

The Construction of Effective Multi-Dimensional Computer Designs of Experiments Based on a Quasi-Random Additive Recursive R_d -sequence

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Abstract – Uniform multi-dimensional designs of experiments for effective research in computer modelling are highly demanded. The combinations of several one-dimensional quasi-random sequences with a uniform distribution are used to create designs with high homogeneity, but their optimal choice is a separate problem, the solution of which is not trivial. It is believed that now the best results are achieved using Sobol's LP_r-sequences, but this is not observed in all cases of their combinations. The authors proposed the creation of effective uniform designs with guaranteed acceptably low discrepancy using recursive Ra-sequences and not requiring additional research to find successful combinations of vectors set distributed in a single hypercube. The authors performed a comparative analysis of both approaches using indicators of centred and wrap-around discrepancies, graphical visualization based on Voronoi diagrams. The conclusion was drawn on the practical use of the proposed approach in cases where the requirements for the designs allowed restricting to its not ideal but close to it variant with low discrepancy, which was obtained automatically without additional research.

Keywords – Computer designs of the experiment, generalized discrepancy, LP_r-sequence, parameterless additive recursive Ra-sequences, quasi-random expanding sequences, uniformity of distribution, Voronoi diagrams.

I. INTRODUCTION

Computer designs of experiment [1], by which we mean the numerical techniques of obtaining finite sequences of points that uniformly fill unit hypercube with an arbitrary number of its first elements, are characterised by significant applied capabilities. The general theoretical significance of this problem is confirmed by the extension of its field of application to such areas as stochastic global optimization [2], surrogate optimization [3], approximation of the Pareto set for multi-criteria optimization [4], quasi-Monte Carlo simulation [5], cryptography, some computer graphics applications, etc.

Despite considerable attention of researchers to the design of experiments, not all theoretical questions on their creation have been resolved. In particular, studies [6], in which questions of cost-optimal designs have been studied are of interest. Particularly great difficulties arise when creating multidimensional designs. Moreover, it is certainly relevant.

II. RESEARCH ANALYSIS

In the future, we will focus on applications to optimization problems, in which a point in the search space is associated with a certain set of variation parameters. Then the computer design of the experiment is a specification of points in hyperspace (points sampling), the selection strategy of which ensures the detection of global and local trends in the topology of the multi-dimensional response surface. As an optimal design of experiment, we will consider one, which obtains the maximum amount of information concerning the response hypersurface by generating a set of points. Due to the fact that this information is not a priori usually known, it makes sense to ensure that unit hypercube is filled with points with high qualities of uniformity, since the transition by stretching to the multi-dimensional parallelepiped of the real factor space is simple and does not significantly change the quality of the distribution characteristics. The uniformity of the distribution increases the probability that at least some of the points fall into the region of extremes or inflections of the response hypersurface. For these reasons, the mathematical description of a multidimensional surface turns out to be more rigorous than if probing was carried out at points in a different way. With an increase in the dimension of space to more than three, the problem of constructing a design is significantly complicated. It is also important to make a compromise between the limited number of the used observation points and the amount of information that can be obtained using carefully selected points. Methods of generating one-dimensional quasi-random expandable sequences, characterised by a low generalized discrepancy and a reduced probability of local inhomogeneity, have been well processed by researchers [1]. It should be noted that quasi-random sequences are used in cases where the preference is given to obtaining distributions of random numbers with a high degree of uniformity, and their correlation is not important. The discrepancy is a quantitative characteristic used to measure the deviation of the distribution of the existing sequence from the ideal uniform distribution, that is, it performs the function of a measure of inhomogeneity [7]. The smaller the discrepancy, the more homogeneous is the sequence. Using the discrepancy, we

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can also characterise the multi-dimensional designs of experiments [8]. Most often, in the process of creating multi-dimensional designs of experiments with low discrepancy certain combinations of several one-dimensional sequences are used, but their optimal choice is a separate problem, the solution of which is not trivial, that is noted, for example, in [9]. In the future, as effective we will consider the multi-dimensional design of the experiment if the choice of the set of vectors distributed in a single hypercube is realized without alternative, providing it with guaranteed low discrepancy without additional research on the composition of the combinations.

Currently, a number of quasi-random sequences with low discrepancy [8], [10] are known, including the van der Corput sequences, Halton sequences, Faure sequences, Sobol's LP_r-sequences, Niederreiter sequences, etc. When generalizing to higher-dimensional designs, all of them have the need for an optimized choice of the so-called basic parameters (for example, guide numbers for Sobol's sequences), which requires additional effort and is a disadvantage that makes their practical application difficult.

Martin Roberts [11] proposed one of the new modern variants of quasi-random sequences with a qualitatively low discrepancy indicator – the parameterless additive recursive R-Kronecker sequence using irrational numbers, which in turn are obtained on the basis of the generalized Fibonacci sequence (golden ratio). It is shown that the R-sequence is characterised by a small amount of generalized discrepancy even with a significant increase in the sample volume of the generated points. However, in the author's article, only the results of subjective studies of the quality of the uniform distribution of two-dimensional R₂-sequences are presented; it is not convincing enough when using multi-dimensional designs.

Therefore, the aim of the article is to study the creation of effective multi-dimensional computer designs of point sampling in unit hypercube using parameterless additive recursive R_d-sequences, their comparison with designs on combinations of LP_r-sequences, as the most effective among others, based on an analysis of objective numerical indicators of generalized discrepancy.

III. DESIGNING COMPUTER EXPERIMENTS

A recursive R_d-sequence in a *d*-dimensional space can be mathematically written as:

$$\mathbf{R}_d(\phi_d): \mathbf{t}_n = \{N \cdot \alpha\}, \quad (1)$$

where *N* is a number of design points *N* = 1, 2, 3, ... ;

α is an irrational number, $\alpha = \left(\frac{1}{\phi_d}, \frac{1}{\phi_d^2}, \frac{1}{\phi_d^3}, \dots, \frac{1}{\phi_d^d} \right)$;

ϕ_d is a unique positive root of the equation $\mathbf{x}^{d+1} = \mathbf{x} + 1$.

For *d* = 1, $\phi_1 = 1.618033\dots$; for *d* = 2, $\phi_2 = 1.324717\dots$; for *d* = 3, $\phi_3 = 1.220744\dots$

As a quantitative measure of the heterogeneity of the set of vectors that are distributed in unit hypercube, two varieties of discrepancy regarding L₂ norm (the centred discrepancy and the wrap-around discrepancy), which are invariant by remarking and ordering factors and regarding the rotation of coordinates, are used.

Discrepancy indicators for *N* design points in *d*-dimensional space are calculated in accordance with the ratios [12]:

a) centred discrepancy

$$\begin{aligned} (\mathbf{CD}(\mathbf{D}_n))^2 = & \left(\frac{13}{12}\right)^d - \frac{2}{N} \cdot \sum_{k=1}^N \prod_{j=1}^d \left[1 + \frac{1}{2} \cdot \left| \mathbf{x}_{kj} - 0.5 \right| - \right. \\ & \left. - \frac{1}{2} \cdot \left| \mathbf{x}_{kj} - 0.5 \right|^2 \right] + \\ & + \frac{1}{N^2} \cdot \sum_{k=1}^N \sum_{j=1}^N \prod_{i=1}^d \left[1 + \frac{1}{2} \cdot \left| \mathbf{x}_{ki} - 0.5 \right| + \right. \\ & \left. + \frac{1}{2} \cdot \left| \mathbf{x}_{ji} - 0.5 \right| - \right. \\ & \left. - \frac{1}{2} \cdot \left| \mathbf{x}_{ki} - \mathbf{x}_{ji} \right| \right]; \end{aligned} \quad (2)$$

b) wrap-around discrepancy

$$(\mathbf{WD}(\mathbf{P}))^2 = \left(\frac{4}{3}\right)^d + \frac{1}{N^2} \cdot \sum_{k=1}^N \sum_{j=1}^N \prod_{i=1}^d \left[\frac{3}{2} - \left| \mathbf{x}_{ki} - \mathbf{x}_{ji} \right| \cdot \left(1 - \left| \mathbf{x}_{ki} - \mathbf{x}_{ji} \right| \right) \right]. \quad (3)$$

It is considered that a lower value of the discrepancy when comparing the designs of the experiment is characteristic of a more uniform, and, accordingly, a more desirable design. For greater clarity, we will also use a graphical representation of the generated data in the form of Voronoi diagrams. Firstly, two-dimensional designs will be considered, on the basis of which it is easy to work out a reliable research methodology, which will subsequently be extended to three- and other multi-dimensional spaces. In numerical experiments, the following initial data from Tables I and II were used.

The set of sequences shown in Table 2 was chosen according to the results of numerical experiments for a visual demonstration of the most indicative designs described below in terms of their homogeneity. In the experiments, a complete iteration of combinations (ξ_i, ξ_j) *i* = 1...6, *j* = 1...20 for two-dimensional designs and (ξ_i, ξ_j, ξ_k), *i* = 1...6, *j* = 1...20, *k* = 1...20 for three-dimensional designs was carried out. Four-dimensional and five-dimensional designs were created similarly based on previously obtained two- and three-dimensional plans, where ($\xi_i, \xi_j, \xi_k, \xi_m$), *m* = 1...20 and ($\xi_i, \xi_j, \xi_k, \xi_m, \xi_l$), *l* = 1...20. In this case, changes in the indices *i, j, k* were carried out within the previously specified limits.

TABLE I
THE INITIAL DATA FOR R_d -SEQUENCES OF DIMENSION D

No.	$R_2; d = 2$		$R_3; d = 3$			$R_4; d = 4$			
	x2	y2	x3	y3	z3	x4	y4	z4	q4
1	0.255	0.07	0.319	0.171	0.05	0.357	0.234	0.129	0.039
2	0.009755	0.64	0.138	0.842	0.599	0.213	0.968	0.757	0.577
3	0.765	0.21	0.958	0.513	0.149	0.07	0.702	0.386	0.116
4	0.52	0.779	0.777	0.184	0.699	0.927	0.436	0.015	0.654
5	0.274	0.349	0.596	0.855	0.249	0.783	0.169	0.644	0.193
6	0.029	0.919	0.415	0.526	0.798	0.64	0.903	0.272	0.732
7	0.784	0.489	0.234	0.197	0.348	0.497	0.637	0.901	0.27
8	0.539	0.059	0.053	0.868	0.898	0.353	0.371	0.53	0.809
9	0.294	0.629	0.873	0.539	0.447	0.21	0.105	0.158	0.347
10	0.049	0.198	0.692	0.21	0.997	0.067	0.839	0.787	0.886
...
120	0.085	0.881	0.801	0.025	0.464	0.301	0.567	0.945	0.132
121	0.84	0.451	0.62	0.696	0.014	0.158	0.301	0.574	0.67
122	0.595	0.021	0.439	0.367	0.563	0.014	0.035	0.202	0.209
123	0.35	0.59	0.258	0.038	0.113	0.871	0.769	0.831	0.747
124	0.105	0.16	0.077	0.709	0.663	0.728	0.503	0.46	0.286
125	0.86	0.73	0.897	0.38	0.213	0.584	0.236	0.088	0.825
126	0.615	0.3	0.716	0.051	0.762	0.441	0.97	0.717	0.363
127	0.369	0.87	0.535	0.723	0.312	0.298	0.704	0.346	0.902
128	0.124	0.44	0.354	0.394	0.862	0.154	0.438	0.974	0.44

TABLE II
THE INITIAL DATA OF LP_r -SEQUENCES (N = 128) [13]

ξ_1	ξ_2	ξ_3	ξ_4	ξ_6	ξ_7	ξ_9	ξ_{10}	ξ_{11}	ξ_{13}	ξ_{20}
0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5
0.25	0.75	0.25	0.75	0.75	0.25	0.25	0.75	0.25	0.25	0.75
0.75	0.25	0.75	0.25	0.25	0.75	0.75	0.25	0.75	0.75	0.25
0.125	0.625	0.875	0.875	0.125	0.375	0.875	0.625	0.625	0.875	0.125
0.625	0.125	0.375	0.375	0.625	0.875	0.375	0.125	0.125	0.375	0.625
0.375	0.375	0.625	0.125	0.875	0.125	0.625	0.375	0.875	0.625	0.875
0.875	0.875	0.125	0.625	0.375	0.625	0.125	0.875	0.375	0.125	0.375
0.0625	0.9375	0.6875	0.3125	0.0625	0.4375	0.8125	0.6875	0.0625	0.4375	0.9375
0.5625	0.4375	0.1875	0.8125	0.5625	0.9375	0.3125	0.1875	0.5625	0.9375	0.4375
0.3125	0.1875	0.9375	0.5625	0.8125	0.1875	0.5625	0.4375	0.3125	0.1875	0.1875
...
0.117188	0.117188	0.664063	0.648438	0.523438	0.929688	0.960938	0.210938	0.773438	0.257813	0.617188
0.617188	0.617188	0.164063	0.148438	0.023438	0.429688	0.460938	0.710938	0.273438	0.757813	0.117188
0.367188	0.867188	0.914063	0.398438	0.273438	0.679688	0.710938	0.960938	0.523438	0.0078125	0.367188
0.867188	0.367188	0.414063	0.898438	0.773438	0.179688	0.210938	0.460938	0.023438	0.507813	0.867188
0.242188	0.742188	0.289063	0.273438	0.648438	0.554688	0.085938	0.585938	0.398438	0.632813	0.742188
0.742188	0.242188	0.789063	0.773438	0.148438	0.054688	0.585938	0.085938	0.898438	0.132813	0.242188
0.492188	0.492188	0.039063	0.523438	0.398438	0.804688	0.335938	0.335938	0.148438	0.882813	0.492188
0.992188	0.992188	0.539063	0.023438	0.898438	0.304688	0.835938	0.835938	0.648438	0.382813	0.992188
0.00390625	0.996094	0.308594	0.574219	0.347656	0.675781	0.035156	0.097656	0.449219	0.074219	0.253906

IV. THE RESULTS OF NUMERICAL EXPERIMENTS

The research results are illustrated (Figs. 1–3) first for two-dimensional and three-dimensional designs, respectively.

The obtained indicators of centred discrepancy (2) and wrap-around discrepancy (3) for two-dimensional designs, namely, for parameterless R_2 -sequences and some combinations of LP_r -sequences are given in Table III.

Figure 1 contains Voronoi diagrams of design variants of experiments with the best indicators of discrepancy based on LP_r -sequences and R_2 -sequences. Note that for designs of experiments with close homogeneity based on LP_r -sequences the evaluation of the results for both indicators of discrepancy is not always unambiguous. At the same time, the associative relationship on the homogeneity of the distribution between graphic images and numerical indicators is not always clearly

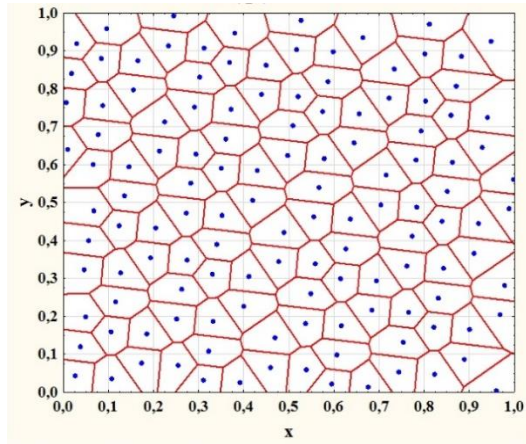
seen, as it is demonstrated by examples of R_2 - and (ξ_4, ξ_9) LP_τ -sequences. Although two-dimensional LP_τ -sequences refer to sequences with a small discrepancy, there are combinations of them that do not demonstrate it, for example, the combinations shown in Fig. 2. Therefore, the selection of the “best” and “worst” pairs of LP_τ -sequences requires additional studies, the time costs for which to obtain positive results are difficult to assess due to chance. The results of the calculation of the discrepancy indicators regarding L_2 norm for two-

dimensional designs (Table III) and the visual analysis of Voronoi diagrams make it possible to verify that there are combinations of LP_τ -sequences that have both better and slightly worse indicators of generalized discrepancy compared to parameterless R_2 -sequences.

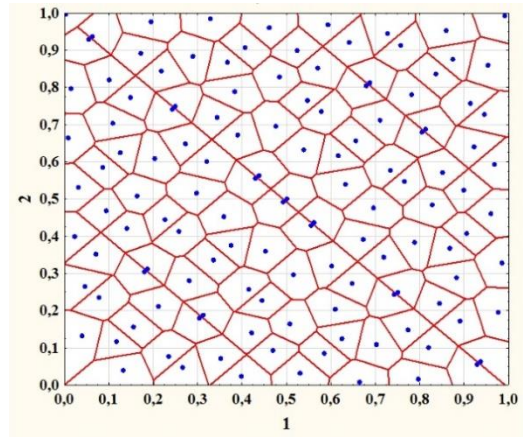
The indicators of centred discrepancy and wrap-around discrepancy for three-dimensional designs are obtained and given in Table IV.

TABLE III
INDICATORS OF GENERALIZED DISCREPANCY FOR TWO-DIMENSIONAL DESIGNS

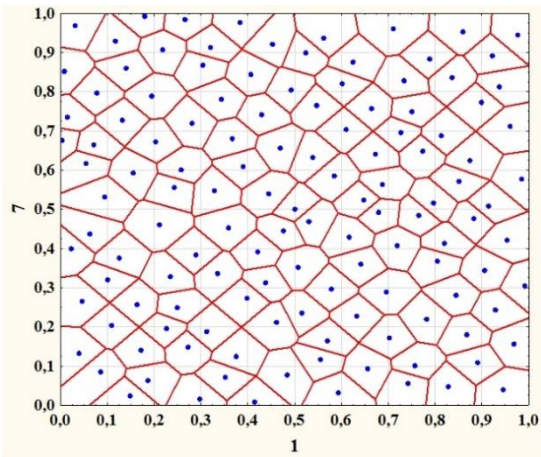
Indicators	Quasi-sequences							
	R_2	LP_τ						
		(ξ_1, ξ_2)	(ξ_1, ξ_7)	(ξ_4, ξ_{11})	(ξ_2, ξ_{10})	(ξ_3, ξ_{13})	(ξ_2, ξ_{20})	(ξ_4, ξ_9)
Centred discrepancy $\cdot 10^{-4}$	5.261	0.7805	0.9471	0.6876	65.55	4.588	7.141	5.102
Wrap-around discrepancy	3.555938	3.555628	3.555688	3.555708	3.557398	3.557328	3.556283	3.556143



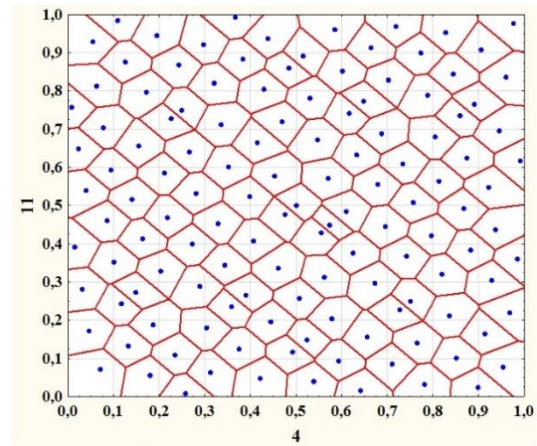
a) R_2 -sequence



b) LP_τ -sequences (ξ_1, ξ_2)



c) LP_τ -sequences (ξ_1, ξ_7)



d) LP_τ -sequences (ξ_4, ξ_{11})

Fig. 1. Visualization of the uniformity of two-dimensional designs in the form of Voronoi diagrams.

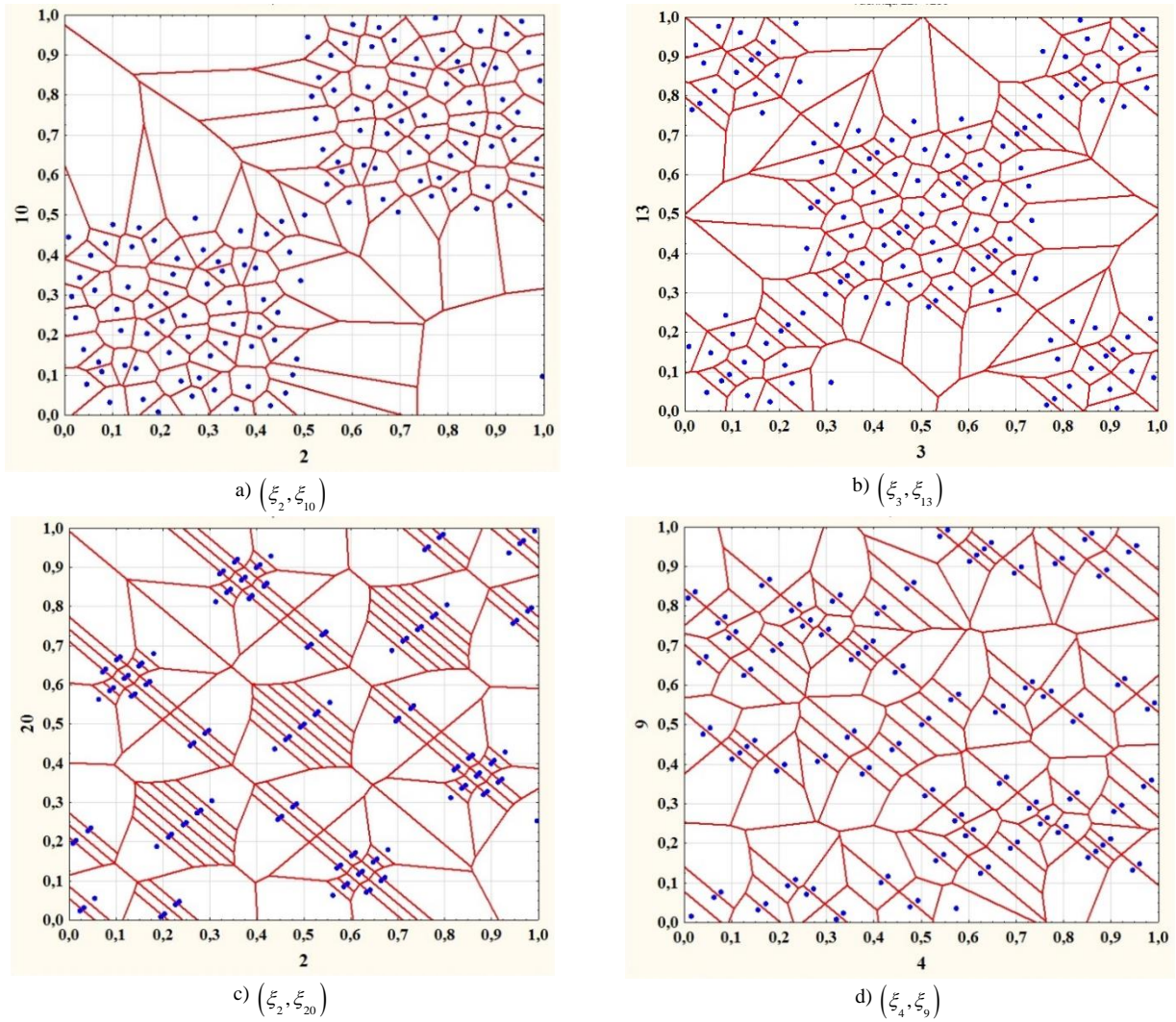
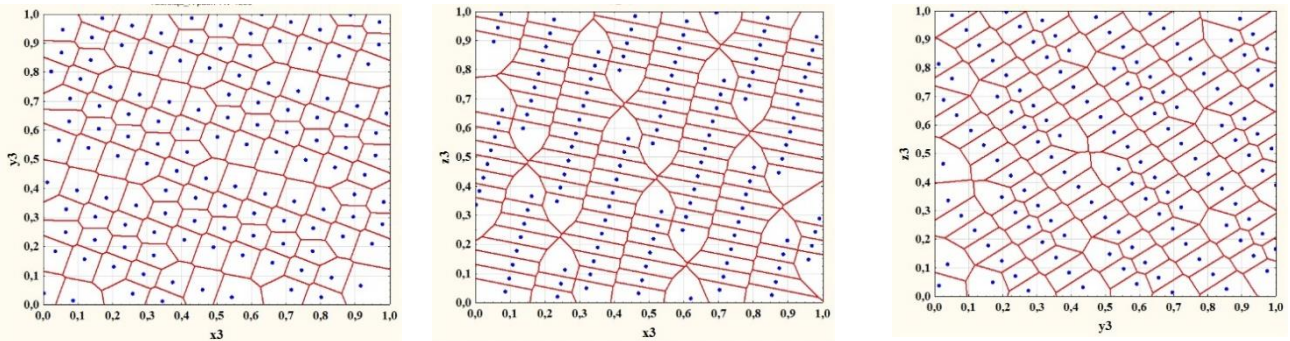


Fig. 2. Visual analysis of the uniformity of two-dimensional designs in the form of Voronoi diagrams formed by LP_τ -sequences.

TABLE IV
INDICATORS OF GENERALIZED DISCREPANCY FOR THREE-DIMENSIONAL DESIGNS

Indicators	Quasi-sequences		
	R_3	LP_τ	
		(ξ_6, ξ_7, ξ_{12})	(ξ_3, ξ_4, ξ_9)
Centred discrepancy $\cdot 10^{-4}$	7.859	1.769	80.93
Wrap-around discrepancy	4.741793	4.741183	4.744208



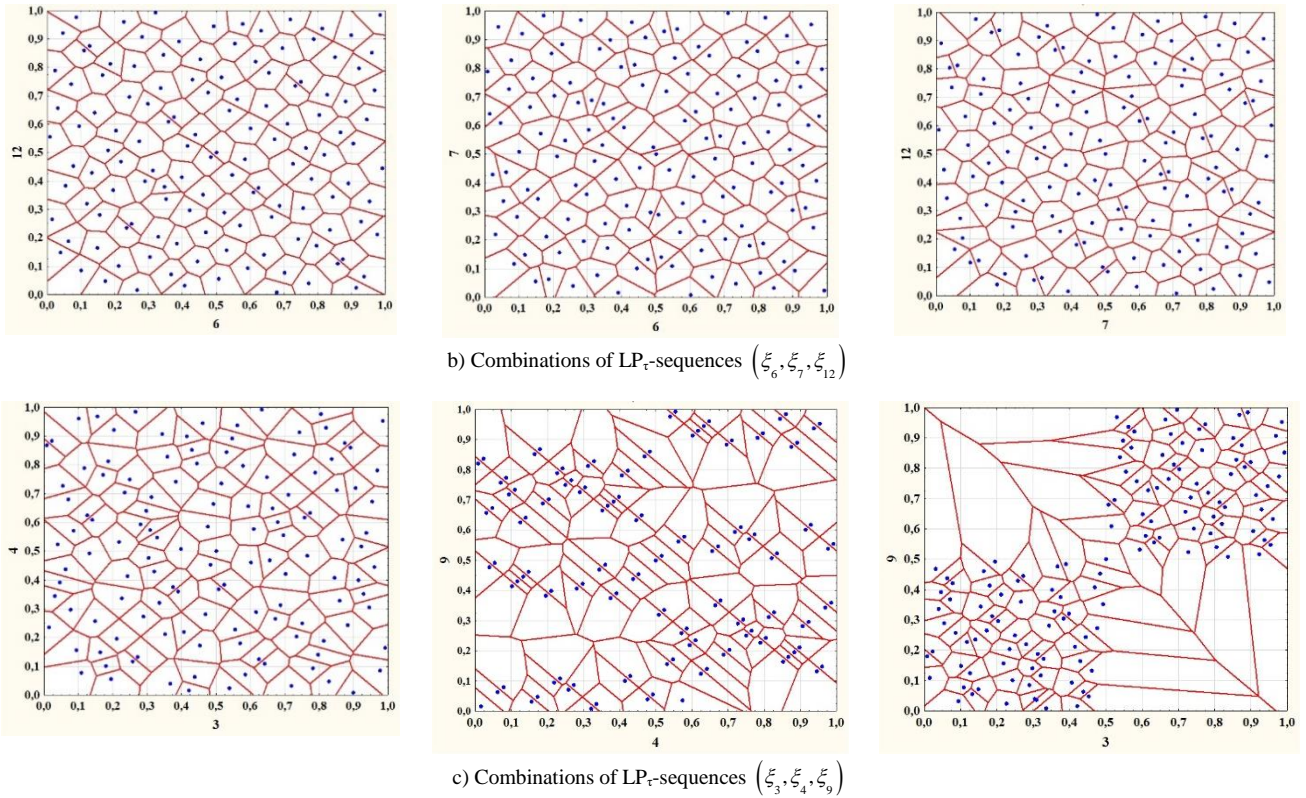


Fig. 3. Voronoi diagrams for projections of three-dimensional designs.

Here, it is possible to observe a clearly expressed unambiguity in estimates of inhomogeneity with the help of numerical indicators of discrepancy for plans of experiments with close homogeneity based on R_3 - and (ξ_6, ξ_7, ξ_{12}) LP_τ -sequences, and even more for “worse” design (ξ_3, ξ_4, ξ_9) . The same conclusions can be drawn from an analysis of the

corresponding Voronoi diagrams. In conclusion, we will try to summarise the research results in compliance with the previously proposed paradigm for creating multi-dimensional designs of experiments. Tables V and VI contain the calculation results.

TABLE V
INDICATORS OF GENERALIZED DISCREPANCY FOR FOUR-DIMENSIONAL DESIGNS

Indicators	Quasi-sequences						
	R_4	LP_τ					
		$\left(\begin{matrix} \xi_1, \xi_2, \\ \xi_5, \xi_7 \end{matrix}\right)$	$\left(\begin{matrix} \xi_1, \xi_2, \\ \xi_3, \xi_5 \end{matrix}\right)$	$\left(\begin{matrix} \xi_5, \xi_7, \\ \xi_{12}, \xi_{14} \end{matrix}\right)$	$\left(\begin{matrix} \xi_1, \xi_2, \\ \xi_{10}, \xi_{19} \end{matrix}\right)$	$\left(\begin{matrix} \xi_2, \xi_6, \\ \xi_{20}, \xi_{10} \end{matrix}\right)$	$\left(\begin{matrix} \xi_1, \xi_2, \\ \xi_{10}, \xi_{15} \end{matrix}\right)$
Centred discrepancy $\cdot 10^{-4}$	3.613	0.5245	0.4528	0.4573	8.248	10.143	8.092
Wrap-around discrepancy	6.326442	6.322127	6.322074	6.32235	6.325789	6.330247	6.325179

TABLE VI
INDICATORS OF GENERALIZED DISCREPANCY FOR FIVE-DIMENSIONAL DESIGNS

Indicators	Quasi-sequences						
	R_5	LP_τ					
		$\left(\begin{matrix} \xi_1, \xi_2, \\ \xi_3, \xi_5 \end{matrix}\right)$	$\left(\begin{matrix} \xi_1, \xi_2, \\ \xi_3, \xi_5 \end{matrix}\right)$	$\left(\begin{matrix} \xi_6, \xi_7, \\ \xi_{12}, \xi_{14}, \\ \xi_3 \end{matrix}\right)$	$\left(\begin{matrix} \xi_1, \xi_2, \\ \xi_5, \xi_7, \\ \xi_{10} \end{matrix}\right)$	$\left(\begin{matrix} \xi_1, \xi_2, \\ \xi_{10}, \xi_{19}, \\ \xi_{16} \end{matrix}\right)$	$\left(\begin{matrix} \xi_2, \xi_6, \\ \xi_{20}, \xi_{10}, \\ \xi_{16} \end{matrix}\right)$
Centred discrepancy $\cdot 10^{-4}$	1.959	0.973	0.946	0.971	9.391	11.113	12.357
Wrap-around discrepancy	8.431419	8.430584	8.430845	8.430928	8.435925	8.44094	8.446635

A comparison of obtained results of discrepancy does not allow drawing conclusions regarding the unambiguous choice of designs when using at the same time a combination of two indicators, as evidenced, for example, by comparing pairs of R_4 - and $(\xi_1, \xi_2, \xi_{10}, \xi_{15})$ LP_τ -sequences for four-dimensional design

or $(\xi_1, \xi_2, \xi_3, \xi_5, \xi_7)$ and $(\xi_6, \xi_7, \xi_{12}, \xi_{14}, \xi_3)$ LP_τ -sequences and others for five-dimensional designs. It can be argued that, based on the LP_τ -sequences, it is possible to create the best multi-dimensional designs of experiment in terms of homogeneity. However, an arbitrary combination of vectors in the design does

not automatically lead to the desired result. At the same time, if the requirements for the design allow us to restrict ourselves to its not ideal variant with a guaranteed low discrepancy, then this can be done using R_α -sequences without the risk of obtaining “anomalous” varieties, as is the case with LP_τ -sequences.

V. CONCLUSIONS

For multi-dimensional designs with an increase in the dimensionality of space, it is increasingly difficult to find combinations of LP_τ -sequences that have the best indicators of generalized discrepancy and require significant time resources. However, the use of combinations of LP_τ -sequences still shows the best results due to a successful choice of guide numbers.

To summarise, we can draw conclusions regarding the concept of rational use of designs for a multi-dimensional factor space based on a combination of parameterless additive recursive one-dimensional R -sequences. In the case of an increase in the dimensionality of space, the concept provides the automatic creation of new versions of experimental designs with quite acceptable, but not the best characteristics of homogeneity by the formation of new vectors without additional research to determine the value of the discrepancies. Discrepancy indicators will be considered acceptable ones when they are worse than the best ones obtained using LP_τ -sequences in successful designs, but better than in their unsuccessful varieties.

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