of the implementation of the research idea in [20] for the situations related to the high dimensionality of the space in comparison with the number of points of the sequence used. Summarising, we note that in all the mentioned cases, the optimization was carried out as a result of a computer search using certain filtering techniques of such sets of direction numbers that would provide the best distribution of sequences. Unfortunately, the authors cited only the indirect results of the performed studies, limiting them only to the values of test calculations of multidimensional integrals. At the same time, they failed to demonstrate the objective numerical characteristics of the obtained homogeneous distributions in the form of discrepancy indicators, to conduct a statistical and graphical analysis of the projection properties for 2D measurements.

In the paper [21], the authors proposed an algorithm for creating groups of experimental designs with uniform filling of the multidimensional design space with high-quality projections in terms of homogeneity in one and two dimensions. Sobol’s sequences are used for this purpose, which, according to the authors, allows preserving the indicated properties of the designs as a whole when combining groups. The algorithm uses optimization techniques with the maximin distance criterion and a new optimality criterion based on the spread of the minimum distance of each point from all others, as well as a perturbation strategy when combining groups into a single one to effectively achieve homogeneity in the design hyperspace. A crucial requirement for the given space-filling design is also emphasized, which is critically applied in, at least, sequences with a uniform 1D projection. The research considers the creation of uniform multidimensional designs with an increasing number of points, and, in fact, the projection properties of the obtained designs are not addressed, especially for the cases of many dimensions, which leaves the issue of their quality unresolved.

Therefore, a critical analysis of the sources of information regarding the problem under consideration showed the need for additional research of new designs, conditioned by the use of such sets of direction numbers for Sobol’s quasi-sequences, which guarantee not only general volumetric homogeneity of the created designs of experiments, but also their qualitative projection properties in 2D dimensions.

Given the sometimes contradictory information about the guide numbers of the Sobol's LPτ-sequences found by previous researchers, the *goal of this research* is to develop a methodology for constructing more advanced quasi-experimental designs based on them, characterised by improved 2D projection properties and low volumetric discrepancy rates.

II. Research Methodology

The research methodology was as follows. For conducting numerical experiments, the first 20 modified Sobol’s sequences were used, the direction numbers for which were calculated according to [22]. Designs of experiments with different number of points were formed from one-dimensional sequences as a result of sequential component-wise selection. The generation of designs started with two-dimensional ones and was carried out by a complete sorting of all possible combinations of the 20 specified sequences. To create three-dimensional designs, the two-dimensional one best in terms of homogeneity and projection properties was used, assuming that the next dimensional design can be obtained from the previous one. The algorithm involved fixing a combination of sequences for a two-dimensional variant and a full review of the added sequences until the best three-dimensional combination was found. The evaluation of the quality of the candidate design was implemented by calculating the indicators of discrepancies both for the design as a whole and for each of its 2D projections.

Therefore, for a comprehensive assessment of the homogeneity of the designs, indicators of both the classic centered CD and wrap-around WD discrepancies [1], as well as the novel mixed MD [23] and weighted symmetrized centred WSCD discrepancies [24] were calculated, the expressions for calculating which are given in the APPENDIX.

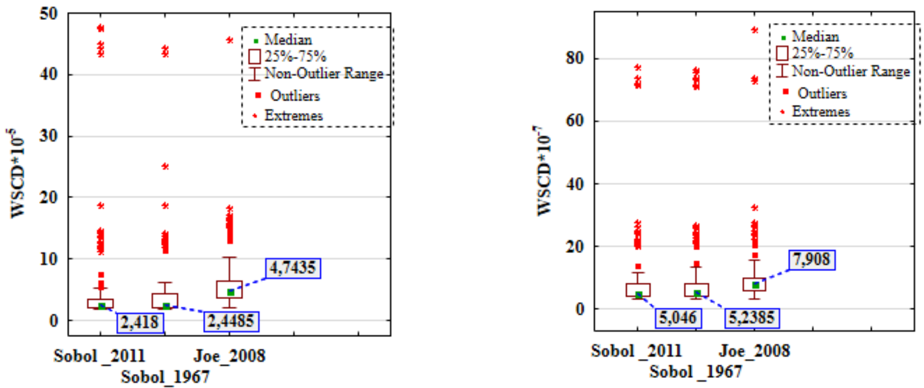
The WSCD indicator should be especially noted for its ability to adjust weighting coefficients for spaces of different dimensions and the presence of advantages of the new function of the divergence calculation kernel, which in the complex to a certain extent eliminates the known disadvantages of using classical indicators. The selected best designs were compared according to the relevant indicators with those obtained on the basis of recommendations [15], [17], which were generated by the codes borrowed from [25] for the optimality criterion $D^{(6)}$ and from [22]. Graphical analysis based on Voronoi diagrams was performed for the received 2D projections of the designs. In addition, histograms of the distribution of discrepancies of all low-dimensional projections of each variant of the design were subject to visual analysis, by means of which their quality was assessed. Based on the obtained statistical indicators of discrepancies of 2D projections, i.e., median, lower and upper quartiles, non-outlier range, etc., in combination with the results of graphic analysis, conclusions were drawn regarding the acceptability of the design variant.

Therefore, the task was to find new quasi-DOE variants with improved projection properties, more perfect in terms of indicators than those established by the authors [15] and [25], [17] and [22].

III. Numerical Experiments

For an empirical study of the projection properties of the improved Sobol's sequences, recognized according to the review of publications as the most perfect, a number of numerical experiments were conducted on their analysis. Experiments were performed for sequence variants, for which the following designations were introduced for clarity: Joe_2008, which corresponds to the sequences proposed by S. Joe and F.Y. Kuo [25], and Sobol_2011, obtained by Sobol and co-authors in [22]. Designs created on the first 20 of these sequences with the number of points 127 and 1023 were selected for calculations. Conclusions regarding the homogeneity of 2D design projections were made as a result of statistical analysis of the WSCD discrepancy indicators, which were calculated for all design projections. For example, Table I, Table II and Table III (Appendix) are given, which contain the values of these indicators calculated for two-dimensional projections of the design with 1023 points.

The results of the observations are graphically demonstrated by box plots presented in Fig. 1. A comparative analysis of research results with similar designs of experiments performed on classic Sobol's sequences with a set of direction numbers borrowed from [26] and designated as Sobol_1967 was also carried out. This made it possible to advance the view of the degree of improvement of the low-dimensional projection properties of the analysed varieties of Sobol's sequences.



(a) (b)

Fig. 1. Box-and-whisker plot diagrams for designs with different number of points: (a) $N = 127$ and (b) $N = 1023$.

Some WSCD values are not displayed on the diagrams, which differ significantly, even by orders of magnitude, from those given, which is explained by the choice of an adequate scale that allows detailed visual analysis of the situation. Therefore, these emissions for the design with 1023 points are: for Sobol_1967 sequences – $272.19\cdot10^{-7}$ on the projection (ξ_3, ξ_{11}), $279.9\cdot10^{-7}$ on the projection (ξ_8, ξ_{15}) (see Table I); Sobol_2011 – $4332\cdot10^{-7}$ on the (ξ_{10}, ξ_{18}) projection (see Table III). A similar situation is observed for the design with 127 points, where the emissions on the projections (ξ_2, ξ_{10}) and (ξ_3, ξ_9) on the Sobol_1967 sequences take the same values and are equal to $172.2\cdot10^{-5}$.

At the same time, a visual analysis of the quality of the 2D projections of the designs, namely the homogeneity of the distribution of points was carried out using Voronoi diagrams to assess the degree of homogeneity in terms of the area of all formed segments. Figures 2–4 (Appendix) illustrate the worst pairwise projections with the largest *WSCD* scores for the designs on all kinds of Sobol's sequences.

All the projections shown on them demonstrate the tendency of the distribution points to group into clusters, which is also confirmed by the associative relationship with the calculated corresponding values of the weighted symmetrized centred discrepancy, shown in the same figures.

TABLE IV

NEW COMBINATIONS OF SOBOL'S SEQUENCES WITH MORE ADVANCED PROJECTION PROPERTIES

LP_τ	ξ_1	ξ_2	ξ_3	ξ_4	ξ_5	ξ_6	ξ_7	ξ_8	ξ_9	ξ_{10}	ξ_{11}	ξ_{12}	ξ_{13}	ξ_{14}	ξ_{15}	ξ_{16}	ξ_{17}	ξ_{18}	ξ_{19}	ξ_{20}
Three-factor uniform design of experiment																				
3LPτ–1		■								■							■			
3LPτ–2	■					■								■						
3LPτ–3	■	■	■																	
3LPτ–4	■	■					■													
Four-factor uniform design of experiment																				
4LPτ–1		■						■		■							■			
4LPτ–2	■					■								■			■			
4LPτ–3	■	■	■	■																
4LPτ–4	■	■		■			■													
Five-factor uniform design of experiment																				
5LPτ–1		■					■	■		■							■			
5LPτ–2	■	■				■								■			■			
5LPτ–3	■	■	■	■			■													
5LPτ–4	■	■		■			■								■					
Six-factor uniform design of experiment																				
6LPτ–1		■					■	■		■				■			■			
6LPτ–2		■	■				■	■		■							■			
6LPτ–3		■					■	■		■						■	■			
6LPτ–4	■	■	■			■								■			■			
6LPτ–5	■	■			■	■								■			■			
6LPτ–6	■	■				■							■	■			■			
6LPτ–7	■	■				■	■							■			■			
6LPτ–8	■	■	■	■	■		■													
6LPτ–9	■	■	■	■			■								■					
Seven-factor uniform design of experiment																				
7LPτ–1	■	■	■		■	■								■			■			
7LPτ–2	■	■			■	■				■				■			■			
7LPτ–3	■	■		■	■	■								■			■			
7LPτ–4	■	■			■	■	■							■			■			
7LPτ–5	■	■			■	■			■					■			■			
7LPτ–6	■	■			■	■							■	■			■			
7LPτ–7	■	■			■	■								■			■	■		
Eight-factor uniform design of experiment																				
8LPτ–1	■	■	■		■	■				■				■			■			
8LPτ–2	■	■	■	■	■	■								■			■			
8LPτ–3	■	■	■		■	■	■							■			■			
8LPτ–4	■	■	■		■	■							■	■			■			
8LPτ–5	■	■	■		■	■								■			■	■		
8LPτ–6	■	■	■		■	■								■			■		■	
Nine-factor uniform design of experiment																				
9LPτ–1	■	■	■		■	■	■							■			■	■		
9LPτ–2	■	■	■	■	■	■	■							■			■			
9LPτ–3	■	■	■		■	■	■							■			■		■	
9LPτ–4	■	■	■	■	■	■								■			■	■		
9LPτ–5	■	■	■		■	■								■			■		■	

Empirical comparative analysis of 2D projections of experimental designs on the most famous improved Sobol's sequences demonstrates the imperfection of the design variants created on their basis. At the same time, it is worth noting the convincing advantages of both designs with different numbers of points built on the Sobol_2011 sequences over others. Therefore, it is advisable to further search for new sets of sequences that would provide lower rates of volumetric and two-dimensional projection design discrepancies.

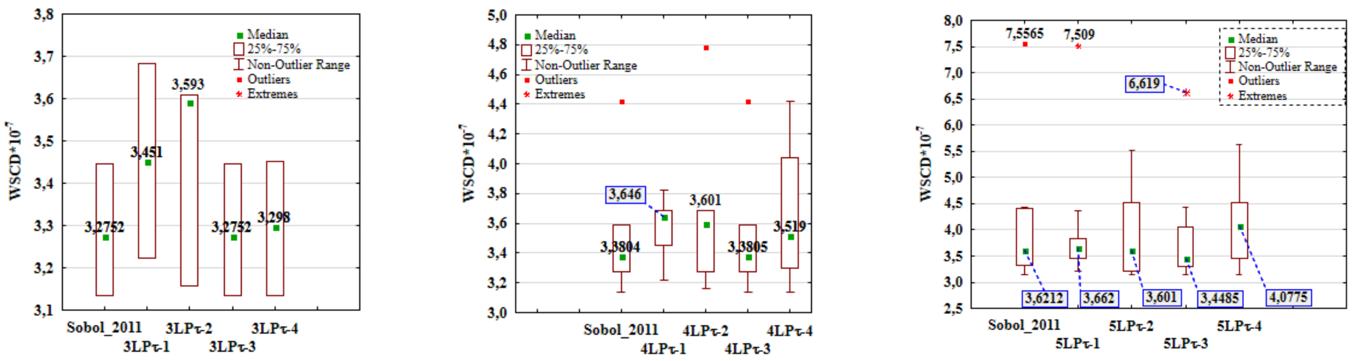
According to the proposed methodology, the authors created designs of experiments based on their established best set Sobol_2011 selected according to the above-mentioned homogeneity criteria to ensure acceptable projection properties.

The search for their more perfect variants with 1023 points was carried out for factor spaces from two to nine dimensions. Table IV shows the best obtained combinations of Sobol's sequences, which are highlighted in colour, and their coding is introduced.

As a result of statistical calculations, the results of which are shown in Fig. 5 in a graphic form, a comparative analysis of the combinations of sequences with prototypes proposed by the authors for different factor spaces was carried out.

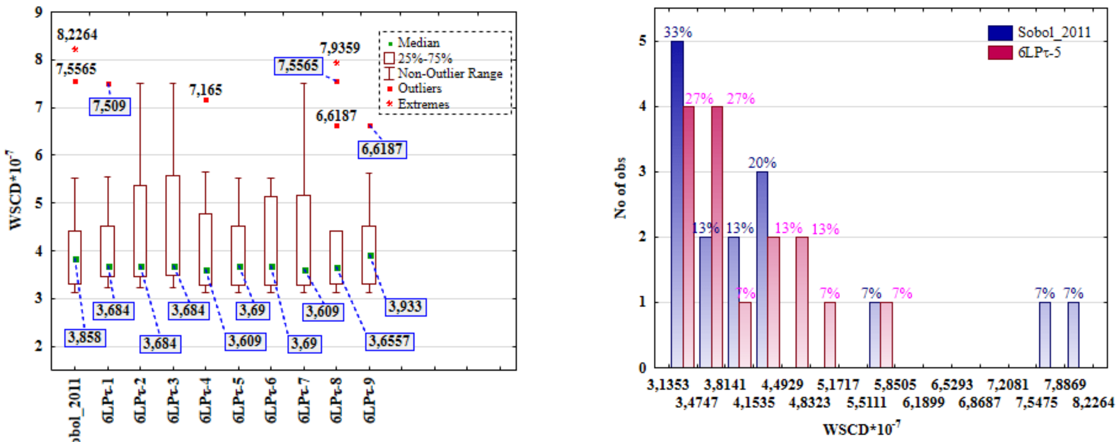
If for the three-, four- and five-factor designs for their best options, the results are actually identical in quality to the prototypes, then already on the six-factor design there is a certain improvement of the candidate design for the 6LPτ−5 combination (Fig. 6). It should be noted that in order to find this version of the design, it was necessary to investigate a certain hierarchical structure of the formation of applicant designs: on the basis of 5LPτ−1, applicants 6LPτ−1 – 6LPτ−3 were created; based on 5LPτ−2 – respectively 6LPτ−4 – 6LPτ−7, etc.

The expediency of choosing this particular combination of Sobol's sequences for creating a six-factor experimental design is confirmed by the histograms of the distributions of discrepancies for the analysed variety and the corresponding prototype (Fig. 6b). Both of these designs show almost the same indicators of homogeneity of projections. However, the prototype has two outliers forming the sequences (ξ_4, ξ_5) and (ξ_4, ξ_6), unlike the design on the sequence combination 6LPτ−5, for which all WSCD values of the projections are within the non-outlier range.



(a) (b) (c)

Fig. 5. "Box with whiskers" diagrams for designs of different dimensions with $N = 1023$: (a) is three-factor and (b) is four-factor and (c) is five-factor.



(a) (b)

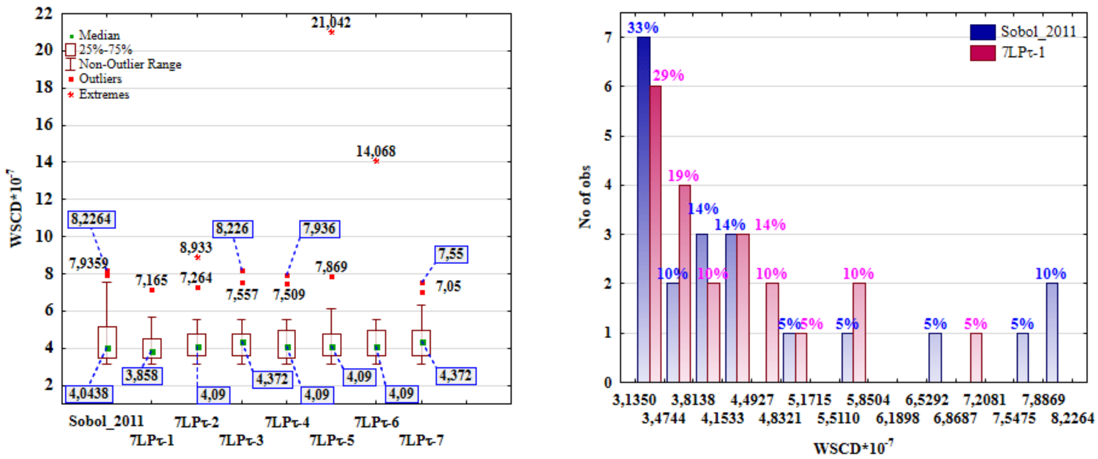
Fig. 6. The analysis of statistical indicators for six-factor designs: (a) is "box with whiskers" diagrams of *WSCD* projection indicators and (b) is histograms of the distribution of indicators of discrepancies of 2D projections.

Table V contains the numerically calculated volume measures of *CD*, *WD*, *MD*, and *WSCD* discrepancies for designs with different numbers of points in the six-factor space. For all cases of design evaluation with conflicting indicators of discrepancies, the *WSCD* indicator was preferred due to its greater perfection [24].

TABLE V
INDICATORS OF VOLUMETRIC DISCREPANCIES FOR THE PROPOSED BEST OPTIONS OF SIX-FACTOR DESIGNS OF EXPERIMENTS ON NEW COMBINATIONS OF SEQUENCES

Combinations of sequences	Number of points of the design	$CD(P)^2 \cdot 10^{-3}$	$WD(P)^2$	$MD(P)^2 \cdot 10^{-3}$	$WSCD(P)^2 \cdot 10^{-3}$
6LPτ−1	$N = 31$	28.709761	11.310316	144.171298	0.320782
	$N = 127$	5.68399	11.255842	32.397446	0.04849905
	$N = 511$	0.45081	11.238943	2.520635	0.003071041
	$N = 1023$	0.094527	11.23764	0.453312	0.0003291458
6LPτ−5	$N = 31$	18.812932	11.299139	109.346919	0.237927
	$N = 127$	2.186651	11.246012	12.552014	0.018057
	$N = 511$	0.431165	11.23892	2.408089	0.002751995
	$N = 1023$	0.095705	11.237635	0.447015	0.0003171118
6LPτ−9	$N = 31$	15.650665	11.288267	89.731476	0.212231
	$N = 127$	2.624273	11.244994	12.846477	0.020728
	$N = 511$	0.207117	11.238016	1.009143	0.001118348
	$N = 1023$	0.072899	11.23757	0.342922	0.0002955792
Sobol_2011	$N = 31$	16.121807	11.28917	92.531943	0.2162901
	$N = 127$	1.782498	11.24324	8.927928	0.01401179
	$N = 511$	0.193313	11.238015	0.969702	0.00108588
	$N = 1023$	0.063502	11.237552	0.321374	0.0003135235

The further search for designs of higher dimensionality was performed on the basis of the newly found set of 6LPτ−5 sequences. For the variants of the seven-factor designs found by a complete search of the sequence added to the main combination calculations of the corresponding statistical characteristics were performed according to the algorithm similar to the previous experiments. Figure 7 made it possible to isolate a promising combination of 7LPτ−1 sequences for the further research. Volume indicators of disagreements together with the indicators of some good aggregates in the seven-factor space are presented in Table VI.



(a) (b)

Fig. 7. The analysis of statistical indicators for seven-factor designs: (a) is "box with whiskers" diagrams of *WSCD* projection indicators and (b) is histograms of the distribution of indicators of discrepancies of 2D projections.

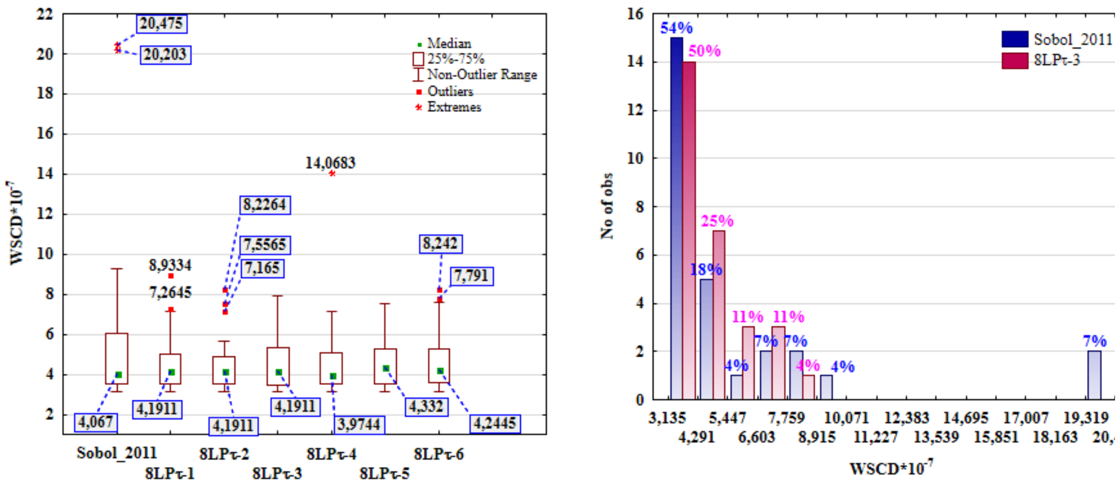
TABLE VI

Indicators of Volumetric Discrepancies for the Proposed Best Options of Seven-Factor Designs of Experiments on New Combinations of Sequences

Combinations of sequences	Number of points of the design	$CD(P)^2 \cdot 10^{-3}$	$WD(P)^2$	$MD(P)^2 \cdot 10^{-3}$	$WSCD(P)^2 \cdot 10^{-3}$
7LPτ−1	$N = 31$	27.764583	15.09819	236.127016	0.30377
	$N = 127$	4.015851	15.000214	31.537308	0.028634
	$N = 511$	0.657797	14.985909	5.047348	0.003506745
	$N = 1023$	0.157093	14.983722	1.038758	0.0004488243
7LPτ−4	$N = 31$	29.15454	15.098286	240.503813	0.314502
	$N = 127$	3.738329	15.000705	30.213014	0.024719
	$N = 511$	0.708433	14.985927	5.137145	0.003363344
	$N = 1023$	0.222409	14.983803	1.293564	0.0005254929
7LPτ−5	$N = 31$	30.52608	15.101158	250.3278	0.325074
	$N = 127$	3.625625	14.999033	27.756465	0.0235
	$N = 511$	0.663962	14.985932	5.05543	0.00345667
	$N = 1023$	0.211747	14.983844	1.322887	0.0005580185
Sobol_2011	$N = 31$	26.622533	15.086056	216.993973	0.2944844
	$N = 127$	3.140208	14.994981	21.999524	0.02005147
	$N = 511$	0.359587	14.984643	2.540841	0.001547291
	$N = 1023$	0.129471	14.983632	0.879688	0.000456143

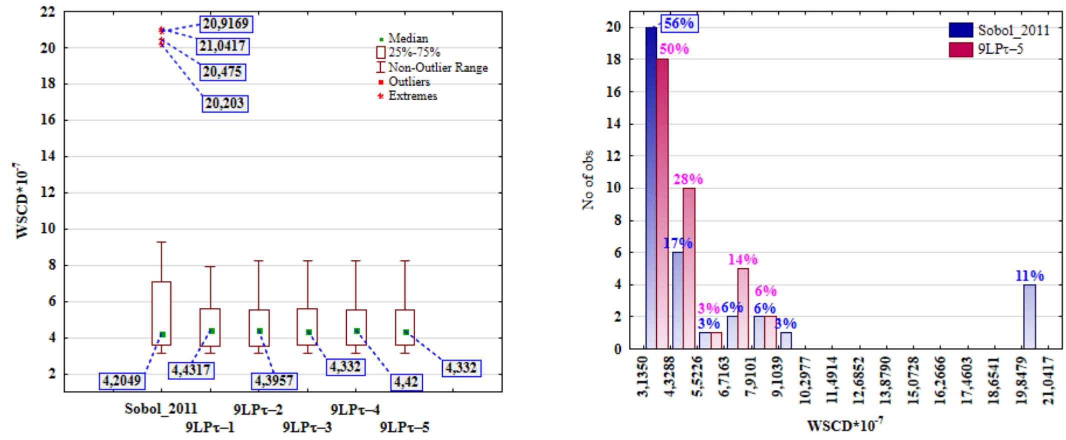
The creation of designs for eight- and nine-factor spaces was carried out in the same way. The best seven-factor sequence combination of 7LPτ−1 was used as the basis for constructing the next eight-factor design. As a result, two aggregates were selected – 8LPτ−2 and 8LPτ−3, which have practically the same indicators of projection discrepancies and which serve as the basis for creating nine-factor designs. As in the previous cases, for designs of smaller dimensions, the selection and analysis of new combinations of sequences was carried out using scale diagrams (Figs. 8a and 9a) and for designs on the selected aggregates, the histograms of distributions of *WSCD* projection indicators were constructed (Figs. 8b and 9b). Accordingly, Table VII and Table VIII show the volume differences for the best sequence combinations found for the eight- and nine-factor designs.

Therefore, the proposed methodology for finding new combinations of Sobol's quasi-sequences ensures the necessary homogeneous projection properties of designs and the absence of the effect of unwanted grouping of points into clusters.



(a) (b)

Fig. 8. The analysis of statistical indicators for eight-factor designs. (a) is "box with whiskers" diagrams of *WSCD* projection indicators and (b) is histograms of the distribution of indicators of discrepancies of 2D projections.



(a) (b)

Fig. 9. The analysis of statistical indicators for nine-factor designs: (a) is "box with whiskers" diagrams of *WSCD* projection indicators and (b) is histograms of the distribution of indicators of discrepancies of 2D projections.

TABLE VII

INDICATORS OF VOLUMETRIC DIFFERENCES FOR THE PROPOSED BEST OPTIONS OF EIGHT-FACTOR DESIGNS OF EXPERIMENTS ON NEW COMBINATIONS OF SEQUENCES

Combinations of sequences	Number of points of the design	$CD(P)^2 \cdot 10^{-3}$	$WD(P)^2$	$MD(P)^2 \cdot 10^{-3}$	$WSCD(P)^2 \cdot 10^{-3}$
8LPτ–2	$N = 31$	41.801831	20.179579	500.049228	0.39116
	$N = 127$	6.202748	20.007122	65.24872	0.034757
	$N = 511$	0.979025	19.982362	10.310375	0.004103681
	$N = 1023$	0.291468	19.978804	2.664993	0.0006569325
8LPτ–3	$N = 31$	42.525733	20.186607	510.692672	0.396249
	$N = 127$	6.315941	20.009777	69.788755	0.03655
	$N = 511$	1.15486	19.982538	11.029995	0.004280242
	$N = 1023$	0.332366	19.97884	2.840957	0.000701116
8LPτ–5	$N = 31$	43.777951	20.183487	513.672709	0.398842
	$N = 127$	7.344476	20.009389	73.38338	0.042357
	$N = 511$	1.418529	19.983353	12.930556	0.005074828
	$N = 1023$	0.312688	19.978919	2.879081	0.0006739865
Sobol_2011	$N = 31$	39.298077	20.161438	460.138167	0.37228556
	$N = 127$	5.373487	20.000598	51.01718	0.02622118
	$N = 511$	0.706348	19.980819	6.744938	0.00226884
	$N = 1023$	0.286071	19.978708	2.564797	0.0008006

TABLE VIII

INDICATORS OF VOLUMETRIC DISCREPANCIES FOR THE PROPOSED BEST OPTIONS OF NINE-FACTOR DESIGNS OF EXPERIMENTS ON NEW COMBINATIONS OF SEQUENCES

Combinations of sequences	Number of points of the design	$CD(P)^2 \cdot 10^{-3}$	$WD(P)^2$	$MD(P)^2 \cdot 10^{-3}$	$WSCD(P)^2 \cdot 10^{-3}$
9LPτ–3	$N = 31$	67.232965	27.016216	1129.27	0.52973
	$N = 127$	10.661591	26.694216	153.832956	0.051675
	$N = 511$	2.120955	26.646693	26.37223	0.006021832
	$N = 1023$	0.560823	26.639486	6.904157	0.0009819638
9LPτ–5	$N = 31$	70.3771	26.997248	1103.327	0.558465
	$N = 127$	10.224223	26.694576	150.898447	0.046483
	$N = 511$	1.856867	26.64589	24.16055	0.00531544
	$N = 1023$	0.62457	26.639544	7.37461	0.0010498648
Sobol_2011	$N = 31$	61.564693	26.980562	1027.54246	0.499997
	$N = 127$	9.140274	26.682701	123.055175	0.038443
	$N = 511$	1.439116	26.643266	16.910987	0.003331481
	$N = 1023$	0.496914	26.63914	6.187372	0.00117735

IV. Conclusions

Summarising the results of the research, it can be noted that the authors' empirical analysis of the low-dimensional projection properties obtained by the predecessors of the improved Sobol sequences showed that they did not manage to fully solve the problem of guaranteeing highly homogeneous two-dimensional projections in multivariate homogeneous designs of experiments within the framework defined by them. It turned out that generally quite good designs of experimental created on these sequences are characterised in some 2D projections by sometimes even a "catastrophic" ability to group points into clusters. Such projections may not manifest themselves abnormally in cases where the factor hyperspace is significantly multidimensional and characterised by thousands of dimensions. However, in modelling practice, there are other cases where the presence of such projections in the designs is a significant obstacle. For such cases, it is desirable to have sets of Sobol's quasi-sequences with no tendency to cluster in projections.

Prospects for a possible further solution to the mentioned problem, according to the authors, consist in the search for new Sobol's sequences as combinations of those containing the best prototype followed by their cataloguing. Numerous examples of the implementation of this idea give reason to believe that it is fruitful. It was possible to obtain a number of combinations of six-, seven-, eight- and nine-component Sobol's sequences that allowed for the creation of computer uniform designs with better projection properties than the best prototype. However, it turned out that the identified positive trend was not universal, that is, during the creation of variants of experimental designs based on the found new sets of sequences, it became clear that they lost their advantages as a result of changing the number of points in the design. In other words, the found combinations of sequences have a specialized purpose and can be successfully used only for the number of design points for which they were searched. This fact certainly somewhat limits their wider use, but does not exclude their use in a number of cases where it is important to obtain high-quality design projections.

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APPENDIX

The expressions for calculating discrepancies [1. 23]: centred L_2-discrepancy (CD) –

$$\left[CD(P)\right]^2=\left(\frac{13}{12}\right)^d-\frac{2}{N}\cdot\sum_{k=1}^{N}\prod_{j=1}^{d}\left[1+\frac{1}{2}\cdot\left|x_{kj}-0.5\right|-\frac{1}{2}\cdot\left|x_{kj}-0.5\right|^2\right]+\frac{1}{N^2}\cdot\sum_{k=1}^{N}\sum_{j=1}^{N}\prod_{i=1}^{d}\left[1+\frac{1}{2}\cdot\left|x_{kj}-0.5\right|+\frac{1}{2}\cdot\left|x_{ji}-0.5\right|-\frac{1}{2}\cdot\left|x_{kj}-x_{ji}\right|\right]$$

wrap-around L_2-discrepancy (WD) - $\left[WD(P)\right]^2=\left(\frac{4}{3}\right)^d+\frac{1}{N^2}\cdot\sum_{k=1}^{N}\sum_{i=1}^{N}\prod_{j=1}^{d}\left[\frac{3}{2}-\left|x_{ki}-x_{ji}\right|\cdot\left(1-\left|x_{ki}-x_{ji}\right|\right)\right].$

mixture L_2-discrepancy (MD) –

$$\left[MD(P)\right]^2=\left(\frac{19}{12}\right)^d-\frac{2}{N}\sum_{i=1}^{N}\prod_{j=1}^{d}\left[\frac{5}{3}-\frac{1}{4}\cdot\left|x_{ij}-\frac{1}{2}\right|-\frac{1}{4}\cdot\left|x_{ij}-\frac{1}{2}\right|^2\right]+\frac{1}{N^2}\sum_{i=1}^{N}\sum_{k=1}^{N}\prod_{j=1}^{d}\left(\begin{array}{l}\frac{15}{8}-\frac{1}{4}\cdot\left|x_{ij}-\frac{1}{2}\right|-\frac{1}{4}\cdot\left|x_{kj}-\frac{1}{2}\right|-\frac{3}{4}\cdot\left|x_{ij}-x_{kj}\right|+\\+\frac{1}{2}\cdot\left|x_{ij}-x_{kj}\right|^2\end{array}\right).$$

weighted symmetrized centred discrepancy ($WSCD$) -

$$\left[WSCD(P)\right]^2=\left[1+\left(\frac{2}{3}\right)\cdot\omega\right]^d-\left[\left(\frac{2}{N}\right)\cdot\sum_{i=1}^{N}\prod_{j=1}^{d}\left[1+\omega\cdot\left[\left(\frac{1}{2}\right)+x_{ij}-x_{ij}^2\right]\right]\right]+\frac{1}{N^2}\cdot\left[\sum_{k=1}^{N}\sum_{i=1}^{N}\prod_{j=1}^{d}\left[1+\omega\cdot\left[1-\left|x_{ij}-x_{kj}\right|\right]\right]\right],$$

where N is the number of points of the experimental design, d is the dimensionality of space, ω is a weight that takes the value of 1/4 for low-dimensional designs of experiments and 1/20 for high-dimensional designs.

TABLE I

DISCREPANCY VALUES OF $WSCD\cdot 10^{-7}$ FOR DESIGN ON THE SOBOL_1967 SEQUENCES

	ξ_2	ξ_3	ξ_4	ξ_5	ξ_6	ξ_7	ξ_8	ξ_9	ξ_{10}
ξ_1	3.135271	3.446261	3.586738	3.655722	3.157862	3.450995	20.20318	4.733149	7.264484
ξ_2		3.27521	4.420583	4.419499	5.515511	3.29763	3.642641	3.450114	3.679757
ξ_3			3.314533	3.858025	4.292092	6.618729	4.842493	21.45324	4.966227
ξ_4				7.556529	8.226353	4.043833	3.932138	5.596591	5.701185
ξ_5					4.090172	7.935852	20.47511	21.63889	21.23221
ξ_6						5.16709	9.251812	4.39926	21.5892
ξ_7							3.674877	4.045617	4.31512
ξ_8								3.92267	21.0705
ξ_9									24.15898
ξ_{10}									
ξ_{11}									
ξ_{12}									
ξ_{13}									
ξ_{14}									
ξ_{15}									
ξ_{16}									
ξ_{17}									
ξ_{18}									
ξ_{19}									

	ξ_{11}	ξ_{12}	ξ_{13}	ξ_{14}	ξ_{15}	ξ_{16}	ξ_{17}	ξ_{18}	ξ_{19}	ξ_{20}
ξ_1	4.776211	21.58757	5.313264	4.317837	7.246687	3.298493	3.690371	4.443629	7.790726	4.433307
ξ_2	8.234781	5.761331	9.53217	5.952952	5.209362	26.66922	3.221957	7.04957	4.196881	4.506192
ξ_3	272.1966	23.53816	24.57291	6.663328	5.052704	4.938041	7.165084	4.667765	8.242427	4.799243
ξ_4	3.441723	3.618375	71.19144	76.26067	4.161565	11.70234	4.645157	6.682162	4.277706	6.170309
ξ_5	7.180612	5.634211	12.38862	3.451816	8.504796	5.53103	4.372423	6.321572	4.189077	20.23596
ξ_6	4.194298	7.897992	5.267591	20.01587	4.137402	21.25421	4.785323	7.550409	4.680258	3.95661
ξ_7	4.38662	5.090417	7.772068	3.521008	8.245029	22.74584	7.50879	7.139842	3.619694	20.99323
ξ_8	3.577598	4.561826	5.428419	4.409712	279.9596	4.707672	3.648729	3.292502	4.566422	4.426012
ξ_9	3.821121	8.280628	7.706479	3.669583	3.483265	5.887212	3.330872	4.193432	3.291396	21.20911
ξ_{10}	4.021908	3.977921	3.450031	5.015911	10.88844	4.171001	3.665614	73.46166	5.999559	26.31009
ξ_{11}		3.298475	4.40806	21.3764	19.97826	71.61944	9.667457	7.17474	21.38016	5.280181
ξ_{12}			4.044699	7.262044	73.75374	7.927747	13.33699	25.71056	3.39636	4.397036
ξ_{13}				3.597228	6.457606	7.339785	4.415319	7.666438	4.921669	8.404516
ξ_{14}					20.44443	3.668402	3.424172	12.81079	8.801858	6.473425
ξ_{15}						9.512942	4.392525	4.193861	75.69399	4.290341
ξ_{16}							14.73467	4.377707	4.629005	8.297501
ξ_{17}								5.536856	7.54368	3.480233
ξ_{18}									10.03214	5.6842
ξ_{19}										24.51987

TABLE II

DISCREPANCY VALUES OF *WSCD* · 10^{-7} FOR DESIGN ON THE JOE_2008 SEQUENCES

	ξ_2	ξ_3	ξ_4	ξ_5	ξ_6	ξ_7	ξ_8	ξ_9	ξ_{10}
ξ_1	6.07952	5.173161	4.462667	4.514601	5.621243	3.809093	5.058498	21.456978	7.459557
ξ_2		8.560936	6.761909	6.844661	9.022332	7.302943	17.394579	8.582609	11.12089
ξ_3			5.874076	6.255624	7.400787	6.347632	8.454173	7.659716	12.42753
ξ_4				7.348459	8.860304	3.382962	6.525121	5.133513	12.416441
ξ_5					4.677235	3.65814	5.811236	5.274983	7.382682
ξ_6						5.889926	7.083168	10.369522	9.781544
ξ_7							6.104199	3.868105	8.959195
ξ_8								7.185477	10.530805
ξ_9									12.778902
ξ_{10}									
ξ_{11}									
ξ_{12}									
ξ_{13}									
ξ_{14}									
ξ_{15}									
ξ_{16}									
ξ_{17}									
ξ_{18}									
ξ_{19}									

	ξ_{11}	ξ_{12}	ξ_{13}	ξ_{14}	ξ_{15}	ξ_{16}	ξ_{17}	ξ_{18}	ξ_{19}	ξ_{20}
ξ_1	8.899532	20.349856	12.750539	6.381515	6.381515	5.317316	3.847379	8.095746	5.30034	7.782563
ξ_2	9.076746	8.55609	6.658351	10.01775	8.565456	7.879552	10.718573	14.93764	10.060482	11.842014
ξ_3	8.297442	6.758906	26.199112	9.790689	10.450336	8.140247	27.65486	14.331752	7.437651	24.181083
ξ_4	6.922296	7.34811	4.702787	8.853243	6.052472	9.547748	5.202914	9.631521	7.151582	4.856908
ξ_5	23.514363	5.418481	6.066549	6.076401	8.384584	5.228337	4.984077	7.936029	7.30586	5.851847
ξ_6	7.304917	23.674174	5.51932	11.256906	5.392946	14.788289	6.434512	8.908644	7.062925	6.714404
ξ_7	8.418274	4.879356	4.169602	6.946566	4.778555	5.439054	5.85908	9.154483	9.200837	3.82683
ξ_8	8.258958	5.947349	6.435293	9.732339	7.659161	7.59419	8.426515	10.804007	8.164208	9.756372
ξ_9	9.438028	3.976547	4.852622	6.257823	5.947816	5.341221	15.570131	9.33989	7.521185	5.618402
ξ_{10}	10.970445	8.158907	8.155839	10.769644	8.086096	12.792888	9.262765	32.562993	9.384904	13.823929
ξ_{11}		6.173936	6.746424	10.059056	10.90312	7.698906	24.78481	10.884554	7.844262	73.654829
ξ_{12}			4.42556	8.643193	4.945183	5.560573	3.848321	12.378489	9.148992	3.72115
ξ_{13}				8.169775	4.073376	6.463288	26.195181	8.629196	5.244579	4.612301
ξ_{14}					7.792285	89.187338	10.320001	12.716166	26.881124	8.53127
ξ_{15}						73.016964	9.065372	9.273948	5.925364	8.959646
ξ_{16}							15.691358	10.891428	7.028169	22.443878
ξ_{17}								8.33157	5.797317	7.025411
ξ_{18}									10.348238	26.53023
ξ_{19}										11.675859

TABLE III

DISCREPANCY VALUES *WSCD* · 10^{-7} FOR DESIGN ON THE SOBOL_2011 SEQUENCES

	ξ_2	ξ_3	ξ_4	ξ_5	ξ_6	ξ_7	ξ_8	ξ_9	ξ_{10}
ξ_1	3.135271	3.446261	3.586738	3.655722	3.157862	3.450995	20.203178	7.868513	7.264484
ξ_2		3.27521	4.420583	4.419499	5.515511	3.29763	3.642641	3.445448	3.450845
ξ_3			3.314533	3.858025	4.292092	6.618729	4.842493	4.188611	5.362813
ξ_4				7.556529	8.226353	4.043833	3.932138	4.026576	24.606687
ξ_5					4.090172	7.935852	20.475111	21.041678	4.510269
ξ_6						5.16709	9.251812	4.39926	8.933427
ξ_7							3.674877	20.916865	4.357111
ξ_8								4.221276	3.825997
ξ_9									24.158983
ξ_{10}									
ξ_{11}									
ξ_{12}									
ξ_{13}									
ξ_{14}									
ξ_{15}									
ξ_{16}									
ξ_{17}									
ξ_{18}									
ξ_{19}									

	ξ_{11}	ξ_{12}	ξ_{13}	ξ_{14}	ξ_{15}	ξ_{16}	ξ_{17}	ξ_{18}	ξ_{19}	ξ_{20}
ξ_1	5.522727	21.587565	5.163961	3.608647	4.111322	3.298493	3.690371	4.443629	7.790726	4.433307
ξ_2	5.286045	8.747392	3.858653	4.525241	5.629277	7.404457	3.221957	7.04957	4.196881	4.506192
ξ_3	4.416827	4.492691	3.437189	5.650867	3.932931	3.44501	7.165084	4.667765	8.242427	4.799243
ξ_4	8.751314	3.319769	7.550999	5.491008	5.076047	9.1222	4.645157	6.682162	4.277706	6.170309
ξ_5	3.597338	3.793	14.068279	4.963509	3.269856	10.346055	4.372423	6.321572	4.189077	20.235958
ξ_6	10.358882	4.631987	5.267591	3.593118	20.159489	8.915712	4.785323	7.550409	4.680258	3.95661
ξ_7	4.423946	3.816675	11.429993	5.555263	4.519451	3.481079	7.50879	7.139842	3.619694	20.993226
ξ_8	22.016528	5.275681	22.299666	4.409712	3.821247	7.25049	3.648729	3.292502	4.566422	4.426012
ξ_9	3.821121	8.280628	7.706479	3.669583	3.483265	5.887212	6.144301	4.345068	4.48582	22.441446
ξ_{10}	4.021908	3.977921	3.450031	5.015911	10.888441	4.171001	3.684277	4332.9478	72.13149	26.366083
ξ_{11}		3.298475	4.40806	21.3764	19.978255	71.619443	7.497897	4.335065	5.106125	9.777936
ξ_{12}			4.044699	7.262044	73.753745	7.927747	6.245093	8.671346	3.638977	5.404832
ξ_{13}				3.597228	6.457606	7.339785	5.131507	8.578586	3.35457	24.827855
ξ_{14}					20.444432	3.668402	3.274869	3.367372	7.570108	7.294009
ξ_{15}						9.512942	3.310078	4.417816	77.410977	5.260811
ξ_{16}							5.571196	21.510236	8.781497	27.740144
ξ_{17}								5.536856	7.54368	3.480233
ξ_{18}									10.032143	5.6842
ξ_{19}										24.519874

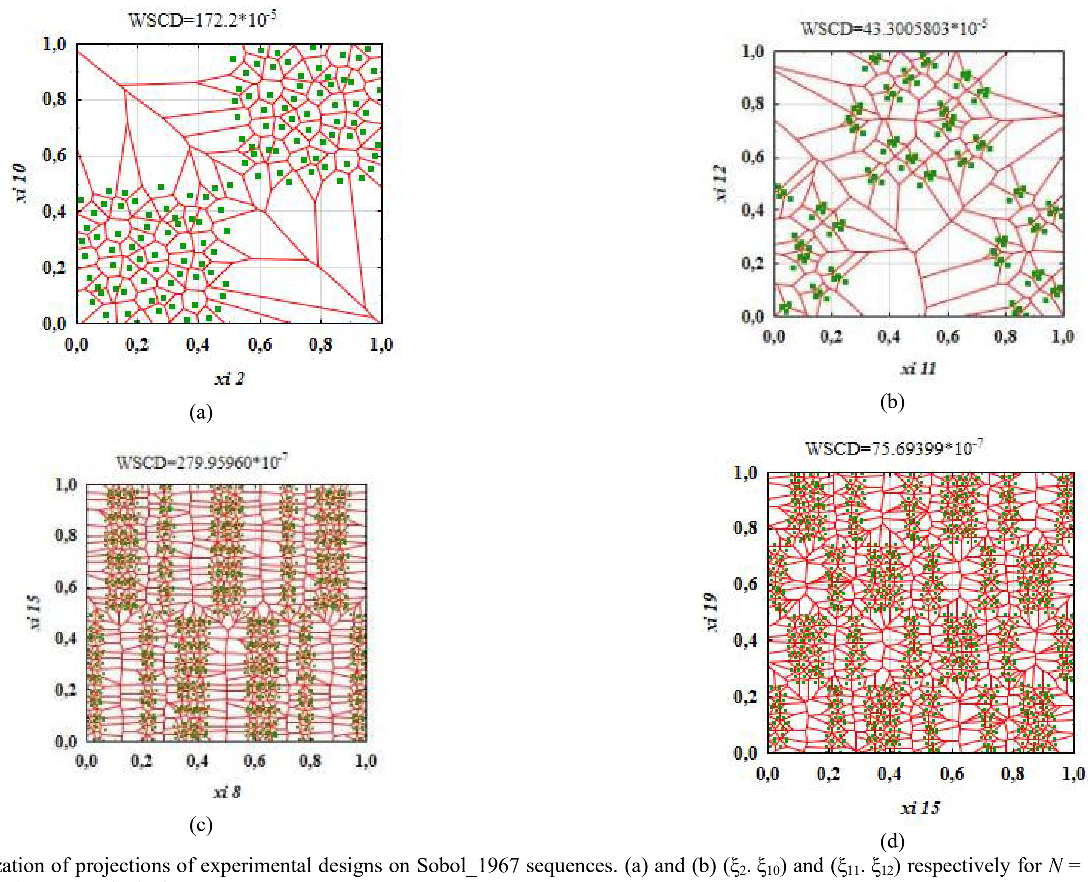

Fig. 2. Visualization of projections of experimental designs on Sobol_1967 sequences. (a) and (b) (ξ_2. ξ_{10}) and (ξ_{11}. ξ_{12}) respectively for N = 127. (c) and (d) (ξ_8. ξ_{15}) and (ξ_{15}. ξ_{19}) respectively for N = 1023.

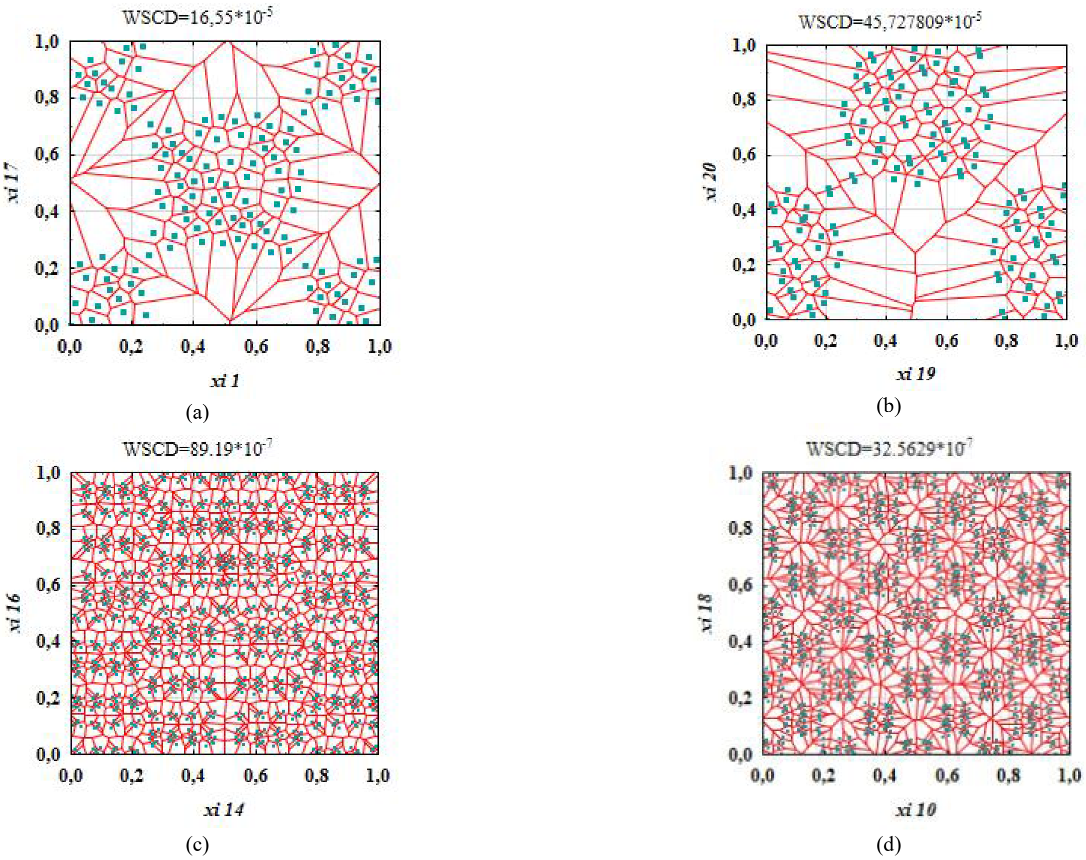

Fig. 3. Visualization of projections of experiment designs on Joe_2008 sequences. (a) and (b) (ξ_1. ξ_{17}) and (ξ_{19}. ξ_{20}) respectively for N = 127. (c) and (d) (ξ_{14}. ξ_{16}) and (ξ_{10}. ξ_{18}) respectively for N = 1023.

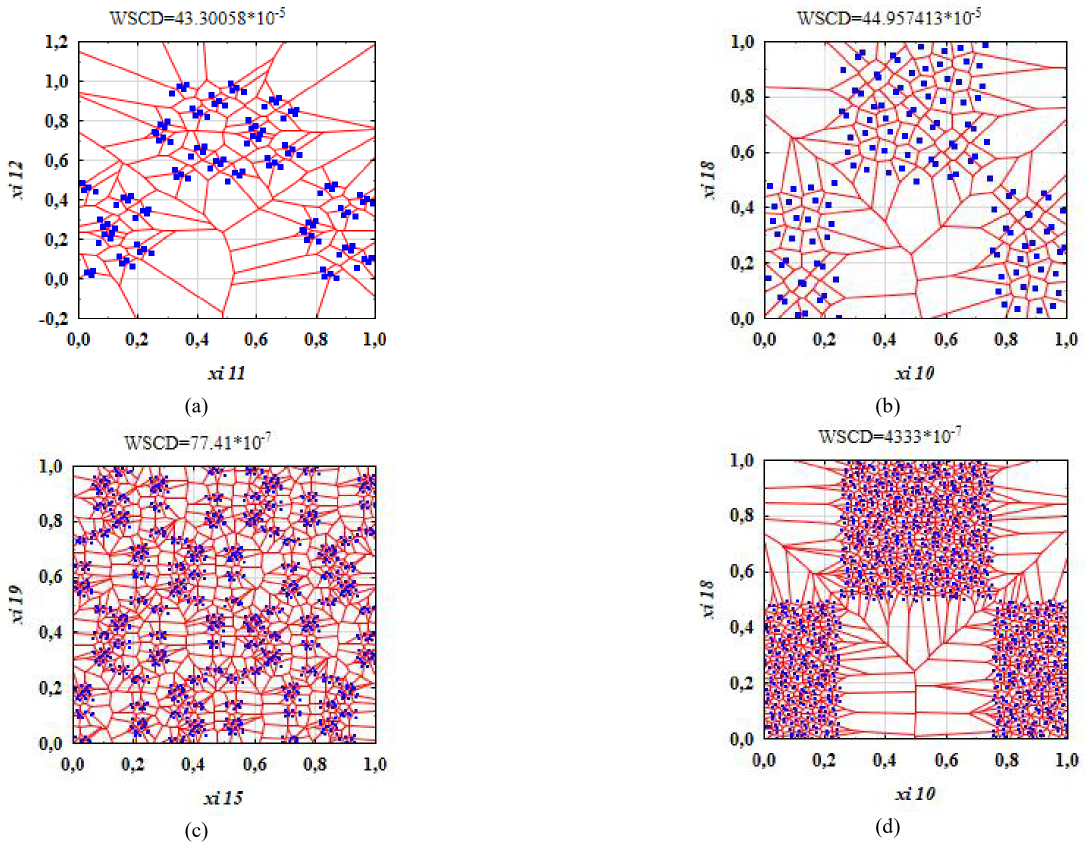

Fig. 4. Visualization of projections of experimental designs on Sobol_2011 sequences. (a) and (b) (ξ_{11}. ξ_{12}) and (ξ_{10}. ξ_{18}) respectively for N = 127. (c) and (d) (ξ_{15}. ξ_{19}) and (ξ_{10}. ξ_{18}) respectively for N = 1023.