ISSN 1407-8015

TRANSPORT AND ENGINEERING MAŠĪNZINĀTNE UN TRANSPORTS 20

2008-8015

MECHANICS MEHĀNIKA

NEW SEQUENTIAL DESIGNS OF EXPERIMENTS FOR METAMODELING AND OPTIMIZATION

JAUNI SECĪGIE EKSPERIMENTU PLĀNI METAMODELĒŠANAI UN OPTIMIZĀCIJAI

Janis Auzins, leading research associate, Dr. sc. ing. Riga Technical University, Institute of Mechanics Address: 6 Ezermalas Street, Riga, LV-1006, Latvia Phone +371 67089396 E-mail: auzinsjp@latnet.lv

Janis Janushevskis, doctoral student, Mg. sc. comp. Riga Technical University, Institute of Mechanics Address: 6 Ezermalas Street, Riga, LV-1006, Latvia Phone +371 67089396 E-mail: janisj@latnet.lv

Keywords: experimental design, sequential sampling, metamodeling, global optimization

1. Introduction

Experimentation and approximation are essential for efficiency and effectiveness in engineering analyses of complex systems in which designers have to deal with multidisciplinary and multi-objective analysis using very complicated and expensive-to-run computer analysis codes. This process of experimentation and approximation is called metamodeling, in which we need: (a) choosing an experimental design for generating data, (b) choosing a model to represent the data, (c) fitting the model to the data, and (d) solving the constrained optimization problem. The datasets may include both computer experiments (with or without deterministic noise) and natural experiments made under uncertainty. For the analysis of deterministic computer experiments the use of classical D, A, I-optimal designs of experiments (DOE), which need repeated runs, is not effective. In the past decades the Latin Hypercube (LH) experimental designs [1, 24] and non-parametric approximation methods (Kriging, Radial Basis Functions, Local Polynomial Methods) [6, 15, 16, 17, 21, 22, 23] have been generally recognized. However the LHs must be completely designed before the experimentation begins. At this time the optimal number of runs for metamodel building is unknown, but the adding of additional runs damages the uniformity of LHs. The classical hierarchical guasi-random sequences which allow adding new sample points (experimental runs, trials), like Halton [11] and Sobol [30] sequences, give highly correlated components for 4, 5 or more dimensions. Good results are given by adaptive experimental designs, in which the approximation or optimization information obtained from previous experimental runs is used for the choice of additional runs [17]. And yet this approach loses effectiveness in the practical engineering case when several responses must be simultaneously observed and used

in optimization for quality criterion and constraint functions. In this work a new approach for the creation of hierarchical DOEs and the modification of local polynomial approximation method is proposed, which gives almost the same or better accuracy of prediction than the metamodels built with adaptive sampling methods and Kriging or RBF approximations.

2. Space and sub-space filling uniformity measures

For the analysis of deterministic computer experiments, V. Eglajs [1] proposed the principle that the number of levels for each factor is equal to the number of runs and each level is used only once. In the situation when the response depends mainly on one factor (the number of which is unknown before experimentation) this principle provides the maximum amount of information about this dependency. Later McKay et al. [24] introduced the name "Latin Hypercube" for DOEs of this type and showed that random LHs give better accuracy for the Monte Carlo integration than pseudo-random samples. The second principle proposed in [1] was that the experiments must fill the area of interest as uniformly as possible. For the measure of the uniformity Eglajs [1] introduced the first space filling criterion – the potential energy criterion

$$\Phi = \sum_{i=1}^{N} \sum_{j=i+1}^{N} \frac{1}{d_{ij}^2},$$
(1)

where *N* is the number of experimental points (runs) and d_{ij} is the Euclidean distance between points *i* and *j*. The LH designs with minimal value of the criterion Eq. (1) have good spacefilling properties, however the experimental points tend to spread out to the corners of the unit cube. Eglajs also proposed the first coordinate exchange algorithm for construction of LHs with minimal value of potential energy criterion. The other category of designs are constructed by algorithmic approaches under certain optimality criteria, such as Minimax and Maximin designs [19], maximum entropy designs [7, 29], integrated mean squared-error (IMSE) designs [28], Mean Square Error (MSE) and uniform designs [10]. Morris and Mitchell [25] introduced a generalization of Eglajs criterion:

$$\Phi_{p} = \left[\sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \frac{1}{d_{ij}^{p}}\right]^{1/p},$$
(2)

where

$$d(x_{i}, x_{j}) = d_{ij} = \left[\sum_{k=1}^{m} |x_{ik} - x_{jk}|^{t}\right]^{1/t}, t = 1 \text{ or } 2.$$
(3)

Park [26] introduced optimal LHDs based on either the maximum entropy criterion or the IMSE criterion; Fang, et al [8, 9] introduced optimal LHDs based on the Centered L_2 discrepancy criterion and wrap-around discrepancy criterion. Searching the optimal LH design of experiments according to any criterion is very difficult and can be realized with methods of discrete optimization – coordinate exchange, multistart, threshold and simulated annealing methods [2, 16, 176, 20, 23]. The author disagrees with the optimized of understood of UH designs is more tractable than searching in the entire sample space without any restrictions. Our practice shows, that the optimization of DOE without any level restrictions is much easier [2], furthermore for the optimization of DOE in the whole space the methods for optimization of LHs (for example coordinate exchange) can also be used and optimized LHs can be utilized as the initial design for optimization. In this regard, the question arises whether it is necessary to strictly follow the principle of LH– absolute uniformity of one-dimensional projections. Especially since in most cases with a



Fig. 1. Plane x_1 - x_2 of 111-runs 6-factor wrap-around-optimal LH design

number of factors m>2 the two-dimensional projections of optimized LHs are far from uniformity. The second reason to give up on absolute uniformity of one-level projections is that we can't add new experimental runs to the existing design without damaging this property.

The criterion of wrap-around L_p discrepancy [8, 12, 20] is claimed to deal with uniformity over the unit cube *P* and all the projections of *P* over C^u , but the two-dimensional projections of wrap-around-optimized 111-runs 6-factor LH shows middling uniformity, see Fig. 1.

3. Average projection criterion

Due to unsatisfactory projection uniformity of LH designs and known sequential quasirandom sequences it seems reasonable to make the compromise between the space-uniformity and subspace uniformity, including the uniformity of one-dimensional projections. The combined criterion can be built for any known criterion as the weighted sum of criterion for entire space and subspaces. For example, when we are interested in the uniformity of space filling of entire space, all one-dimensional projections and all two-dimensional subspaces, we can build the combined criterion

$$\Phi_{comb} = \Phi + \frac{a}{m} \sum_{k=1}^{m} \Phi_k + \frac{2b}{m(m-1)} \sum_{k=1}^{m-1} \sum_{j=k+1}^{m} \Phi_{kj} \quad , \tag{4}$$

where Φ_k , Φ_{kj} – filling quality criterions for one-dimensional and two-dimensional subspaces, a, b – weighting coefficients for one and two-dimensional uniformity respectively.

For example, using the criterion Eq. (2), Eq. (3), we can build the complex *average projection* criterion

$$\boldsymbol{\Phi} = \left[\sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \left[\frac{1}{\sum_{k=1}^{m} \left|x_{ik} - x_{jk}\right|}\right]^{p} + \frac{a}{m} \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \sum_{k=1}^{m} \left[\frac{1}{\left|x_{ik} - x_{jk}\right|}\right]^{p} + \frac{2b}{m(m-1)} \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \sum_{k=1}^{m-1} \sum_{l=k+1}^{m} \left[\frac{1}{\left|x_{ik} - x_{jk}\right| + \left|x_{il} - x_{jl}\right|}\right]^{p}\right]^{1/p} . (5)$$

The problem is the choice of the weighting coefficients. Using large values of weighting coefficients *a* we can obtain Latin hypercubes (with the level distribution nearly to uniform). Santner et al [35] used the largest diagonal size $\sqrt[p]{d}$ of *d*-dimensional unit cube for scaling the uniformity criteria in different dimensions. Here another approach was used. The analysis of the problem could be facilitated by an approximate expression which describes the



Fig. 2. Optimal values of criterion Eq. (2), Eq. (3)

dependency of the optimal criterion Eq. (2), Eq. (3) values on the number of runs N and the number of factors m. The Fig. 3. shows this dependence graphically for p=50, t=1, $20 \le N \le 200$ and $1 \le m \le 6$. The optimal values of criterion were found using the program Relax [2]. Good approximation of the dependency of optimal criterion values on the number of runs N and number of factors (variables) m gives the expression

$$\Phi_p^{Optimal} = \left(1 + \sqrt{(m-1)(0.04778 + 0.000422N)}\right) (Nm)^{1/p} (N^{1/m} - 1).$$
(6)

This equation can be used for the control of the choice of the weighting coefficients a, b in the complex criterion Eq. (5)

4. Sequential designs obtained from fixed-size DOEs

The complex criterion Eq. (5) can be used for optimization of both fixed-size and sequential DOEs. Figures 3-5 show the 41-run 2-factor fixed-size designs, optimized according to complex criterion using various values of weighting coefficient. All designs were optimized using improved multistart relaxation and exchange method and the program code *Relax* [2].



Fig. 3. Fixed-size Latin Hypercubes optimized according to Eq. (2), Eq. (3), p=50



Fig. 4. 2-factor 41-run design optimized according to Eq. (5), a=0.01, b=0, p=50. Left – plane x_1-x_2 , right – plane x_1-x_1



Fig. 5. 2-factor 41-run design optimized according to Eq. (5), a=0.001, b=0, p=50. Left – plane x_1 - x_2 , right – plane x_1 - x_1

To obtain the sequential design from a fixed-size design, we use the point arranging method. According to this method, the point which gives the minimal worsening of optimality criterion by its elimination is moved out from the *N*-run design to build a *N*-1-run design.



Fig. 6. 2-factor 25-run design obtained from a 41-run design. Left – plane x_1 - x_2 , right – plane x_1 - x_1

It can be seen that the sequential designs obtained in this way are similar to PLS sequential designs [27], see Fig. 7.



Fig. 7. 2-factor 41-run PLS design [27]. Left – plane x_1 - x_2 , right – plane x_1 - x_1

5. Sequential DOEs created by adding one point at time

Sequential designs can be obtained in a traditional way – by adding new experimental points to the existing design. The designs are called "adaptive", when the information about responses in previously created experimental points is used. In the work [17], the cross validation approach is used in which a point with the largest prediction error is selected as the new sample point. The problem is to find good assessment for the prediction error and the fact that in usual engineering optimization tasks several responses must be simultaneously

approximated. We also tried to add direct the point in which the largest prediction error occurs for some test functions (Six Hump Camel, Branin) and found that only the maximal



Fig. 8. 41-run sequential design. Left – plane x_1 - x_2 , middle – plane x_1 - x_1 , right – plane x_2 - x_2 prediction error measure was better than by using fixed-size experimental designs or sequential designs without adaptation. Therefore in this work the non-adaptive sequential designs are used. Figure 8. shows the 2-factor 41-run design, obtained by adding one point at time according to criterion Eq. (5), beginning from a 9-run optimal LH design. This design is hierarchical – new points can be added.

6. Approximation test problem

The proposed method of DOE was tested on many common test problems, both for approximation and for unconstrained and constrained global optimization. Only few of the calculated problems will be shown here. First we will look only at the metamodel building problem. The measures for the prediction accuracy assessment of metamodels are listed in Table 1.

Name	Equation
Max. Absolute Error	$\max \left F_i - \hat{F}_i \right $
(MAE)	
Average Absolute Error	$1\sum_{i=1}^{n} E_{i} - \hat{E} $
(AAE)	$\frac{-n}{n}\sum_{i=1}^{n} \mathbf{r}_i-\mathbf{r}_i $
Mean Square Error (MSE)	$\frac{1}{n}\sum_{i=1}^n \left(F_i - \hat{F}_i\right)^2$
Root Mean Square Error (RMSE)	$\sqrt{\frac{\sum_{i=1}^{n} \left(F_{i} - \hat{F}_{i}\right)^{2}}{n}} = \sqrt{MSE}$
Relative Root Mean Square Error (RRMSE)	$100\% \sqrt{\frac{MSE}{Variance}} = 100\% \sqrt{\frac{\frac{1}{n} \sum_{i=1}^{n} (F_i - \hat{F}_i)^2}{\frac{1}{n} \sum_{i=1}^{n} (F_i - \overline{F})^2}}$

Table 1. Error measures for accuracy assessment

Here *n* is the number of confirmation points over the domain, in which the values of exact function F_i and its prediction \hat{F}_i are calculated. \overline{F} stands for the mean of exact function values in confirmation points. Usually a large number of randomly selected LH sample points was used (1000-100000), which give 3-4 correct decimal digits of global average error measures.

The two-dimensional test problem is taken from the work [27].



Fig. 9. Exact function Eq. (7)
$$f(x_1, x_2) = \left[0.8r + 0.35\sin\left(2.4\pi \frac{r}{\sqrt{2}}\right)\right] \left[1.5\sin(1.3\Theta)\right]$$
(7)

in the domain $0 \le x_1, x_2 \le 1$,

where
$$r = \sqrt{x_1^2 + x_2^2}$$
, $\Theta = \arctan\left(\frac{x_2}{x_1}\right)$.

Table 2. shows the approximation results, using several experimental designs and approximation methods.

Method	Mo	ving	Local quadratic with Gaussian weighting						Local cubic with		
	Le	east	coefficient						Gaussian weighting		
	Squ	ares							coefficient		
	[2	27]									
Exp.	CVT	PLS	PLS	MSE	Sobol	Halto	New 1	New	New	New 2	MSE
Design				LH		n		2	1		LH
AAE	0.01	0.019	0.006	0.006	0.008	0.008	0.006	0.005	0.004	0.0038	0.00360
	33	1	48	17	41	71	26	98	13	7	

Table 2. Results of approximation using 41 runs

Here CVT is the Central Voronoi Tessellation design [27], PLS is the Progressive Lattice Sampling [27], MSE LH is the LH design optimized according the Mean Square Error [2, 10], New 1 is the design Fig. 5., New 2 is the design Fig. 8.

It can be seen that Local quadratic approximation gives better results than Moving Least Square [27]. The new sequential designs give the prediction error approximately equivalent to the error obtained by using fixed-size MSE-optimal Latin Hypercube. The best results for this function can be obtained using local cubic approximation.

7. The optimization examples

Here we show two optimization examples – with two and with six variables. Similar to other authors, the optimization approach is based on the sequential metamodeling. At each stage the metamodel is built, the optimum of metamodel function is found and the search region is reduced. The metamodels are built using first, second or third order local polynomial approximation with Gaussian weighting function [2]. The best type of approximation is chosen using leave-one-out cross-validation. Because this cross-validation method suggests increased bandwidth value (decreased coefficient in the exponential weighting function

respectively), the suggested value was corrected using a multiplier which was found by analysis of great number of approximation examples for various numbers of variables, runs and level of noise [2]. The optimization of the metamodel was carried out using a simple multistart random search method, which needs a large number of approximated function evaluations but gives a good reliability of search results [14]. Using the iteration method for solving a system of linear algebraic equations, the calculation of approximated functions is very fast and allows 10^5 - 10^6 function evaluations in a few seconds for number of variables $m \le 12$. Only the use of local cubic approximation becomes unpractical for problems with m > 5. We did not carry out research to achieve optimization with the minimal possible number of experimental runs (evaluations of exact function). For each next stage the range of each variable was decreased two times, values calculated in the previous stages were not used. The relative error of minimum found is defined as

$$E = 100\% \frac{\left|F_{\min} - F_{\min exact}\right|}{\left|F_{\min exact}\right|}$$
(8)

7.1. Two-dimensional example

Here we show a simple very well-known optimization example – Six Hump Camelback function which was used for metamodel and optimization testing in [5, 21, 22, 31, 32, 33]. It is defined as:

$$F(x) = \left(4 - 2.1x_1^2 + \frac{x_1^4}{3}\right)x_1^2 + x_1x_2 + \left(4x_2^2 - 4\right)x_2^2,$$

$$x_1 \in [-2, 2], x_2 \in [-1, 1].$$
(9)

This function has six local optima with the global optimum equal to -1.031628 at (0.0898 -0.7127) and (-0.0898 0.7127).

Let us assume that the function is unknown to the designer and that the function value can only be obtained through computation-intensive analysis. Therefore, the goal is to identify the global design optimum with a small number of function evaluations. We use the design space reduction in three stages.



Fig. 10. Camel Back function. Left – exact function, right – the first approximation stage (25 sample points)



Fig. 11. Contour plot of first stage metamodel with experimental points and second stage search region shown

The second stage was executed in the region $x_1 \in [-0.5, 0.5]$, $x_2 \in [-0.9, 0.9]$, the four points from the first stage, which fall in the reduced region, are not used. The cubic local approximation with Gaussian weighting function was used, RMSE=0.059064, RRMSE=12.51%. Two optima at points (0.0945584, -0.708366), (-0.0945565, 0.7083668), exact function value at those points



Fig. 12. Contour plot of second stage metamodel

F=-1.03137, approximated values $\hat{F} = -1.008363$.

The third stage should be made at two subregions to specify two optima points, but it is not necessary because the found minimal value -1.03137 differs from exact minimum -1.0316 by 0.025%, which is more than sufficient in usual engineering practice.

In the third stage over the region $x_1 \in [0, 0.2]$, $x_2 \in [-0.8, -0.6]$, 12 experimental points are added, previously created points were not used. Local cubic approximation, RMSE=4.16E-5, MAE=0.00015, optima at point (0.08984, -0.71265), *F*=-1.0316284.

Table 3. Comparison of the results of Camel Back function optimization

	NEW	NEW	РСК	Prev. ARSM	Impr ARSM I	Impr ARSM II	WHDSRO	SA
Evalu- ations	51	63	45	100	39	44	97*	11276
E (%)	0.025	< 0.001	0.16	16	0.54	0.25	< 0.01	< 0.01

In the Table 3., NEW is the proposed method, PCK – Polynomial–Clustering–Kriging, the result is taken from [32], Prev. ARSM, Impr ARSM I, Impr ARSM II are the results taken from [31], WHDSRO – Working-Hotelling Domain Spanning Robust Optimization [5], result with 98% successful convergence, SA – Simulated Annealing, result taken from [33].

It can be seen that the proposed method gives very good results – high precision and a low number of function evaluations.

7.2. Six-dimensional optimization example

This example is the Hartman 6 function Eq. (10). This function was also optimized in [3, 31, 32, 33, 34]. In the region $0 \le x_i \le 1$, *i*=1,..., 6 the function has global minimum: $f_{H6}(0.201690, 0.150011, 0.476874, 0.275332, 0.311652, 0.657300) = -3.32237$.

$$F_{H6}(x) = -\sum_{i=1}^{4} c_i e^{-\sum_{j=1}^{5} \alpha_{ij} (x_j - p_{ij})^2}$$
(10)

with coefficients given in Table 4.

· ·			
ĺ	α_i	C_i	p_i
1	(10, 3, 17, 3.5,	1.0	(0.1312, 01696, 0.5569, 0.0124,
	1.7, 8)		0.8283, 0.5886)
2	(0.05, 10, 17, 0.1,	1.2	(0.2329, 0.4135, 0.8307, 0.3736,
	8, 14)		0.1004, 0.9991)
3	(3, 3.5, 1.7, 10,	3.0	(0.2348, 0.1451, 0.3522, 0.2883,
	17, 8)		0.3047, 0.6650)
4	(17, 8, 0.05, 10,	3.2	(0.4047, 0.8828, 0.8732, 0.5743,
	0.1, 14)		0.1091, 0.0381)

Table 4. Coefficients for Hartman 6 function



Fig. 13. Hartman 6 function. Left – exact function, right – local quadratic approximation. All the variables that are not used for plotting are fixed at 0.5

For the approximation of this function the first 54 runs from fixed-size 111-run experimental design were used. The 111-run design was optimized according to complex criterion Eq. (5) with the coefficients a=0.001, b=0.1. The projections of the 111-run design and the 54-run design are shown in Fig. 14. 15.



Fig. 14. Projections of 6-factor 111-run design. Left – plane x_1 - x_2 , right – plane x_1 - x_1



Fig. 15. Projections of first 54 runs from 6-factor 111-run design. Left – plane x_1 - x_2 , right – plane x_1 - x_1

The optimization was provided in four sequential stages, at each next stage the search region was reduced two times at each dimension. The local quadratic approximation with Gaussian weight function was used for metamodel building.

	1-stage	2-stage	3-stage	4-stage
RMSE of prediction	0.2977	0.1617	0.0350	0.002746
F_{\min}	-0.0806	-2.6436	-3.31678	-3.32233
Error of minimum found	92%	20%	0.17%	0.001%
Total number of function evaluations	54	108	162	216

Table 5. The convergence history

Table 6. shows the comparison with results obtained by other authors.

Table 6. Comparison of the results of Hartman function optimization

	New	New	rbf- Solve	DIR- ECT	MCS	Prev. ARSM	Impr ARSM I	Impr ARSM II	WHD SRO	WSN	SA
Eva- luati- ons	163	217	87	213	74	1248	158	105	591	82	11081
E (%)	<1	< 0.01	<1	<1	<1	<0.1	20	26	< 0.01	<1	95

In the Table 6., ARSM, Impr ARSM I, Impr ARSM II are the results taken from [31], rbfSolve is taken from [3]. DIRECT is an algorithm developed in [18] for finding the global minimum of a multi-variate function subject to simple bounds, using no derivative information. The result is taken from [3]. MCS (Multilevel Coordinate Search) by Huyer and Neumaier [13] is a Matlab program for bound constrained global optimization using function values only, results are taken from [3]. WHDSRO – Working-Hotelling Domain Spanning Robust Optimization [5], result with 78% successful convergence. WSN – result taken from [34]. SA – Simulated Annealing, result taken from [33]

It can be seen from Table 6. that the proposed method gives the minimal number of function evaluations for finding the optimum with E<0.01%, as well as a good performance for finding the optimum with E<1%.

8. Conclusions

The proposed complex space filling criterion approach allows creating designs of experiments with good space filling properties over the whole domain and all its one- and two-dimensional subspaces. This approach allows to construct both fixed-size and sequential experimental designs. Sequential designs can be obtained by adding new points to the existing design or by arranging the points of a large optimized fixed-size design.

Optimized LHDs can be used as the initial design for the search of optimal designs without level restrictions.

The accuracy of metamodels which are built using proposed sequential experimental designs is comparable to the accuracy of metamodels built by using fixed-size optimal designs or adaptive-sequential designs with the same number of runs. Kriging gives the average best accuracy of metamodels which are built using deterministic experiments, but local polynomial approximations with Gaussian weighting function give almost the same accuracy and may be the most effective for approximation of functions with noise.

Future research will be directed at the development of a method for the optimal choice of weighting coefficients of complex space-filling quality criterion in dependence of the sample size and the number of input variables.

References

- 1. Audze P. and Eglajs V. New approach for planning out of experiments // In: Problems of Dynamics and Strength, Vol. 35 Zinatne, Riga, 1977 p. 104-107 (in Russian).
- 2. Auzins J. Direct optimization of experimental designs // In: Proceedings of 10th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference Albany, New York, 2004, AIAA paper No. 2004-4578.
- 3. Björkman M., Holmström K. Global Optimization of Costly Nonconvex Functions Using Radial Basis Functions // In: Optimization and Engineering, 2000, No. 1 p. 373–397.
- 4. Branin F., and Hoo S. A Method for Finding Multiple Extrema of a Function of n Variables // In: Numerical Methods for Non-Linear Optimization, edited by F. Lootsma, Academic Press - New York, 1972 - p. 231-237.
- 5. Branscome C. and Mavris D. A Regression Confidence Band Approach to Global Optimization // In: 10th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference, September 2004 Albany, New York, AIAA 2004-4463.
- 6. Cleveland W. and Devlin S. Locally Weighted Regression: An Approach to Regression Analysis by Local Fitting // In: Journal of the American Statistical Association, Vol. 83, 1988 p. 596-610.
- Currin C. Mitchell T., Morris M. and Ylvisaker D. Bayesian Prediction of Deterministic Functions, With Applications to the Design and Analysis of Computer Experiments // In: J. Amer. Statist. Assoc., Vol. 86, 1991 - p. 953-963.
- Fang K., Lu X. and Winker P. Lower bounds for centered and wrap-around L₂discrepancies and construction of uniform design by threshold accepting // In: Journal of Complexity, 2003., 19 – p. 692-711.
- 9. Fang K., Ma X. and Winker P. Centered L_2 -discrepancy of random sampling and Latin hypercube design, and construction of uniform designs // In: Mathematics of Computation, 2002, 71 p. 275–296.
- 10. Fang K.T. and Wang Y. Number-Theoretic Methods in Statistics, Chapman & Hall London, 1994.
- 11. Halton J. H. On the efficiency of certain quasi-random sequences of points in evaluating multi-dimensional integrals, Numer. Math. 1960, 2 p. 84–90.

- 12. Hickernell F.J. A generalized discrepancy and quadrature error Bound // In: Mathematics of Computation, 1998, 67 p. 299–322.
- 13. Huyer W. and Neumaier A. Global optimization by multilevel coordinate search // In: Journal of Global Optimization, 1999, vol. 14 p. 331–355.
- 14. Janushevskis A., Akinfiev T., Auzins J. and Boyko A. A comparative analysis of global search procedures // In: Proceedings of the Estonian Academy of Sciences, 2004, Vol. 10, No. 4 p. 236–250.
- Jin R., Chen W. and Simpson T. Comparative Studies of Metamodeling Techniques under Multiple Modeling Criteria // In: Journal of Structural Optimization, Vol. 23, No. 1, 2001 - p. 1-13
- 16. Jin R., Chen W., Sudjianto A. An Efficient Algorithm For Constructing Optimal Design Of Computer Experiments // In: Proceedings of DETC'03 ASME 2003 Design Engineering Technical Conferences and Computers and Information in Engineering Conference -Chicago, Illinois USA, September 2-6, 2003, DETC2003/DAC-48760, 10 pages, available also at URL: http://ideal.mech.northwestern.edu/metamodeling.html [cited August 2003].
- Jin R., Chen W., and Sudjianto A. On Sequential Sampling for Global Metamodeling in Engineering Design // In: ASME 2002 Design Engineering Technical Conferences and Computer and Information in Engineering Conferenc - Montreal, Canada, September 29-October 2, 2002. Paper No. DETC2002/DAC-34092.
- Jones D.R., Perttunen C.D., and Stuckman B.E. Lipschitzian optimization without the Lipschitz constant // In: Journal of Optimization Theory and Applications, vol. 79, No. 1, 1993 - p. 157–181.
- 19. Johnson M.E., Moore L.M. and Ylvisaker D. Minimax and Maximin Distance Designs // In: Journal of Statistical Planning and Inference, Vol. 26, 1990 p. 131-148.
- 20. Ma C. and Fang K. T. A new approach to construct of nearly uniform designs // In: Int. J. Materials and Product technology, Vol. 20, Nos. 1-3, 2004 p. 115-126.
- 21. Martin J.D. and Simpson T.W. Use of Kriging Models to Approximate Deterministic Computer Models // In: AIAA Journal, 2005, Vol. 43, No. 4 p. 853-863.
- Martin J.D. and Simpson T.W. A Study on the Use of Kriging Models to Approximate Deterministic Computer Models // In: Proc. of DETC'03, 2003, Chicago, DETC 2003/ DAC- 48762.
- 23. Meyer R.H. and Nachtsheim C. J. The Coordinate-Exchange Algorithm for Constructing Exact Optimal Experimental Designs // In: Technometrics, Vol. 37, 1995 p. 60-69.
- 24. McKay M.D., Conover W. J., and Beckman R. J. A comparison of three methods for selecting values of input variables in the analysis of output from a computer code // In: Technometrics, Vol. 21, No. 2, 1979 p. 239-245.
- 25. Morris M.D. and Mitchell T.J. Exploratory Designs for Computational Experiments // In: Journal of Statistical Planning and Inference, Vol. 43, No. 3, 1995 p. 381-402.
- 26. Park J.S. Optimal Latin-Hypercube Designs for Computer Experiments // In: J. Statistical Planning and Inference, Vol. 39 No. 1, 1994 p. 95-111.
- 27. Romero V.J., Burkardt J.S., Gunzburger M.D., Peterson J.S., Krishnamurthy T. Initial Application and Evaluation of a Promising New Sampling Method for Response Surface Generation: Centroidal Voronoi Tessellation // In: Proc. of 44th Structures, Structural Dynamics, and Materials Conference (5th AIAA Non-Deterministic Approaches Forum), Apr. 7-10, 2003, Norfolk, AIAA-2003-2008
- 28. Sacks J., Welch W.J., Mitchell T. J. and Wynn H. P. Design and analysis of computer experiments // In: Statistical Science, Vol. 4, No. 4, 1989 p. 409-435.
- 29. Shewry M. and Wynn H. P. Maximum Entropy Sampling // In: J. Appl. Statist., Vol. 14, 1987 p. 165-170.
- 30. Sobol I. M. The distribution of points in a cube and approximate evaluation of integrals.

Zh. Vychisl. Mat. Mat. Fiz. 1967, 7 - 784-802.

- 31. Wang G.G. Adaptive Response Surface Method Using Inherited Latin Hypercube Design Points. Transactions of the ASME // In: Journal of Mechanical Design, Vol. 125, June 2003 p. 210-220.
- Wang G.G. and Simpson T.W. Fuzzy Clustering Based Hierarchical Metamodeling for Design Space Reduction and Optimization // In: Engineering Optimization, Vol. 36, No. 3, June 2004 – p. 313–335.
- 33. Wang, G.G. Improvement on the Adaptive Response Surface Method for Highdimensional Computationintensive Design Problems // In: ASME Design Engineering Technical Conferences - Design Automation Conference (Diaz, A.), Pittsburgh, PA, ASME, September 9-12, 2001. DETC2001/DAC-21141.
- 34. Williams B. J., Santner T. J. and Notz W. I. Sequential Design Of Computer Experiments To Minimize Integrated Response Functions // In: Statistica Sinica 10, 2000 p. 1133-1152.
- 35. Santner T. J, Williams B. J, Notz W. I.. The Design and Analysis of Computer Experiments, Springer-Verlag New York, 2003.

Auziņš J., Januševskis J. Jauni secīgie eksperimentu plāni metamodelēšanai un optimizācijai

Darbā piedāvātas jaunas secīgo iztvērumu pieejas eksperimentu plānu veidošanai. Galvenā ideja ir jaunu eksperimentu plāna punktu pievienošana vai eksistējoša plāna punktu sakārtošana, izmantojot kritēriju, kas ir sava veida kompromiss starp telpas aizpildes vienmērīguma kritēriju visā eksperimentālajā apgabalā un tā maza dimensiju skaita projekciju apakštelpās.

Secīgie iztvērumi var tikt lietoti gan metamodeļu veidošanai, gan uz metamodeļiem balstītai optimizācijai. Darbā lietotas lokāli svērto polinomu aproksimācijas metodes un rezultāti salīdzināti ar citu autoru rezultātiem, kas iegūti ar radiālo bāzes funkciju un Kriginga metodi, pielietojot tās labi zināmiem aproksimācijas un optimizācijas testa uzdevumiem. Vairumā gadījumu jaunie datoreksperimentu plāni rada mazāku prognozes kļūdu, salīdzinājumā ar zināmajiem secīgajiem plāniem.

Auzins J., Janushevskis J. New Sequential Designs of Experiments for Metamodeling and Optimization

In this work, a new sequential sampling approach for creating designs of experiments is proposed, the main idea of which is the adding of new experimental points or arranging points in existing experimental design according to a criterion, which achieves a compromise between the space filling quality in whole space and lowdimensional subspaces. Sequential samplings can be used both for global metamodeling and metamodel-based design optimization. The authors use locally weighted polynomial approximation method and compare results with the results of other authors, obtained by using RBF and Kriging methods on a number of well-known common approximation and optimization test problems. Kriging gives the average best accuracy of metamodels which are built using deterministic experiments, but local polynomial approximations with Gaussian weighting function give almost the same accuracy. In most cases the new designs for computer experiments give smaller prediction errors when compared with existing sequential designs.

Аузиньш Я., Янушевскис Я. Новые последовательные планы эксперимента для метамоделирования и оптимизации

Предложен новый подход к образованию последовательных экспериментальных выборок. Основная идея состоит в добавлении новых экспериментальных точек или упорядочивании точек существующего плана эксперимента согласно критерию, который представляет собой компромисс между критерием равномерности заполнения всего экспериментального пространства и ее подпространств низкоразмерных проекций. Последовательные планы могут использоваться как для создания метамоделей, так и для оптимизации на базе метамоделирования. В работе использованы методы локально взвешенных полиномиальных аппроксимаций для хорошо известных тестовых задач аппроксимации и оптимизации, и результаты сравнены с результатами других авторов, полученными методами Радиальных базовых функций и Кригинга. В большинстве случаев новые планы компьютерных экспериментов дают меньшую ошибку прогноза.