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COMPARING THE EFFECTS OF APPLICATION OF THE SMART AND TRADITIONAL DESIGNS OF EXPERIMENT

PORÓWNANIE EFEKTÓW ZASTOSOWANIA ELASTYCZNYCH I TRADYCYJNYCH PLANÓW EKSPERYMENTU

A b s t r a c t

This paper presents an analysis of comparing the effects of the application of the smart and traditional designs of experiment. The smart designs of experiment generated according to two various methods were compared to the central composite designs for two and three inputs. To check how the use of selected designs will affect the results of the experiment a computer simulation was performed, where a real research object was replaced by two special testing functions whose values were compared to the values predicted by the neural networks trained with the use of data sets based on compared smart and traditional designs of the experiment.

Keywords: *smart design of experiment, central composite design, experimental research*

S t r e s z c z e n i e

W artykule przedstawiono wyniki porównania efektów zastosowania elastycznych i tradycyjnych planów eksperymentu. Plany elastyczne były generowane z użyciem dwóch różnych metod i porównane z planem centralnym kompozycyjnym. W celu zbadania wpływu zastosowanego planu eksperymentu została wykonana symulacja komputerowa, w której rzeczywisty obiekt badań został zastąpiony dwoma funkcjami testowymi, których wartości były porównywane z wartościami aproksymowanymi za pomocą sieci neuronowych, uczonych na zbiorach opartych o porównywane plany.

Słowa kluczowe: *elastyczny plan eksperymentu, plan centralny kompozycyjny, badania eksperymentalne*

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1. Introduction

Scientific experiment seems nowadays to be a very important source of obtaining information. It is caused by the need of experimental validation of various devices, systems and processes, and on the other hand, planning and execution of an experiment is strongly supported by the use the various techniques of conducting and analyzing the experiment. These techniques known as the design of experiment methodology (DoE) are particularly useful when the researcher seeks for a way to limit the cost or time of the planned experiment without reducing its quality [1–2]. The goal of research determines using various types of experimental designs. One can mention, for example, full factorial designs, fractional designs, dedicated for mixtures or based on the response surface analysis. Choosing the traditional designs of experiments determines the number of the design's units and the number of inputs' levels. The other approach to the planning of an experiment is the main idea of the smart designs of the experiment which allows the researcher to set a number of design's units and the number of inputs' levels.

2. The Idea of Smart Designs of Experiments

Smart designs of an experiment are generated in a dedicated computer application, based on three important principles: adaptation, randomness and equipartition [3]. The first principle means the possibility of adjusting the design's characteristics to the conditions of the experiment and characteristics of the object under research. The researcher is able, for example, to set a number of design's units and levels for each input. The second principle means that smart designs are created in a non-deterministic manner: both the generation of input's levels and the selection of design's units are conducted with the using of pseudo-random numbers. However, there are some limitations put on the random way of generating design's units [3–4]:

– a parameter called ”important difference” (Δx), a minimal permissible distance between the currently generated value and the existing values of each input factor levels,
– a parameter called the ”minimal Euclid's distance” (*esmin*) – it is the Euclid's distance to the nearest ”neighbour-unit” in the input's space, calculated for each design's unit, where each unit must fulfill the condition: $es \geq esmin$.

Both parameters described above are based on the conception of the Euclid's distance and use the fact that a set of design units in the space of inputs is equivalent to the set of points in the orthogonal coordinate system as well as the combinations of inputs' levels (which make up the units of designs) are equivalent to the point coordinates. The Δx and *esmin* parameters support equipartition of the design's units in the inputs' space.

There are three ways to generate the inputs' levels [4]. In the first method (Z-method), inputs' levels are generated as pseudo-random values from the normalized range [–1, 1] and checked if they pass the important difference condition test. If a value fails the test, it is removed and the next one is generated to reach the demanded amount of input's levels. In the R-method, the levels of inputs are calculated by dividing the inputs' ranges by the demanded numbers of input's levels. The smallest level is calculated as the minimum of the input's range, whereas the biggest level is calculated as the maximum of the input's range. For example, in case of 5 levels the set of values consists of the following values: {–1.0, –0.5, 0, 0.5, 1.0} (see Fig. 1). In the R2-method, the idea of level calculation is that each level should be the center point of equal areas of influence. The first and the last levels are not equal to the minimum or maximum of the input's range. In case where 5 levels are assumed, the set of inputs' levels consists of the following values: {-0.8, -0.4, 0.0, 0.4, 0.8} (see Fig. 1).

The third rule fulfilled by the smart design is equipatition of their units. If there are no other assumptions, design's units should cover regularly the whole inputs' space. To estimate the regularity of the distribution of the design's units, the method of the equipartitional analysis (EPA, [3]) is used. The analyzed (created) experimental design is compared to the master-design, the units of which are distributed perfectly regularly in the inputs' space ([5], Fig. 2).

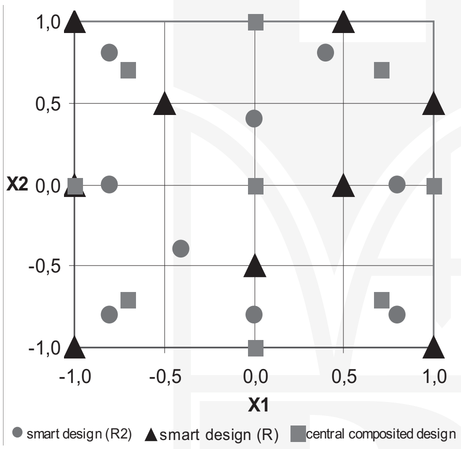

Fig. 1. 2-inputs smart designs (R and R2-method) and central composited design

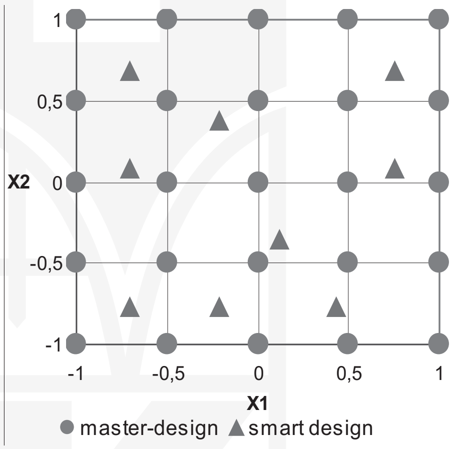

Fig. 2. 2-inputs master-design and smart design

The master-designs have the same number of inputs as the analyzed designs and the same number of various input's levels, but the number of design's units is often significantly higher and equal to the product of numbers of all input's levels. However, the levels of the master-design are calculated for each input by dividing the length of the input range by the number of input's levels. For each unit of the master-design, one can evaluate the Euclid's distance to the nearest unit of the analyzed design. For such a collection (called equipartitional set), one can evaluate a lot of statistical parameters (e.g. descriptive statistics [6]) or make one of the statistical tests [7]. Each of them could be an equipartition criterion in this analysis. Two parameters have been used: the maximal (*e1max*) and mean (*e1mean*) value of an equipartitional set. The *e1mean* parameter describes the central tendency of an equipartitional set and the *e1max* parameter gives the information whether there are some huge empty areas in the inputs' space (without design's units), which is important when taking into consideration the assumption that the design's units should cover the whole inputs' space.

The following steps are performed while generating the smart designs of an experiment [5]:
– defining characteristics of the design: the number of inputs (factors), the number of designs' units, the number of inputs' levels;
– generating the inputs' levels according to the chosen method;
– generating the sets of levels of inputs' factors;
– generating the set of all possible design's units by permuting all inputs' levels;
– completing the design by selecting from the set of all possible design's units only the ones which fulfill the *esmin* condition;
– equipartitional analysis to evaluate the quality of the design (quality means regular and equipartitional distribution of design's units in inputs' space).

The smart design's generator in the current version has implemented the functionalities which support an automatic selection of the optimal values of important generation's parameters – the important difference (Δx, used in Z-method of levels' generating) and the minimal Euclid's distance (*esmin*, used to ensure high regularity and equipartition of design's units in the inputs' space) [5]. Using previous versions of the generator, a researcher had to set it himself.

To increase the probability of obtaining high-quality designs, they are generated in the series and each design has to fulfill the *esmin* condition. If at least one design can be created, the *esmin* value is automatically increased and new designs are generated again. If any design is created, the *esmin* value is automatically decreased and designs are generated again [5]. The design of better quality is selected on the basis of the described above equipartitional parameters: *e1max* and *e1mean.*

The smart designs of an experiment are multiple-generated [8]. The reason is the application of pseudo-random numbers in the algorithm of designs generating. The designs generated with the same seed of a pseudo-random number generator, the same parameters of generation (Δx, method of input's levels generating) and the same design's characteristic (the number of inputs, the number of input's levels, the number of design's units) will be identical. But if the seed value is changed or just if one tries to generate it next time even with the same generation parameters, they could be different and the difference of the design's quality could be sometimes significant. To avoid such a problem, it seems to be necessary to generate several designs and choose one, based on the EPA-parameters (*e1max* and *e1mean*). Each design generating is repeated up to 20 times to get 10 designs.

3. Computer Simulation

The main aim of this study was to compare the effects of use the traditional and smart designs in an experiment conducted according to these designs. The central composited designs and smart designs were analyzed for two (Fig. 1) and three inputs. The smart designs were designed with the same numbers of units (9 for 2 inputs and 15 for 3 inputs) and the same numbers of each levels (5) as compared to central composited designs. The smart designs were generated with the application of the R-method and R2-method of generation the inputs' levels. In the previous studies [9] both methods allow for the best results of experiments as the Z-method.

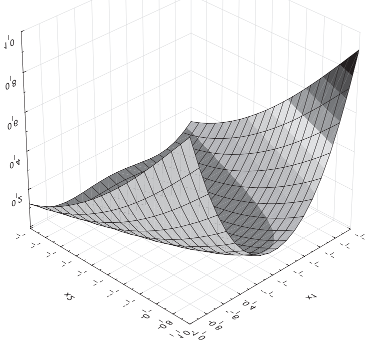

Fig. 3. Rosenbrock's function

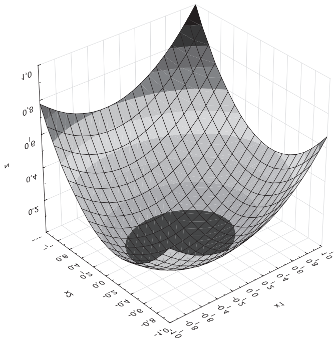

Fig. 4. SumOfSquare function

The research was carried out as a computer simulation where a real research object was simulated by two special testing functions – Rosenbrock's (1) and SumOfSquare (2) known very well as testing functions in optimization [10].

$$f(x)=\sum_{i=1}^{N-1}\left((1-x_i)^2+100\cdot(x_{i+1}-x_i^2)^2\right) \tag{1}$$

$$f(x)=\sum_{i=1}^{N}\left((i+1)\cdot x_i^2\right) \tag{2}$$

For the testing functions simulating the real research object one can evaluate easily its values for each point in the input's space and compare them to the values predicted by neural networks trained with the use of data sets based on the studied designs of the experiment. It was assumed that the values predicted by the neural network will be significantly influenced by a training set which was built on the basis of the analyzed design. The comparison of the values predicted by the neural network with the values of the testing function calculated as absolute differences for a special testing sets (simulation errors) allows indirectly evaluate the quality of information gain in computer simulation of an experiment conducted according to the designs, and at the same time evaluate the influence of the design on the quality of information gained in the conducted experiment.

Neural approximation is one of the popular methods of approximation. The advantages of this method are an easy implementation and a lack of additional assumptions, which is important especially when the function of a real object being the subject of experimental research is poorly known, or not known at all. The neural networks were created in the Statistica Automated Neural Networks module. For all the neural networks, the same methods of learning were applied, so the same influence on the results are assumed. The Automated Network Search tool enabled the automated evaluation and selection of multiple network architectures. The learning cases were selected randomly. 70% cases was assigned to a training set and 30% to a testing set. However, the small size of the learning set should be noted, as they were 9-elements for 2-inputs designs and 15-elements for 3-inputs designs.

The multi-layer perceptron type of nets consist of between 3 and 10 hidden neurons and learns with application of the BFGS algorithm. Various activation functions were checked while searching for the best net: linear, logistic, hyperbolic tangent and exponential. The Automated Network Search tool trains 20 nets with various settings (the number of hidden neurons, activation functions) and saves the best five. On the basis of nets' quality parameters (sum of squares with errors) which were calculated for learning and testing sets, the best was selected and applied to the prediction of the data.

The compared neural approximated and real values were calculated for special testing sets, consisting of 121 (for two inputs designs) and 1331 (for three inputs designs) units. The sets were built as combinations of 11 levels for each input. The levels were calculated by dividing regularly the input range [–1, 1] into 10 subranges: –1, –0.8, –0.6 ... 1. For each error set (a collection of the absolute differences between real and approximated values), statistical parameters were calculated: the maximal and average error, the percent of testing cases where error values were higher than 0.1 (10% of output range [0, 1]) and standard deviation. To check whether the approximated values sets and testing function sets differ significantly, the nonparametric two-samples Kolmogorov-Smirnov test [7] was conducted. This test does not require any assumption about normality or homogeneity of sample variance and is known to be sensitive to any kind of distributional difference.

4. Results of Simulation

The results of simulation are shown in Table 1. There are the following symbols used in the table: Ros means Rosenbrock's function, SoS means SumOfSquare function, CC means central composited design, R2 means smart design generated according to the R2-method and R means smart design generated according to the R-method. Errors means a set of absolute differences between testing function values and the values predicted by neural nets calculated for special testing sets consisting of 121 cases for 2 inputs and 1331 cases for 3 inputs.

The average values of the error parameters calculated for all three compared designs' types are shown in Table 2.

Taking into consideration the average values of errors, the best results were obtained for smart designs generated according to the R2-method. The error average values for all types of designs seem to be relatively low for the output range [0, 1]. However, the maximal values of absolute differences are in the same time definitely to high, especially in the case of a central composited design. It should be noted that the maximal value as a descriptive statistic parameter means only one value calculated sometimes for a huge set and not always describes adequately the analyzed data. As in the case of the average error, also the lowest value of maximal error was obtained for the R2-design but the difference compared to the other two designs was significant (about 30%). The question is which type of statistical parameters is more important for the researcher. Taking into consideration the percentage of cases where the absolute difference between the real (obtained for testing functions) and the approximated (predicted by neural net) values were higher than 0.1 (10% of [0, 1] output range length), you can notice a similar trend as in the case of an average error. The best result was obtained for 2 and 3-inputs designs generated according to the R2-method. Standard deviation indicates whether the cases tend to be very close to the mean value (low value) or rather are spread out over a large range of values (high value). The calculated values are quite similar, however the lowest value was obtained for designs generated with application of the R2-method.

Table 1

Simulation errors

number of inputs	testing function	type of design	maximal error	average error	errors > 0.1 [%]	standard deviation	K-S test
2	Ros	CC	0.87	0.10	40	0.12	$p > .10$
2	Ros	R2	0.59	0.09	31	0.10	$p > .10$
2	Ros	R	0.60	0.13	41	0.14	$p < .10$
2	SoS	CC	0.56	0.17	63	0.13	$p < .001$
2	SoS	R2	0.57	0.19	72	0.13	$p < .001$
2	SoS	R	0.83	0.18	64	0.16	$p < .10$
3	Ros	CC	0.71	0.10	36	0.10	$p < .001$
3	Ros	R2	0.83	0.11	30	0.12	$p < .001$
3	Ros	R	0.60	0.10	34	0.10	$p < .001$
3	SoS	CC	1.44	0.26	69	0.29	$p < .001$
3	SoS	R2	0.48	0.12	51	0.08	$p < .001$
3	SoS	R	0.86	0.18	68	0.13	$p < .001$

Table 2

Average values of simulation errors

type of designs	maximal error	average error	errors > 0.1 [%]	standard deviation
CC	0.90	0.16	52	0.16
R	0.73	0.15	52	0.13
R2	0.62	0.12	46	0.11

The last statistical parameter calculated to evaluate the effects of the application both types of designs was *p-value* parameter for the Kolmogorov-Smirnov test. The assumed significant level of the test (α) was equal to 0.05. If the *p-value* is smaller than the α-*value*, it suggests rejecting the null hypothesis (that two compared samples come from the same distribution) and accepting the alternative hypothesis. Unfortunately, the results (Table 1) are not very optimistic. In most cases the obtained p-values are smaller than the ones used in test $\alpha = 0.05$. But you should remember that the learning sets were extremely small and it was probably not enough to learn the neural nets successfully.

5. Conclusions

The study of the simulation results leads to two main conclusions. The first conclusion is that the errors obtained in the simulation of an experiment conducted according to smart designs of an experiment are less than in the cases of using two- and three-input central composited designs. The difference is especially significant for maximal error statistic. The best results were obtained for the smart designs generated according to the R2-method. The second conclusion is that the researcher must consider the problem of the minimal number of design's units, because setting the number which is too low may cause a decrease of the amount of information gain in an experimental research. The idea of smart designs of an experiment is that the researcher can define the number of design's units and the only limitation is the ability to carry out the experiment according to the design generated with the assumed number of units. Generally speaking, the problem is that the purpose of experimental research is often searching for unknown dependences like for example research object function which determines the output depending on the inputs.

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