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Optimized Experimental Designs for Metamodeling: Algorithm

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***Abstract* - The paper is focused on direct optimization of experimental designs of continuous or discrete variables according to any optimality criterion. D-optimality criterion and space filling criteria such as Mean Square Error (MSE), Eglajs criterion, entropy criterion, discrepancy criterion and others can be used. Univariate relaxation and coordinate exchange algorithm with improved multistart is used for optimization.**

The proposed univariate relaxation and exchange algorithm with improved multistart method gives a good effectiveness for direct optimization of continuous and discrete experimental designs according to any optimization criterion. In cases of low dimensions the known D-optimal discrete and continuous designs were confirmed. For a larger number of variables many designs with better D-efficiency were found. The algorithm works very well also for Latin hypercube designs.

***Keywords* - Experimental Design, Latin Hypercube Design, Design Optimization, Metamodeling, D-optimal Design.**

I. INTRODUCTION

ALPHABETICALLY-optimal designs are often generated by an algorithm implemented using a computer. The most commonly used algorithms for their construction, described by Dykstra [1], St. John and Draper [2], Johnson and Nachtsheim [3], and Meyer and Nachtsheim [4], are based on the exchange of points from an initial design and a suitable candidate set. This sequential exchange can be performed one coordinate or experimental run at a time or by simultaneously exchanging multiple design points. Other approaches, such as simulated annealing (Haines [5]), also perform searches of this type but have not been as successful as the more structured methodologies.

In most cases it is impossible to categorically declare that the located designs are optimal (*D*-optimal, *I*-optimal etc), especially for $m>10$. Quite the reverse – for a large number of parameters and runs it is certainly possible to find designs with better values of criteria. It must be noted, though, that an improvement of the criteria in the third or fourth decimal digit does not have practical value. However, the criteria values of the located designs can be used to judge the effectiveness of the optimization methods employed (though occasionally also of computer productivity and time spent for calculation), therefore these designs should be published in public Internet pages. It is hard work to find optimal designs in large dimensions, but this must be done only once for each variant, and the results should be placed in a library accessible to all.

Such libraries have already been created, for example, N. J. A. Sloane [6]–, R. W. Mee [7], K. T. Fang [8] (uniform designs).

II. NOMENCLATURE

D_{eff}	=	*D*-efficiency criterion,
$(D_C)^2$	=	L_2 discrepancy criterion,
E	=	entropy criterion,
f, g	=	generic functions,
$\bar{f}$	=	mean value of function *f*,
Φ_2	=	Eglajs' potential energy criterion,
i, j, l	=	indices,
L	=	number of coefficients in regression function,
n	=	number of experimental runs (points),
N	=	number of training sample points for *MSE* criterion and number of confirmation points for σ_{test} and R^2 calculations,
m	=	number of factors (dimensions),
MinDist	=	minimal distance criterion,
MSE	=	mean square error criterion,
R^2	=	R square error measure,
$\boldsymbol{\sigma_{test}}$	=	relative prediction error of approximation,
$\boldsymbol{x_i}$	=	vector-row of *m* coordinates of experimental design.

III. OPTIMIZATION CRITERIA

In this paper we will pay attention chiefly to the criterion of *D*-optimality for second order polynomial approximation problem. Let's suppose that we wish to construct a design for a full quadratic response surface model

$$y = \beta_0 + \sum_{i=1}^{m} \beta_i x_i + \sum_{i=1}^{m} \sum_{j=i}^{m} \beta_{ij} x_i x_j + \varepsilon , \qquad (1)$$

where there are m variables $x_1,\ldots,$ xm, $L=(m+1)(m+2)/2$ unknown coefficients β, and the errors ε are independent with mean 0 and variance σ^2. Let the design consist on $n \geq L$ points

$$[x_{j1},...,x_{jm}] \quad \text{for} \quad 1 \leq j \leq n , \qquad (2)$$

chosen from a certain *region of measurement* $\boldsymbol{O}$. Let $\boldsymbol{X}$ be the $n \times L$ expanded design matrix, containing one row

$$f(x) = [1, x_1,..., x_k, x_1x_1, x_1x_2,..., x_m x_m] \qquad (3)$$

for each design point $x=[x_1,\ldots,xm]$, and let

$$M_X = X'X \tag{4}$$

denote the matrix of moments of the design measure (the prime indicates matrix transposition).

The prediction variance at an arbitrary point x is

$$\text{var } \hat{y}(x) = \frac{\sigma^2}{n} f(x) M_X^{-1} f(x)' . \tag{5}$$

D-optimal designs are those which maximize D-efficiency D*ef*

$$D_{ef} = \frac{100}{n} \times \left| M_X \right|^{1/p} . \tag{6}$$

D*ef* is the relative number of runs (in %) required by a possibly non-existent orthogonal design to achieve the same value of determinant [9]. D-efficiency defined in such a way is numerically different from the relative D-efficiency used by many other authors, but this does not influence the D-optimality of designs.

Myers and Montgomery [10] identified the pitfalls of the *D*-optimality designs, which have only model-dependent *D*-efficiency and do not address prediction variance. Moreover, for second-order models, the *D*-criterion often does not allow any (or many) center runs. We will not discuss this problem in further detail here, because the proposed algorithm allows the optimization of experimental designs according to any other criterion. For comparison with other designs, four additional criterions have been used:

Eglajs' criterion (Audze and Eglajs [11], Eglajs [12], later proposed also by Morris and Mitchell [13] in a more general form:

$$\Phi_2 = \sqrt{\sum_{u=1}^{n-1} \sum_{v=u+1}^{n} 1 \Big/ \sum_{i=1}^{m} \left(x_{ui} - x_{vi} \right)^2} . \tag{7}$$

Here x_{ui} denotes *i*-th component of point of experimental design number *u*.

The MINDIST criterion [14], which seeks to maximize the minimum distance between any pair of points in the design:

$$\text{MinDist} = \min_{u,v=1,\ldots,n} \sum_{i=1}^{m} \left(x_{ui} - x_{vi} \right)^2 . \tag{8}$$

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

$$\mathrm{c}_{ij} = \exp\left\{ -\Theta \sum_{u=1}^{m} \left| x_{iu} - x_{ju} \right|^q \right\}, \; 0 < q \le 2 , \tag{9}$$

where *i, j*=1,…,*n*.

Throughout this paper the value $q = 2$ is selected, so the correlation between two points is a function of their Euclidean distance L_2, and Θ is set equal to 2.

The Centered L_2 discrepancy criterion [17], which averages the squared difference in the cumulative density function:

$$\left(D_C\right)^2 = \left(\frac{13}{12}\right)^m - \frac{2}{n} \sum_{u=1}^{n} \prod_{i=1}^{m} \left[1 + \frac{1}{2} \left| x_{ui} - 0.5 \right| - \frac{1}{2} \left| x_{ui} - 0.5 \right|^2 \right] + \\ + \frac{1}{n^2} \sum_{u=1}^{n} \sum_{v=1}^{n} \prod_{i=1}^{m} \left[1 + \frac{1}{2} \left(\left| x_{ui} - 0.5 \right| + \left| x_{vi} - 0.5 \right| - \left| x_{ui} - x_{vi} \right| \right) \right]. \tag{10}$$

Mean Square Error (*MSE*) criterion [18], which gives Root Mean Squared Distance (RMSD) between the mesh points in design space R^m and the nearest point from experimental design *D*:

$$\text{MSE} = \sqrt{\left(\frac{1}{N} \right) \sum_{v=1}^{N} \min_{u=1,\ldots,n} \left[\sum_{i=1}^{m} \left(w_{vi} - x_{ui} \right)^2 \right]} , \tag{11}$$

where w_v are points from a large sample in design space R^m (*v*=1,..., *N*), *N* is the number of points of the experimental design and *n* is the number of mesh points. Approximately *N*=1000000 randomly distributed Latin hypercube points are employed as mesh points. Designs optimized according to the *MSE* criteria give points uniformly distributed in the design space and tend to minimize the expected mean squared error of the local quadratic approximation. For unconstrained designs in the unit cube $[-1,1]^m$ (without fixed levels for factors) the so-called NTLBG algorithm [18] exists, which gives fast convergence to the local minimum of criterion:

1. Generate a training sample w_v (*v*=1,..., *N*) of uniformly randomly distributed points (large random Latin hypercube).
2. Set *k*=0 and generate initial experimental design x_i^k, (*i*=1,…,*n*)
3. Divide the training points in *n* groups so that for all points from the *i*-th group the nearest experimental point is x_i^k. Calculate the sample mean $\overline{W_i}$ of each group.
4. Set $x_i^{k+1} = \overline{W_i}$ .0
5. Let ε be a preassigned small positive number. If $\left\| x_i^k - x_i^{k+1} \right\| > \varepsilon$, *i*=1,…,n, then use k+1 instead of k and return to step 3. Otherwise the process is terminated.

For the purpose of comparison with other designs, the distances and other characteristics of experimental designs are calculated after the designs are scaled into the unit cube $[0, 1]^m$, although the designs are mostly constructed in an m-dimensional cube $[-1, 1]^m$.

IV. ALGORITHM OF OPTIMIZATION

A popular way to seek *D*-optimal designs is the exchange algorithm, which successively removes and adds points starting from an initial arbitrarily chosen design [19, 20]. Also,

genetic algorithms have been successfully applied for determining *D*-optimal designs, see for example Giunta et al. [21].

For the finding of local optima we use the so-called univariate relaxation (coordinate relaxation) algorithm. This is very simple – all $n \times m$ components in turn are checked on whether the value of the criterion is improving by increasing or decreasing the component's value by one level. Continuous variables in this case are taken as discrete variables with large number of levels (see below). When all the components have been thus checked and none have changed, the search for local optimum is finished. This algorithm may be carried out in three ways, depending on the order in which the components are changed. First, all *m* components of the first point may be changed, then of the second point and so on until the *n*-th point. Second, the first component may be changed for all points, then the second component for all points and so on until the *m*-th component. Third, the components may be checked in random order. Our experience shows that the second variant converges slightly faster, but on the average a slightly better local optimum can be obtained with the third variant, changing the order of the components after every $n \times k$ tries.

The problem of optimization of experimental designs is characterized by an immense amount of local extremes.

Since the points can be numbered in any order, then any optima, both local and global, repeats *n*! times. However, there is also a huge amount of extremes with different values of criterion. The common practice in such cases is to use "multistart" or "clustering" methods for global optimization.

It can be automatically run many times from randomly chosen starting points, and the best solution found will be returned as the optimal solution. For some smooth nonlinear problems, multistart methods will converge in probability to the globally optimal solution. For other problems, they often yield very good solutions in an acceptable amount of time. Usually the search process begins with an initial design $\boldsymbol{D}^0$. This initial design may be obtained by choosing *n* random points from the design region, although in the implementation the user has the option of specifying $\boldsymbol{D}^0$ himself. After the first optimum is found, the search process is repeated with a new initial design. Usually the optimal is the best design obtained from several tens or even hundreds of tries, see Hardin and Sloane [22].

Our experience with employment of multistart algorithms shows that even a result obtained from as many as a thousand retries may be very far from the optimum. It is much more effective to employ the approach of annealing. Simulated annealing is an example of a random search algorithm. An initial candidate solution is generated, either at random or via another search algorithm. The current candidate is modified in some small, random way, and then this (possibly less optimal) candidate is accepted with a probability based on the Boltzmann kernel [23, 24].

We proceeded in a similar way. The proposed algorithm, strictly speaking, cannot be classified as simulated annealing, it is rather an improved multistart method with generation of new start points by exchange of randomly selected point coordinates from the previously found best solution. From a randomly selected initial design $\boldsymbol{D}^0$ a local optimum design $\boldsymbol{D}^*$ is found using univariate relaxation algorithm. Then $n \times m$ components of this design are modified with given probability p_d. This means that when a random number, uniformly distributed in [0,1], is less than p_d, then the new value of the component is randomly chosen from a continuous or discrete region of parameter values. Then this design is used as a new start point for the relaxation method. Unlike the classic annealing algorithm, the next local optimum with the worst value of criteria is not accepted. The initial exchange probability decreases starting from $p_d = 1$ to approximately 0.01 at the end of optimization process. Practically all designs optimized according to *D*-criterion or other (10)-(13) criteria with traditional multistart exchange algorithms can be improved.

A. Algorithm for Discrete and Continuous Variables

In this algorithm there are not any considerable differences between continuous and discrete variables. Practically it may be assumed that the continuous variable is the same discrete variable with a large number of levels. In practice 1001 levels are used as number of levels for continuous variables. In addition, the optimization process is organized in such a way that even for the continuous variables the initial number of levels is set as 3 or 5, the optimum is found and then the number of levels is increased. So the three-level design is a good initial estimate for the design with continuous variables and vice versa. In some cases of large dimensions the repeated change of the number of levels from 3 to 101 and back allowed to considerably improve the optimization criterion both for 3-dimensional design and continuous design. It also should be noted that there are not any problems in optimizing designs with a different number of levels for several variables.

B. Algorithm for Latin Hypercubes

The first space filling design for a computer experiment was proposed by Audze and Eglajs [11]. In this work, designs in which the number of levels for each variable is equal to the total number of runs were first proposed. In the same paper [11], the first space filling criterion (10) based on a function similar to the function of the potential energy of gravity was first used. Later, the same kind of experimental designs without any optimization were proposed as a Monte Carlo integration technique by McKay et al. [25], and the name "Latin hypercube samplings" was introduced. Numerous space filling experimental designs have since 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 (LHD) were proposed by many authors: Maximin Latin hypercubes [14], Minimal Integrated Mean Squared Error designs [26], Orthogonal array-based Latin hypercube designs [27], Orthogonal Latin hypercubes [28], Integrated Mean Squared Error (IMSE) optimal Latin hypercubes [29]. For Latin hypercubes it is not possible to use the univariate coordinate relaxation algorithm. The two or more point coordinate-exchange algorithms for optimizing of LHDs have been developed by many authors, beginning with work of

Audze and Eglajs [11]. In this algorithm the modification of all possible point pairs is carried out, attempting to exchange their separate coordinates, see Fig. 1.

$$\{x_{i1}, x_{i2}, x_{i3}, \ldots, x_{ik}, \ldots, x_{in}\}$$
$$\{x_{j1}, x_{j2}, x_{j3}, \ldots, x_{jk}, \ldots, x_{jn}\}$$

Fig. 1. Exchange of one pair of coordinates

A very effective exchange algorithm of randomly selected pairs for the optimization of the discrepancy criterion is proposed in work [30]. To construct optimal LHDs, Park [29] presented an approach based on the exchanges of several pairs of the elements in two rows, see Fig. 2. There are 2^{m-1}-1 exchange variants maximally possible since the first coordinate may remain unchanged. Morris and Mitchell [13] combined the exchange algorithm with simulated annealing algorithm to search for optimal LHDs.

$$\{x_{i1}, x_{i2}, x_{i3}, \ldots, x_{ik}, \ldots, x_{in}\}$$
$$\{x_{j1}, x_{j2}, x_{j3}, \ldots, x_{jk}, \ldots, x_{jn}\}$$

Fig. 2. Multiple exchange of coordinates of two points

$$\{x_{i1}, x_{i2}, x_{i3}, \ldots, x_{ik}, \ldots, x_{in}\}$$
$$\{x_{j1}, x_{j2}, x_{j3}, \ldots, x_{jk}, \ldots, x_{jn}\}$$
$$\{x_{l1}, x_{l2}, x_{l3}, \ldots, x_{lk}, \ldots, x_{ln}\}$$

Fig. 3. Cyclic exchange of one coordinate of three points

We also attempted the third exchange variant between three points of design, see Fig. 3. As many authors already have noted, for example [30], the difficulty of the exchange algorithm rapidly increases with the increase of the number or runs n and number of factors m. In general it can be said that the simultaneous exchange of several factors is not effective if m>5. For the *MSE* criterion, however, it altogether does not provide a possibility of improving the local optimum found by the simplest exchange variant, see Fig. 1. The third variant, three-point cyclic coordinate exchange, rapidly becomes ineffective with the increase of the number of runs n, since there are $m[n(n\text{-}1)(n\text{-}2)/3+n(n\text{-}1)/2]$ variants to be checked.

Therefore after many numerical experiments with LHDs with n up to 500 and m up to 15 we concluded that the first, simplest exchange variant is the most effective, in combination with the improved multistart method – generation of new start points by exchange of randomly selected point coordinates from the previously found best solution. This means that for all points x_i , i=1,…, n of previously found best experimental design and all coordinates (factors) l=1,…m, the coordinate x_{il} is exchanged with coordinate x_{jl} from a randomly selected other point x_j, when the currently generated random number from interval [0,1] is less than the given value p_d. The initial exchange probability decreases starting from p_d =1 to approximately 0.01 at the end of optimization process.

For the Eglajs' criterion Φ_2 and Discrepancy criterion $(D_C)^2$, which are large sums of terms, except in the first iteration, we do not need to recalculate all terms. It is necessary to compare only sums of terms that contain the exchanged coordinates. This accelerates calculations approximately $n/2$ times.

C. The Exchange Algorithm for MSE Criterion

The NTLBG algorithm, mentioned above, cannot be directly used in the case of LHDs. Direct calculation of *MSE* criterion, on the other hand, is time-consuming for large n and m. Therefore steps 4 and 5 of the NTLBG algorithm were modified in the following way:

4. For all i, j, k, (i,j=1,…,n), i>j, k=1,…,m we check whether the exchange of x_{ik} and x_{jk} does not decrease the partial sum $\left\|\overline{W}_i - x_i\right\|^2 + \left\|\overline{W}_j - x_j\right\|^2$. This means, that when

$$\left(\overline{W}_{ik} - \overline{W}_{jk}\right)\left(x_{jk} - x_{ik}\right) > 0 \qquad (12)$$

then the k-th component of i-th and j-th point of the experimental design must be exchanged.

5. If no pair of points is changed, then process is terminated. Otherwise repeat step 3.

This algorithm also gives local optima, which depend on initial design, therefore this was combined with the improved multistart method mentioned above.

A universal program *Relax* for design optimization according to several criteria was created and used in software for metamodeling and optimization EDAOpt, created at Riga Technical University. This allows not only to optimize the experimental designs, but also to examine their effectiveness in metamodeling and analysis of numerical and natural experiments. The program *Relax* optimizes continuous and discrete (including LHD) designs. This program improves many designs found by other authors. In most cases of small-size designs, the optimum found by other authors can only be repeated. For example, the discrepancy-optimized design of 16 runs and 5 factors found in work [31] seems to be globally optimal. In the work [32], the authors proposed the cutting method and found 100x5 LHD with $(D_C)^2$ =0.0012. Program *Relax* found LHD with $(D_C)^2$ =0.000797 in a few seconds.

V. CONCLUSIONS

The proposed univariate relaxation and exchange algorithm with improved multistart method gives a good effectiveness for direct optimization of continuous and discrete experimental designs according to any optimization criterion. In cases of low (3-6) dimensions the known *D*-optimal discrete and continuous designs were confirmed. For a larger number of variables many designs with better *D*-efficiency were found. The algorithm works very well also for Latin hypercube designs.

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Jānis Auziņš, Aleksandrs Januševskis, Jānis Januševskis. Optimizētie eksperimentu plāni metamodelēšanai: Algoritms
Šajā darbā tiek apskatīta nepārtrauktu un diskrētu mainīgo eksperimentu plānu tiešā optimizācija atbilstoši izvēlētam optimalitātes kritērijam. Var tikt izmantots D-optimuma kritērijs un tādi telpas aizpildīšanas kritēriji kā vidējās kvadrātiskās kļūdas (VKK) kritērijs, Eglāja kritērijs, entropijas kritērijs, nesaistes kritērijs uc. Optimizācija tiek veikta, izmantojot viendimensijas relaksācijas un koordinātu apmaiņas algoritmu ar uzlabotu multistartu.
Piedāvātais viendimensijas relaksācijas un apmaiņas algoritms ar uzlabotā multistarta metodi uzrāda labu efektivitāti nepārtrauktu un diskrētu plānu tiešajai optimizācijai saskaņā ar jebkuru no optimizācijas kritērijiem. Nepārtrauktu un diskrētu D-optimālo plānu gadījumos ar mazu dimensiju skaitu tika iegūti un apstiprināti līdz šim jau zināmie plāni. Daudz plānu ar labāku D-efektivitāti tika atrasti gadījumos ar lielāku mainīgo skaitu. Algoritms strādā ļoti labi arī Latīņu hiperkubu plānu gadījumos.

Янис Аузиньш, Александр Янушевскис, Янис Янушевскис. Оптимизированные планы экспериментов для метамоделирования: Алгоритм
В работе рассматривается непосредственная оптимизация планов экспериментов дискретных и непрерывных переменных в соответствии с выбранным критерием качества. Возможно использование критерия D-оптимальности и таких критериев заполнения пространства как критерий среднеквадратичной ошибки (СКО), критерий Эглайса, критерий энтропии, критерий невязок и др. Оптимизация производится, используя алгоритм одномерной релаксации и обмена координат с улучшеным мультистартом.
Предложенный алгоритм одномерной релаксации и обмена с методом улучшенного мультистарта показал хорошую эффективность при непосредственной оптимизации планов экспериментов дискретных и непрерывных переменных в соответствии с любым из критериев качества. В случаях непрерывных и дискретных D-оптимальных планов малых размерностей были получены и подтверждены ранее известные планы. В случаях больших размерностей получено много планов с лучшей D-эффективностью. Алгоритм работает очень хорошо и в случаях планов Латинских гиперкубов.