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NEW EXPERIMENTAL DESIGNS FOR METAMODEL BUILDING

JAUNI EKSPERIMENTU PLĀNI METAMODEĻU BŪVĒŠANAI

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1. Introduction

The nonparametric approximation methods are now widely being used for the construction of metamodels for mathematical systems, – Kriging, Radial Basis Functions, Local polynomial approximations. The simulation results that make up the metamodel can contain statistical errors, when natural experiments are also included. In this case the so-called space-filling experimental designs are used instead of the classical D-optimal designs. The first space filling design for a computer experiment was proposed in [1]. In this work, the designs in which the number of levels for each variable is equal to the total number of runs were first proposed. In [1], the space filling criterion based on a function similar to potential energy of gravity was first used. Later, the same kind of experimental designs was proposed as a Monte Carlo integration technique by McKay et al. [2], and the name “Latin hypercube samplings” was introduced. Numerous space filling experimental designs have been developed in an effort to provide more efficient and effective means for sampling deterministic computer experiments based on Latin hypercubes. Different space filling criteria for Latin hypercube designs was proposed by many authors: Maximin Latin hypercubes [3], Minimal Integrated Mean Square Error designs [4], Orthogonal array-based Latin hypercube designs [5], Orthogonal Latin hypercubes [6], Integrated Mean Square Error (IMSE) optimal Latin hypercubes [7]. The accuracy of prediction of metamodels, built on the basis of local polynomial approximation, depends also on weighting functions, used in the least squares method. We compared several space filling designs in combination with several weighting functions for 2-factors test function and 25-factor NASA HSCT approximation test.

2. Local Quadratic Approximation

In this work, we used local quadratic and linear approximations. Let F^i be the i-th observation of the response, and $\boldsymbol{x}^i$ – the i-th observation of s predictors (factors). The upper index for the variable $\boldsymbol{x}$ denotes the number of the point in the experimental design, while the lower index denotes the component of variable $\boldsymbol{x}$. To predict the value of response function in s-dimensional point $\boldsymbol{x}$, we use a second order polynomial approximation,

$$\widetilde{F}(x) = \beta_0 + \sum_{j=1}^{s} \beta_j x_j + \sum_{j=1}^{s} \sum_{k=j}^{s} \beta_{jk} x_j x_k \ . \tag{1}$$

The coefficients β depend on x and are calculated by minimizing the weighted least squares

$$\beta = \underset{\beta}{\arg\min} \ \sum_{j \in N_X} w(x - x^j) \times \left(F^j - \beta_0 - \sum_{i=1}^{5} \beta_i x_{ji} - \sum_{i=1}^{5} \sum_{k=i}^{5} \beta_{ik} x_i^j x_k^j \right)^2 , \tag{2}$$

where $\beta_{0,} \beta_i, \beta_{ik}$ are coefficients of the local quadratic approximation, N_x is the set of numbers of the nearest neighbors of the point $\boldsymbol{x}$. Here we use a constant number of neighbors – bandwidth N_t. The optimal number of neighbors is determined by leave-one-out crossvalidation [8].
The weight function w depends on the Euclidean distance between the point of interest $\boldsymbol{x}$ and the points of observations $\boldsymbol{x}^j$. Let u be
$u(x, x^j) = \dfrac{\left\| x - x^j \right\|}{\left\| x - x^q \right\|}$, where x^q is the farthest point in the neighborhood of point $\boldsymbol{x}$. An often-used weight function is the *tricube function* [9] $w_1(x, x^j) = \left(1 - u(x, x^j)^3\right)^3$.
We have also tested other weighting functions:
$w_2(x, x^j) = 1$; $w_3(x, x^j) = \dfrac{1}{u}$; $w_4(x, x^j) = \dfrac{1}{u^4}$; $w_5(x, x^j) = \dfrac{1}{u^8}$; $w_6(x, x^j) = (1 - u)^4$,
$w_7(x, x^j) = 1 + 2u^3 - 3u^2$; $w_8(x, x^j) = 1 - 10u^3 + 15u^4 - 6u^5$; $w_9(x, x^j) = e^{-\left(\frac{u}{g}\right)^2}$.
All weighting functions have zero value if u>1, i.e. all farthest N-N_t points are ignored.
Figure 1 shows the graphs of several weighting functions

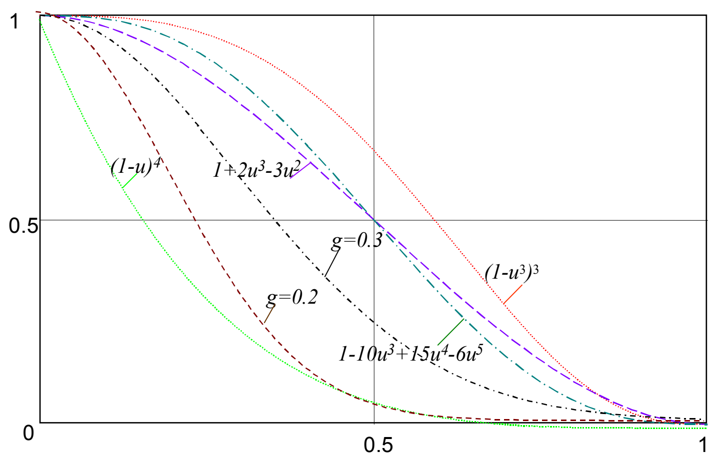

Figure 1. Weighting functions

3. Space Filled Experimental Designs

3.1. Minimal Mean Squared Distance Designs

For the computer experiment, the Minimal Mean Squared Distance (MMSD) experimental designs were employed. The MMSD designs are space filling designs that give the minimal Mean Squared Distance (MSD) between the mesh (training) points in design space *R* and the nearest point from experimental design *D*

$$MSD = \sqrt{\left(\frac{1}{n}\right)\sum_{v=1}^{n} \min_{u=1,\dots,N}\left[\sum_{i=1}^{s}\left(y_i^v - x_i^u\right)^2\right]}, \tag{3}$$

where y^v are points from a large sample in design space R^s (v=1,..., n), N is the number of points of the experimental design and n is the number of mesh points. We used a 1000000-point Latin hypercube sample as training points. These designs give points uniformly distributed in the design space and tend to minimize the expected mean squared error of the local quadratic approximation. Fang and Wang [10] introduced a similar criterion, named the Mean Squared Error (MSE) (the corresponding design is called *mse-rep-points*) and offer several algorithms for optimizing this criterion in the case of unconstrained levels and for Latin hypercube type designs. Although there are several numerical methods that claim to generate mse-rep-points for multivariate case (see [11, 12]), no one has shown that these methods can produce the real mse-rep-points.

When n is not large, Linde, Buzo and Gray [13] suggested an iterative vector quantizer algorithm LGB based on a training sequence. But there are some drawbacks with the approach: the resulting output vectors are only locally optimal and depend on the initial set of output vectors. The training sequence and numerical evaluation of the MSE are based on the Monte Carlo method that has poor efficiency.

Practically all the algorithms are based on the following idea. First, all the training set points y_j, j=1,,,n are partitioned in N parts S_i, i=1,,,N, thus that

$$y_j \in S_i \quad if \ \left\|y_j - x_i\right\| < \left\|y_j - x_k\right\|, k \neq i\,. \tag{4}$$

Then, the sample conditional means are calculated and a new set of mse-rep-points $x_i = \frac{1}{n_i} \sum_{y \in S_i} y_i$ is formed, where n_i is the number of training points falling in S_i. This process provides a nonincreasing MSE, and the algorithm eventually converges to a locally optimal solution. These algorithms converge well with a varied choice of training sequences (see for example Fang and Wang [10])

We use a large sample of Latin hypercube type (N=1000000) for training points.

Some experimental designs in a spherical region (in the case of 2 factors) are shown in Fig. 2.

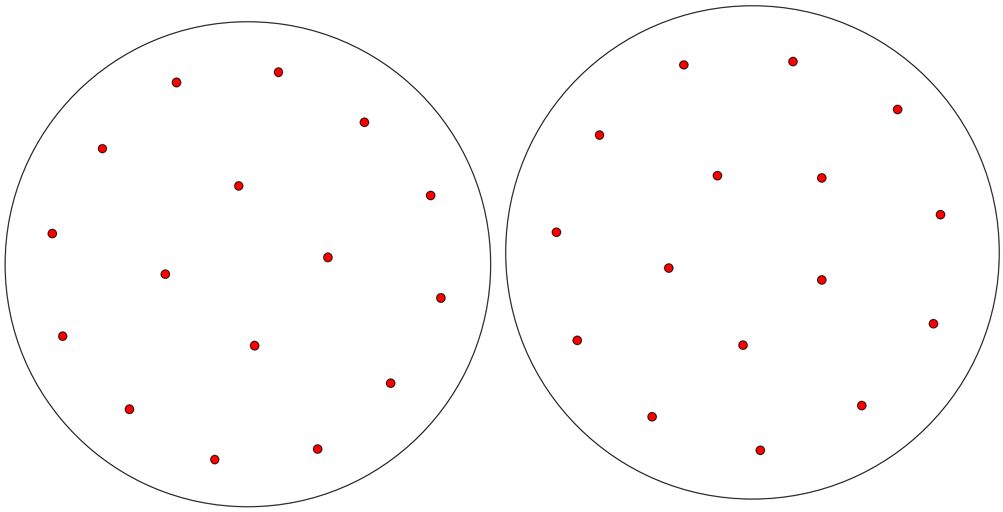

Figure 2. 16-run 2-factor designs in a unit sphere. Left, the design of Fang and Wang [10] *MSD*=0.18247, right, the optimal MSD design, *MSD*=0.1818.

In contrast to designs given in [10], we use spherical rotations to increase the space diversity of designs. The MSE and MSD criteria in unit sphere are invariant by these rotations.

The space diversity L of experimental design shows how uniform the projections of design are on the parameter axis:

$$L = \prod_{j=1}^{s} \sqrt{\frac{\sum_{i=1}^{N-1} \Delta_{ji}^2}{(N-1)(x_{j,\max} - x_{j,\min})^2}} \tag{5}$$

The space diversity of design has maximal value when all projections on axes build equidistant point sequences. This is true according to Latin hypercube designs.

In the case of optimizing the Latin hypercube designs according to the MSD criterion, the method of mean points, mentioned above, is not applicable because the factors have discrete levels of value. A direct minimization of the MSD criterion is highly time-consuming, since the calculation of the criterion itself requires a large amount of calculations.

In the case of the Latin hypercube, we use a modified method of partition of training points. After the calculation of mean values of parts, the total pairwise-columnwise exchange algorithm is used, which changes the components of design points to decrease the summary squared distance between design points and midpoint of the corresponding part of training points. This algorithm works relatively fast and gives results that cannot be improved with the exchange method by direct calculation of MSD criterion. Still, this algorithm, as all the algorithms mentioned above, gives results that are dependant on the initial choice of rep-points. However, using this experimental design, the differences of local quadratic approximation are practically unessential.

3.2 Other Space Filling Designs

For comparing with other space filling designs, four additional criterions have been used:
1. Eglaj`s criterion [1], later proposed also by Morris and Mitchell in a more general form [14]

$$\Phi_2 = \left[\sum_{u=1}^{N-1} \sum_{v=u+1}^{N} \frac{1}{\sum_{i=1}^{s} \left(x_i^u - x_i^v \right)^2} \right]^{1/2} . \tag{6}$$

2. The MINDIST criterion, which seeks to maximize the minimum distance between any pair of points in the data collection plan [3]

$$\text{MINDIST} = \min_{u,v=1,\ldots,N} \sum_{i=1}^{s} \left(x_i^u - x_i^v \right)^2 . \tag{7}$$

3. The entropy criterion first proposed by Shewry and Wynn [15] and then adopted by Currin et al. [16]. The entropy criterion for designs in unit cube $[0,1]^m$ is equivalent to the minimization of $-\log|\mathbf{C}|$, where $\mathbf{C}$ is the $N \times N$ covariance matrix of the design with elements

$$\mathrm{c}_{ij} = \exp\left\{ -\Theta \sum_{k=1}^{m} \left| x_k^i - x_k^j \right|^q \right\}, 0 < q \le 2 , \tag{8}$$

where $i, j=1,\ldots,N$. Throughout this paper the value $q = 2$ is selected thus that the correlation between two points is a function of their Euclidean distance L_2, and Θ is set equal to 2.

4. The discrepancy criterion, which averages the squared difference in the cumulative density function [17]

$$\left(D_C \right)^2 = \left(\frac{13}{12} \right)^s - \frac{2}{N} \sum_{u=1}^{N} \prod_{i=1}^{s} \left[1 + 0.5\left| x_i^u - 0.5 \right| - 0.5\left| x_i^u - 0.5 \right|^2 \right] + \\ \frac{1}{N^2} \sum_{u=1}^{N} \sum_{v=1}^{N} \prod_{i=1}^{s} \left[1 + 0.5\left(\left| x_i^u - 0.5 \right| + \left| x_i^v - 0.5 \right| - \left| x_i^u - x_i^v \right| \right) \right] \tag{9}$$

4. Comparison of Designs and Weighting Functions

4.1. Case of two Parameters

The designs were compared using a two-argument test function

$$f(x,y)=\frac{1}{1+3(x_1-x)^2+(y_1-y)^2}+\frac{-1}{1+3(x_2-x)^2+(y_2-y)^2}+\varepsilon \tag{10}$$

where x_1=0.05, y_1=0.05, x_2=-0.05, y_2=-0.05 and ε is random error with normal distribution and standard deviation σ

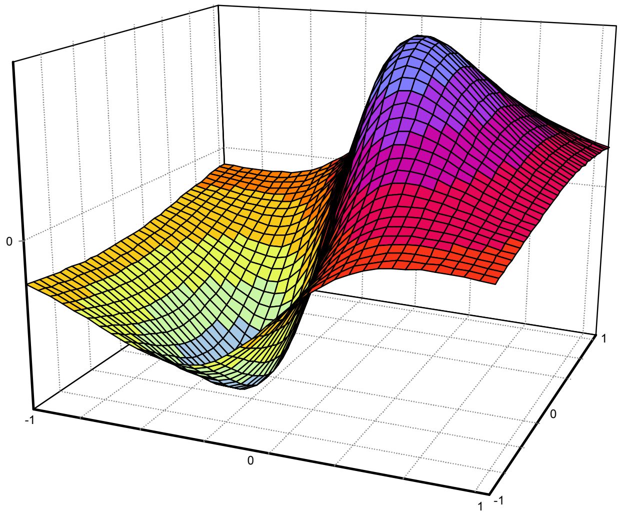

Figure 3. Exact test function (10)

Tables 1, 2 show the mean percentage error (MPE) of 36-run approximations.

$$MPE=\frac{100}{A}\sqrt{\frac{1}{1296}\sum_{i=1}^{1296}\left(f(x_i,y_i)-f(x_i,y_i)\right)^2}\ , \tag{11}$$

where A is the amplitude of the function in test points $A=\max\limits_{i=1,\dots,1296} f(x_i,y_i)-\min\limits_{i=1,\dots,1296} x\ f(x_i,y_i)$

All designs are optimized using 36-run Latin Hypercubes. Here REGULAR stands for 6x6 equidistant lattice and MMSD Latin hypercube

Table 1. Comparison of weighting functions and experimental designs, σ=0

	Discrep	EglKrit	Entrp	MaxMin	Regular	MSDLHS
$(1-u^3)^3$	2.5485 *	2.2315	2.4936	5.8848	2.0807	2.4484
$(1-u)^4$	2.1945	2.1132	2.1678	6.6713	1.9373	1.9814
$1+2u^3-3u^2$	2.4197	2.2435	2.5089	6.2491	2.0326	2.1033
$1-10u^3+15u^4-6u^5$	2.3507	2.2464	2.2361	6.1126	2.1132	2.1375
Const	3.4749	4.5726	2.9689	5.2369	2.9399	3.6178
$1/u$	2.6542	3.0779	3.4234	5.0943	2.0695	2.3194
$1/u^4$	2.5232	2.3923	2.3947	4.6706	2.0183	2.0552
$1/u^8$	2.4205	2.3021	2.0458	4.5728	1.9181	1.9543
$exp(-(u/g)^2)$	2.4988	2.1253	2.1827	6.1128	2.0455	2.2218

* - outlier points exist

Table 2. Comparison of weighting functions and experimental designs σ=0.0077 (3% of A)

	Discrep	EglKrit	Entrp	MaxMin	Regular	MSDLHS
$(1-u^3)^3$	3.1414	3.9615	3.7569	5.2309	3.0908	2.9685
$(1-u)^4$	2.9009	3.3579	3.5047	5.239	3.0401	2.6489
$1+2u^3-3u^2$	2.9207	3.8997	3.7807	4.7263*	3.0678	2.8148
$1-10u^3+15u^4-6u^5$	2.9198	3.799	3.7173	4.9786*	3.1288	3.0155
Const	3.7619	5.0099	4.4419	4.8610*	3.5494	4.1096
$1/u$	3.1052	3.6902	3.5509	4.7632*	3.0409	2.9711
$1/u^4$	3.208	3.3491	3.6638	5.1325	3.1084	3.057
$1/u^8$	3.3807	3.3646	3.6698	5.1605*	3.0658	3.2177
$exp(-(u/g)^2)$	3.1318	3.1181	3.5547	4.802	3.1314	2.6406

* - outlier points exist

As can be seen, MSDLHS with weighting function $(1-u)^4$ gives the best results in both cases. Regular lattice design also gives good results in the case without statistical error, but this design gives the worst results in the case when the function has very small dependence on one factor.

4.2. Case of 25 Parameters (NASA HSCT Approximation Challenge)

See [18] http://www.larc.nasa.gov.MDOB/mdo.test/class2probl
Given: 2490 analysis points, m=25 factors, 1 function of interest.
The challenge: to choose N<= 500 points sample, construct approximation and proof on other 2490-N points.
Table 3: Summary of Results for HSCT Problem

	Response Surfaces (Srivastava et al. [19])			Kriging (Srivastava et al. [19])			Local linear fit MMSD design		
Number of Points	Average Percentage Error	Max Percentage Error	Root Mean Square Error	Average Percentage Error	Max Percentage Error	Root Mean Square Error	Average Percentage Error	Max Percentage Error	Root Mean Square Error
126	207.83	5379.0	667.66	3.15	21.23	4.51	0.77	7.01	1.06
283	0.59	6.12	1.00	2.45	11.91	3.04	0.64	8.43	0.99
372	0.17	2.02	0.24	1.15	7.81	1.41	0.51***	5.97***	0.72***
500	0.49* 0.38**	2.89* 2.55**	0.50**						

* - Khatib et al. [20], ** - Auzins and Janushevskis, *** - Sub-quadratic fit

5. Conclusion

MSD optimal Latin hypercubes and local quadratic or linear approximation using weighting function $(1-u)^4$ can give very good results, which can be better than those given by approximations using other space filling criteria and Kriging or Response surface methods. The choice of bandwidth according to the leave-one-out crossvalidation gives mostly an overvaluation of the optimal number of neighbors, therefore attention must be paid to other, more complicated algorithms of bandwidth choice.

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Auziņš J., Januševskis A. Jauni eksperimentu plāni metamodeļu būvēšanai
Rakstā pētīti eksperimentu plāni telpas aizpildīšanai, kas tiek lietoti lokālām kvadrātiskajām aproksimācijām. Vidējās kvadrātiskās novirzes (VKN) kritērijs tiek piedāvāts, lai optimizētu plānu vienmērīgumu. Citi autori šo kritēriju sauc arī par vidējo kvadrātisko kļūdu. Šī raksta autori piedāvā plānu optimizācijas metodi vienības kuba un sfēras apgabalos, ko var lietot plāniem ar ierobežotām vai neierobežotām līmeņu vērtībām. Arī citi kritēriji, tādi kā entropija, nesaiste, maxmin un Eglāja kritērijs tiek salīdzināti, aproksimējot testa funkciju, pielietojot dažādas svara funkcijas lokālajai aproksimācijai. Tiek parādīts, ka Latīņu hiperkuba tipa plāni, kas optimizēti pēc VKN kritērija, dod vislabākos rezultātus, aproksimējot testa funkciju gan bez statistiskās kļūdas, gan ar normāla sadalījuma statistisko kļūdu. Plānu optimizācijas metode tiek lietota, lai izvēlētos aproksimāciju arī pazīstamajam NASA lielu ātrumu civilā transporta lidmašīnas uzdevumam. Šai gadījumā, izvēloties fiksētu eksperimentu skaitu (no dotajiem 2490) saskaņā ar VKN kritēriju un sekojošu lineāro aproksimāciju, tiek iegūti labi rezultāti, kas ir precīzāki nekā citu autoru iegūtie ar atbildes virsmas un Krīginga metodēm.

Auzins J. , Janushevskis A. New Experimental Designs for Metamodel Building
This paper explores space-filling experimental designs for use with local quadratic approximations. A Mean Squared Distance (MSD) criterion is offered for optimization of the uniformity of designs. The same criterion is also called the Mean Square Error (MSE) criterion by other authors. The authors have proposed a method of optimization of designs in unit cube and spherical regions, which can be used for designs with constrained or unconstrained level values. Also, other criteria such as Entropy, Discrepancy, MaxMin and Eglaj`s criterion are compared by approximation of the test function, using several weight functions for local approximation. It is shown that the Latin Hypercube type designs, optimized according to the MSD criteria, give the best results by approximation of test function both without statistical error and with statistical error with normal distribution. The design optimization method is used also for the well-known NASA High Speed Civil Transport aircraft (HSCT) approximation challenge. For this case, the choice of a fixed number of experiments (from the given 2490) according to the MSD criteria and following local linear approximation gives good results, more accurate than with solutions proposed by other authors, using the Response surface and the Kriging methods.

Аузиньш Я., Янушевскис А. Новые планы экспериментов для построения метамоделей
В статье исследуются методы планирования экспериментов для заполнения пространства в случае локальной квадратичной аппроксимации. Критерий среднеквадратичных отклонений (СКО) предложен для оптимизации равномерности экспериментов. Другие авторы этот критерий также называют среднеквадратичной ошибкой. Авторы настоящей работы предлагают метод оптимизации планов в областях единичных кубов и сфер, которые могут быть использованы как с ограниченными, так и с неограниченными уровнями значений планов. Также другие критерии такие как энтропия, невязка, минимакс и критерий Эглайса сопоставлены при аппроксимации тестовой функции, используя различные весовые функции для локальной аппроксимации. Показано, что оптимизированные согласно критерию СКО планы типа Латинских гиперкубов дают наилучшие результаты для аппроксимации тестовой функции как для случая без статистической ошибки, так и для случая со случайной ошибкой с нормальным распределением. Метод оптимизации планов также используется для известной задачи НАСА по аппроксимации высокоскоростного самолета гражданского транспорта. Для этого случая выбор фиксированного числа экспериментов (из представленных 2490) согласно критерию СКО и последующая локальная линейная аппроксимация дает хорошие результаты, которые более точны, чем решения полученные другими авторами, использующими метод поверхности отклика и метод Кригинга.