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# Optimized Experimental Designs for Metamodeling: Numerical Comparison

Janis Auzins, *Riga Technical University*, Alexander Janushevskis, *Riga Technical University*, Janis Janushevskis, *Riga Technical University*

***Abstract* - The paper is focused on univariate relaxation and coordinate exchange with improved multistart algorithms. The effectiveness of these algorithm are shown for searching of D-optimal designs with continuous and 3-level discrete parameters in 3-15 dimensions with 10 to 300 runs (45 to 4500 optimization parameters) and for optimization of Latin hypercube designs according to several criteria. The optimized designs are compared on many metamodeling test problems. For the case of second order local polynomial approximation, the use of MSE-optimal Latin hypercube designs and modified Gaussian weighting function is proposed. Optimized experimental designs are available in public Internet pages.**

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

## I INTRODUCTION

Formulation of the problem and proposed algorithms are given by authors in [1].

## II . COMPARISON OF THE SEARCH ALGORITHM RESULTS FOR D-OPTIMAL DESIGNS

Here we will look at the search results for *D*-optimal designs in the *m*-dimensional cube. Many authors have been working on the *D*-optimization of experimental designs. Box and Draper [2] used a hill-climbing method to search for *D*-optimal quadratic designs in the square with from 6 to 18 runs, and Haines [3] used simulated annealing to search for *D*-optimal designs in some low-dimensional problems. In particular, she found conjecturally optimal quadratic designs in the square with from 6 to 9 runs. Our program has confirmed the *D*-optimality of the designs found in these two papers as well as in paper of Hardin and Sloane [4].

For three dimensions there are a number of papers dealing with *D*-optimal 3-level designs, see [5], [6-10]. We have used our program *Relax* to search for *D*-optimal designs, both with continuous and with 3-level coordinates, and the designs with from 10 to 15 runs.

For the *D*-optimal 3-level designs our results agree with the above references. We also see from Tables 2-5 that for *D*-optimality it makes little difference whether weuse 3-level or continuous coordinates. Similarly there is not a large difference between $D_{ef}$values in the case of designs with or without center points. First the saturated designs for second order approximations were optimized. In dimensions 2 through 10, a number of authors have attempted to find *D*-optimal designs with the minimal number of runs in a cube. Draper and Lin [11] and Hardin and Sloane [4] give a table comparing the *D*-values of designs found by Box and Draper [12], Draper and Lin [13], Lucas [14], Mitchell and Bayne [8], Notz [15], Katsauonis [16], Rechtschaffner [17] and Hardin

TABLE 1
COMPARISON OF MINIMAL QUADRATIC DESIGNS IN CUBE BASED ON TABLE 7 OF HARDIN AND SLOANE [4]. ENTRY GIVES DEF VALUE

| *m* | Draper and Lin [13] | Lucas [14] | Notz [15] | Mitchell and Bayne [7] | Box and Draper [12] | Recht-schaff-ner [17] | Katsauonis [16] | Hardin and Sloane [4] | New Designs |
|---|---|---|---|---|---|---|---|---|---|
| 3 | 30.3 | 15.2 | 40.0 | 41.0 | 42.3 | 40.0 | 40.95 | 42.3 | 42.347 |
| 4 | 30.8 | 9.6 | 39.2 | 42.5 | 42.3 | 39.2 | 42.5 | 43.2 | 43.240 |
| 5 | 24.1 | 6.6 | 45.9 | 45.6 | 37.4 | 45.0 | 45.9 | 46.7 | 46.721 |
| 6 | 26.3 | 4.8 | 44.6 | | 31.7 | 42.8 | 45.98 | 46.4 | 46.456 |
| 7 | 19.6 | 3.6 | | | 22.7 | 38.3 | 45.10 | 45.8 | 47.604 |
| 8 | 32.1 | 2.8 | | | 19.3 | 33.6 | 44.56 | 45.5 | 48.010 |
| 9 | 20.0 | 2.3 | | | 16.7 | 29.3 | 44.96 | 46.0 | 46.592 |
| 10 | 16.5 | 1.8 | | | 14.6 | 25.5 | | 46.5 | 46.709 |
| 11 | | | | | | | | | 47.085 |
| 12 | | | | | | | | | 46.850 |
| 13 | | | | | | | | | 46.893 |
| 14 | | | | | | | | | 47.854 |
| 15 | | | | | | | | | 47.589 |

TABLE 2

EFFICIENCY OF NEW 3-LEVEL SATURATED DESIGNS

| m | n | $D_{ef}$ | MinDist | E | $\Phi_2$ | $(D_C)^2$ | MSE |
|---|---|---|---|---|---|---|---|
| 3 | 10 | 40.95 | 0.7071 | 0.7948 | 3.548 | 0.1897 | 0.7685 |
| 4* | 15 | 42.50 | 0.7071 | 0.5905 | 4.419 | 0.3171 | 0.9187 |
| 5 | 21 | 45.89 | 0.7071 | 0.6074 | 5.381 | 0.5963 | 1.2075 |
| 6 | 28 | 46.28 | 0.8660 | 0.2643 | 6.486 | 0.7707 | 1.3226 |
| 7 | 36 | 46.33 | 1.0000 | 0.2073 | 7.791 | 0.8611 | 1.5416 |
| 8* | 45 | 47.63 | 1.1180 | 0.0559 | 8.794 | 1.5882 | 1.5355 |
| 9 | 55 | 46.07 | 1.1180 | 0.0276 | 10.095 | 2.0034 | 1.9034 |
| 10 | 66 | 46.08 | 1.1180 | 0.0133 | 11.479 | 2.6819 | 2.0588 |
| 11* | 78 | 46.45 | 1.4142 | 0.0052 | 12.878 | 3.6979 | 1.8667 |
| 12 | 91 | 46.20 | 1.2247 | 0.0033 | 14.228 | 5.2303 | 2.3559 |
| 13 | 105 | 46.35 | 1.2247 | 0.0023 | 15.731 | 6.7866 | 2.4894 |
| 14 | 120 | 47.16 | 1.5000 | 0.0004 | 17.267 | 8.8577 | 2.6384 |
| 15 | 136 | 47.01 | 1.5811 | 0.00015 | 18.829 | 11.6104 | 2.7754 |

* – center point present

TABLE 3

EFFICIENCY OF NEW 3-LEVEL SATURATED DESIGNS WITH ONE CENTER POINT

| m | n | $D_{ef}$ | MinDist | E | $\Phi_2$ | $(D_C)^2$ | MSE |
|---|---|---|---|---|---|---|---|
| 3 | 10 | 40.00 | 0.5000 | 0.8635 | 3.594 | 0.1492 | 0.7204 |
| 4 | 15 | 42.50 | 0.7071 | 0.5905 | 4.419 | 0.3170 | 0.9189 |
| 5 | 21 | 44.81 | 0.7071 | 0.3893 | 5.363 | 0.5358 | 1.0979 |
| 6 | 28 | 46.03 | 0.8660 | 0.2913 | 6.534 | 0.7662 | 1.2519 |
| 7 | 36 | 45.68 | 1.0000 | 0.1411 | 7.815 | 0.8923 | 1.3763 |
| 8 | 45 | 47.63 | 1.118 | 0.0559 | 8.794 | 1.58819 | 1.5355 |
| 9 | 55 | 45.84 | 1.224 | 0.0262 | 10.179 | 1.9606 | 1.6477 |
| 10 | 66 | 45.36 | 1.118 | 0.0167 | 11.538 | 2.7515 | 1.7605 |
| 11 | 78 | 46.45 | 1.4142 | 0.0052 | 12.878 | 3.6979 | 1.8667 |
| 12 | 91 | 46.01 | 1.3228 | 0.0022 | 14.250 | 5.1395 | 2.3551 |
| 13 | 105 | 45.71 | 1.2247 | 0.0028 | 15.814 | 6.7603 | 2.0532 |
| 14 | 120 | 46.63 | 1.4142 | 0.0009 | 17.359 | 8.8413 | 2.1386 |
| 15 | 136 | 46.88 | 1.5811 | 0.0002 | 18.869 | 11.7698 | 2.2215 |

TABLE 4

EFFICIENCY OF NEW DESIGNS WHEN THE POINTS ARE RANGED OVER THE WHOLE CUBE

| m | n | $D_{ef}$ | MinDist | E | $\Phi_2$ | $(D_C)^2$ | MSE |
|---|---|---|---|---|---|---|---|
| 3 | 10 | 42.346 | 0.6705 | 0.7354 | 3.512 | 0.1339 | 0.7132 |
| 4 | 15 | 43.240 | 0.7939 | 0.5903 | 4.456 | 0.2556 | 0.9467 |
| 5 | 21 | 46.721 | 0.6925 | 0.5267 | 5.378 | 0.5570 | 1.2083 |
| 6 | 28 | 46.456 | 0.8238 | 0.2825 | 6.439 | 0.8361 | 1.3757 |
| 7 | 36 | 47.604 | 1.2319 | 0.0778 | 7.705 | 0.9502 | 1.5354 |
| 8 | 45 | 48.010 | 1.1857 | 0.0520 | 8.797 | 1.6144 | 1.5357 |
| 9 | 55 | 46.592 | 1.2226 | 0.0216 | 10.161 | 2.0227 | 1.8613 |
| 10 | 66 | 46.709 | 1.1990 | 0.0088 | 11.476 | 2.8297 | 0.7354 |
| 11 | 78 | 47.085 | 1.3595 | 0.0049 | 12.930 | 3.7927 | 1.8942 |
| 12 | 91 | 46.850 | 1.3325 | 0.0022 | 14.296 | 5.2765 | 2.3537 |
| 13 | 105 | 46.893 | 1.3402 | 0.0010 | 15.806 | 6.8794 | 2.4805 |
| 14 | 120 | 47.854 | 1.5521 | 0.0003 | 17.329 | 9.2363 | 2.6294 |
| 15 | 136 | 47.589 | 1.6700 | 0.0001 | 18.911 | 12.0384 | 2.7572 |

TABLE 5

EFFICIENCY OF NEW DESIGNS WHEN THE POINTS ARE RANGED OVER THE WHOLE CUBE WITH ONE CENTER POINT

| m | n | $D_{ef}$ | MinDist | E | $\Phi_2$ | $(D_C)^2$ | MSE |
|---|---|---|---|---|---|---|---|
| 3 | 10 | 40.573 | 0.6040 | 0.7526 | 3.480 | 0.16547 | 0.7196 |
| 4 | 15 | 42.677 | 0.6363 | 0.6444 | 4.446 | 0.3239 | 0.9212 |
| 5 | 21 | 45.167 | 0.6081 | 0.5013 | 5.389 | 0.5571 | 1.1024 |
| 6 | 28 | 46.447 | 0.8087 | 0.3025 | 6.465 | 0.8569 | 0.7354 |
| 7 | 36 | 46.69 | 1.1316 | 0.1019 | 7.876 | 0.8683 | 1.3655 |
| 8 | 45 | 48.009 | 1.1860 | 0.0522 | 8.797 | 1.6143 | 1.5350 |
| 9 | 55 | 46.460 | 1.2320 | 0.0228 | 10.206 | 2.0256 | 1.6454 |
| 10 | 66 | 46.359 | 1.2038 | 0.0145 | 11.561 | 2.8282 | 1.7592 |
| 11 | 78 | 47.074 | 1.3708 | 0.0051 | 12.943 | 3.7676 | 1.8639 |
| 12 | 91 | 46.672 | 1.2878 | 0.0023 | 14.320 | 5.2119 | 2.3474 |

TABLE 6

EFFICIENCY OF NEW DESIGNS WHEN THE POINTS ARE RANGED OVER THE WHOLE CUBE (DOUBLE NUMBER OF RUNS)

| m | n | $D_{ef}$ | MinDist | E | $\Phi_2$ | $(D_C)^2$ | MSE |
|---|---|---|---|---|---|---|---|
| 3 | 16* | 45.91 | 0.4768 | 3.4032 | 6.186 | 0.1644 | 0.6659 |
| 4 | 30 | 48.23 | 0.4528 | 5.4418 | 9.762 | 0.2725 | 0.7979 |
| 5 | 42 | 49.794 | 0.5130 | 3.1761 | 11.472 | 0.4680 | 1.0182 |
| 6 | 56 | 51.587 | 0.4838 | 2.4806 | 13.534 | 0.7300 | 1.2184 |
| 7 | 72 | 53.273 | 0.6690 | 1.2808 | 15.635 | 1.0865 | 1.3826 |
| 8 | 90 | 54.846 | 0.6991 | 0.9663 | 18.004 | 1.6016 | 1.5884 |
| 9 | 110 | 56.178 | 0.8964 | 0.3593 | 20.485 | 2.1606 | 1.7445 |
| 10 | 132 | 57.373 | 0.9181 | 0.1983 | 23.041 | 3.0380 | 1.9044 |
| 11 | 156 | 58.543 | 1.0426 | 0.0807 | 25.787 | 4.1102 | 2.0597 |
| 12 | 182 | 59.646 | 1.2164 | 0.0297 | 28.581 | 5.4893 | 2.2227 |
| 13 | 210 | 60.324 | 1.1242 | 0.0193 | 31.509 | 7.3919 | 2.3608 |
| 14 | 240 | 60.881 | 1.2208 | 0.0082 | 34.570 | 9.6425 | 2.5017 |
| 15 | 272 | 61.656 | 1.4364 | 0.0021 | 37.609 | 12.7728 | 2.6576 |

* - 16 runs is the maximal number of points in 3-dimensional D-optimal design without repeated points

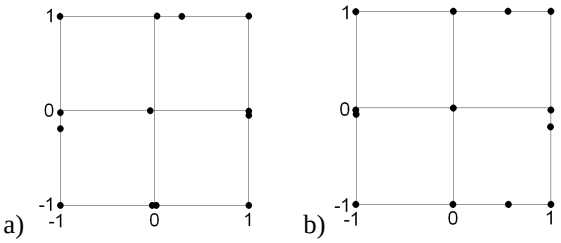


Fig. 1. Continuous D-optimized design with 45 runs and 8 factors: a) *Plane* $x_1$-$x_2$, b) *Plane* $x_4$-$x_7$

and Sloane [4]. We have reproduced this as Table 1, supplemented with an additional column showing the *D*-values of the designs found by *Relax*.

The entries give the $D_{ef}$-values, numbers which are to be made as large as possible. In dimensions $m > 6$ the new designs are better.

For four dimensions, Meyer and Nachtsheim [5] reported that their simulated annealing algorithm found a 17-runs design with $|X'X|$ = 1.4867E13 when the coordinates were restricted to three levels, but that they could only obtain 4.1296E12 when the points ranged over the whole cube. *Relax* found an even better continuous design, with $|X'X|$ = 1.6863 E13 and $|X'X|$=1.5288E13 for the case of three levels. The saturated designs are rarely used in real approximation. The commonly used number of runs in Response surface method with second order polynomial approximation is 1.5 to 2 times greater. Table 6 shows criteria values for *D*-optimal designs with double number of runs.

In the distribution of the points in the design there is a noticeable tendency for the points to be concentrated in the neighborhood of three-level design points, i.e., the point coordinates are close to the values –1, 0, +1. This tendency

can also be noted in designs with 8 variables and 45 runs, see Fig. 1.

## III. Comparison of Space Filling Designs

For various optimal LHDs, (e.g. $\Phi_2$, MinDist, MSE, entropy, and discrepancy), there is no consensus on which criterion is better. In this paper, LHDs optimized according to various criteria were compared for metamodeling using second order local polynomial approximations. Several weighting functions were used:
triweight function suggested by Cleveland [18],

$$W(u) = \left(1-u^3\right)^3, \tag{1}$$

function proposed by the authors

$$W(u) = (1-u)^4, \tag{2}$$

Gaussian kernel

$$W(u) = \exp\left(-\alpha u^2\right). \tag{3}$$

Here u – the Euclidean distance between current point of approximation $x^*$ and point of experimental design, normalized so that the distance between $x^*$ and the nearest point outside the neighborhood of $x^*$ is equal to 1, see [18]. The Gaussian weighting function traditionally is used with coefficient $\alpha = 0.5$, and the smoothness of approximation is controlled by bandwidth $n_t$ (number of neighbors). We used Gaussian kernel with maximal number of neighbors $n_t$ =n, and the smoothness of approximation was controlled only by coefficient α. The optimal constant values of bandwidth $n_t$ and α were found by cross-validation approach.

For comparing a test function is necessary which: 1) badly approximates with second order polynomial approximation (otherwise in place of local approximation the much simpler global polynomial approximation can be employed); 2) is symmetrical in relation to all factors; 3) contains isolated extremes in region of interest; 4) is still simple enough to be approximated with a number of runs that may be comparable to the number of runs required for quadratic approximations. In a m-dimensional cube $[-1, 1]^m$ these requirements are met by the function $f_{test}$

$$f_{test}(x) = \frac{1}{1+\sum_{j=1}^{m}\left(x_j-0.05\right)^2} - \frac{1}{1+\sum_{j=1}^{m}\left(x_j+0.05\right)^2}, \tag{4}$$

which has exactly one minimum and one maximum in this region.

The accuracy of approximation was measured with the relative average prediction error $\sigma_{test}$

$$\sigma_{test} = 100\%\frac{\sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(f_{test}(w_i)-\hat{f}_{test}(w_i)\right)^2}}{\sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(f_{test}(w_i)-\bar{f}_{test}\right)^2}} = 100\%\sqrt{\frac{MeanSquareError}{Variance}} \tag{5}$$

where $w_i$ – confirmation points (i=1,…,N), $\hat{f}_{test}(w_i)$ - approximated value of test function, $\bar{f}_{test}$ - average value of test function in confirmation points. 50000 uniformly randomly selected confirmation points (Latin hypercube sample) in region of interest were used.

Some authors employ the $R^2$ prediction error measure [19]

$$R^2 = 1-\frac{MeanSquareError}{Variance} = 1-\left(\frac{\sigma_{test}}{100}\right)^2 \tag{6}$$

Figures 2-5 show the exact three factor function and its approximations in the plane. Table 7 shows the accuracy of the three-factor test function, approximated with several experimental designs, global second order, global third order polynomial and local quadratic approximations with three different weighting functions. 50000 confirmation points were used. First number in the cell shows the value of relative average prediction error in the case of experimental data without noise. The second number in the cell shows the error value when the function has Gaussian noise with standard deviation equal to 5% from standard deviation of experimental data (the average value of 10 tries). D2 and D3 are determinant values of information matrix $M_X$ for global quadratic and global cubic approximation respectively.

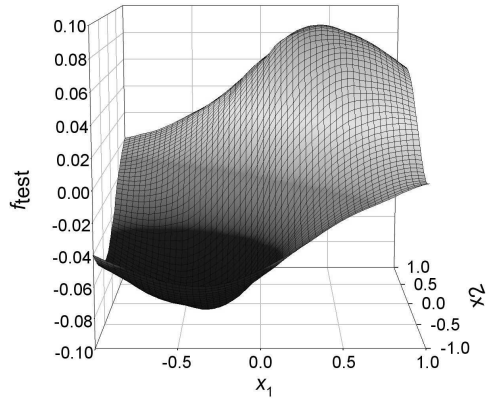


Fig. 2. Exact three argument test function,$x_3$ fixed to zero

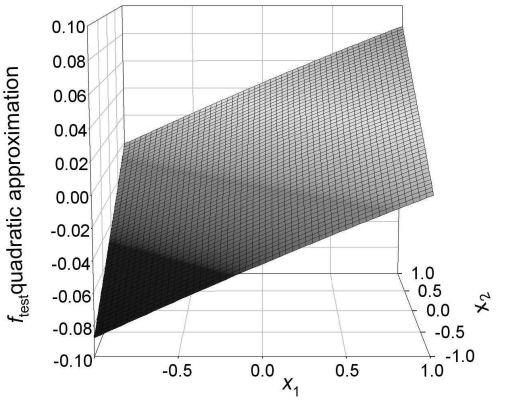


Fig. 3. Global quadratic approximation of three argument test function, $x_3$ fixed to zero

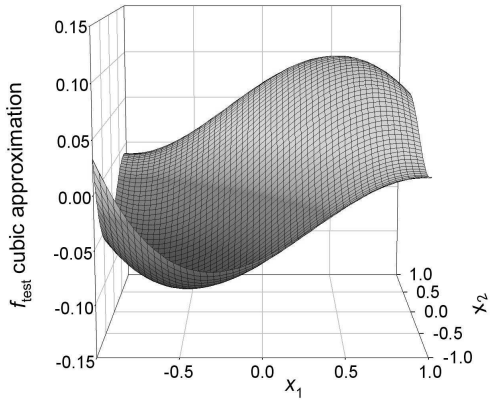


Fig. 4. Global cubic approximation of three argument test function, $x_3$ fixed to zero

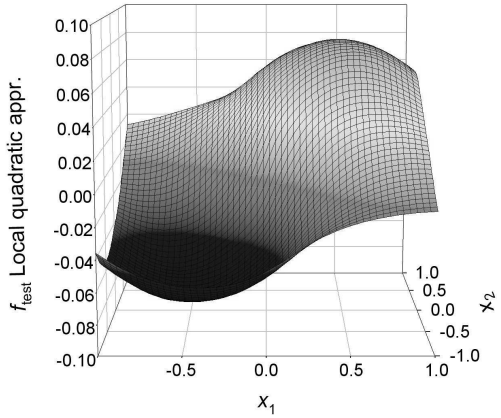


Fig. 5. Local quadratic approximation of three argument test function, $x_3$ fixed to zero

As can be seen, the best prediction accuracy has been obtained by local quadratic approximation using MSE-optimal LHD and Gaussian weighting function. Second order D-optimal LHD design gives noticeably worse accuracy for all approximation methods as for experiments with noise or without noise. It can also be seen that MSE- and E-optimal LHDs have very similar values of criteria and prediction errors. In our experience, in some cases, LHD optimized according to MSE criterion have better entropy criterion values than LHD optimized according to Entropy criterion and vice versa.

The following investigation was carried out with 80 runs 3 factors LHDs. 50 random LHDs were generated without any optimization, and values of optimality criteria, and prediction error values for approximation of test function (4) using local quadratic approximation with weighting function (2) were calculated.

In addition the same values for MSE-optimal, E-optimal, $(DC)^2$-optimal and $\Phi_2$-optimal were calculated. Then Pearson's correlation coefficients between optimality criterions and prediction errors for all 54 designs were calculated. Results are shown in Table 8.

As opposed to other criteria, MinDist criterion must be increased to improve the uniformity of space filling designs, therefore the correlation with other criteria and with the prediction error is negative. Correlation coefficients between optimality criteria and prediction error of approximations are shown also in Fig. 6. The three bars for each criterion show the average value of coefficient and minimal and maximal boundary for confidence interval of 95%. It can be seen that correlation coefficients have large dispersion and the number of tries should be increased.

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TABLE 7

30-RUNS TEST IN 3-DIMENSIONAL CUBE $[-1,1]^3$

| | *MSE* | $(D_C)^2$ | *E* | *Min Dist* | $\Phi_2$ | $D_2$ | $D_3$ | $\sigma_{test}$ Global quadratic | $\sigma_{test}$ Global cubic | $\sigma_{test}$ Local Gaussian | $\sigma_{test}$ Local Tricube | $\sigma_{test}$ Local $(1-u)^4$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| *MSE*-optimal | 0.349 | $173e^{-3}$ | 26.45 | 0.320 | 17.7 | $2.7e^6$ | $3.2e^4$ | 45.1<br>45.3 | 39.7<br>40.7 | 12.2<br>13.0 | 14.3<br>14.9 | 12.5<br>13.2 |
| Uniform (Fang) | 0.373 | $142e^{-3}$ | 30.48 | 0.119 | 18.7 | $4.2e^6$ | $5.4e^4$ | 45.3<br>45.4 | 21.8<br>23.1 | 16.7<br>17.4 | 19.7<br>20.3 | 16.6<br>17.3 |
| $(D_C)^2$-optimal | 0.368 | $137e^{-3}$ | 29.74 | 0.169 | 18.3 | $2.2e^6$ | $1.2e^4$ | 45.8<br>46.1 | 30.2<br>28.8 | 15.7<br>16.3 | 18.4<br>19.0 | 16.2<br>16.8 |
| *E*-optimal | 0.350 | $163e^{-3}$ | 26.39 | 0.320 | 17.7 | $2.4e^6$ | $2.6e^4$ | 45.1<br>45.3 | 38.6<br>38.2 | 12.9<br>13.5 | 14.5<br>15.2 | 13.0<br>13.7 |
| $\Phi_2$-optimal | 0.352 | $163e^{-3}$ | 27.17 | 0.320 | 17.7 | $1.7e^6$ | $3.4e^3$ | 45.1<br>45.2 | 43.8<br>44.6 | 18.6<br>19.2 | 20.0<br>20.4 | 18.2<br>18.9 |
| *D*-opt. LH quadr. | 0.411 | $283e^{-3}$ | 38.74 | 0.060 | 22.8 | $8.5e^6$ | $1.2e^3$ | 48.6<br>48.5 | 58.5<br>58.8 | 25.0<br>25.2 | 28.4<br>28.5 | 25.7<br>26.3 |
| *D*-opt. LH cubic | 0.384 | $211e^{-3}$ | 34.84 | 0.084 | 21.8 | $7.8e^6$ | $6.8e^6$ | 46.1<br>46.3 | 27.0<br>26.7 | 13.1<br>13.5 | 15.3<br>15.6 | 12.9<br>13.3 |

TABLE 8

CORRELATION COEFFICENTS BETWEEN CRITERIA AND PREDICTION ERROR OF APPROXIMATION

| | *E* | *MSE* | *MinDist* | $\Phi_2$ | $(D_C)^2$ | $\sigma_{test}$ |
|---|---|---|---|---|---|---|
| *E* | | 0.9660 | -0.8741 | 0.8249 | 0.7142 | 0.5811 |
| *MSE* | | | -0.8164 | 0.74129 | 0.7188 | 0.6401 |
| *MinDist* | | | | -0.8561 | -0.5345 | -0.3622 |
| $\Phi_2$ | | | | | 0.5491 | 0.3518 |
| $(D_C)^2$ | | | | | | 0.5015 |

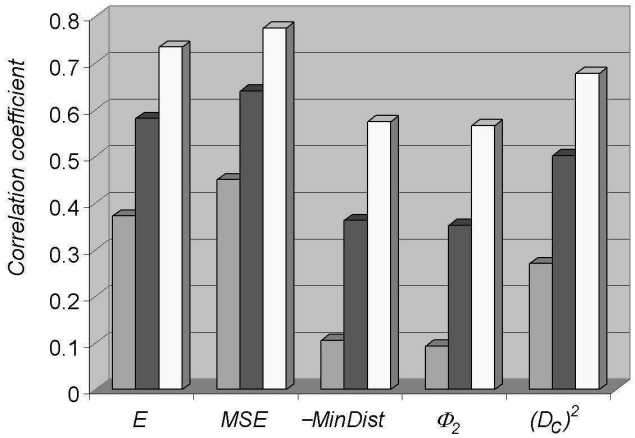


Fig. 6. Correlation between criteria and prediction error of approximation

A comparison of LHDs of this kind was carried out not only on the basis of test function (4), but also with many other functions with number of factors from 2 to 10, as the well-known optimization examples: the Branin function, six-hump camel-back function [20], the Goldstein-Price function and the Hartmn 6 function [21] The results in all cases were similar – the best prediction accuracy of approximation was achieved with *MSE*- or *E*-optimal LHD and local quadratic approximation with weighting functions (2) or (3).

The proposed algorithm for optimization of LHD according to the *MSE* criterion works much faster than the same algorithm for the entropy criterion, because the latter needs calculation of determinant of $n \times n$ matrices, which is computationally difficult for large *n*.

In the conclusion of this analysis we will demonstrate an example of function $F_{10}$ taken from work [19], and transformed to interval [-1,1] for all three factors:

$$F_{10}(x) = \sum_{i=1}^{99} f_i(x)^2 , \qquad (7)$$

where

$$f_i(x) = -0.01i + \exp\left( -\frac{(u_i - 12.8x_2 - 12.8)^{(2.5x_3+2.5)}}{49.95x_1 + 50.05} \right) \qquad (8)$$

and

$$u_i = 25 + \left(-50\ln(0.01i)\right)^{2/3}, \ \text{i=1,…,99} . \qquad (9)$$

This function of three arguments is defined as high-order nonlinear and very difficult for approximation.

Figures 7-9 show the exact function $F_{10}$ and its approximations. The accuracy of approximations is given in the table 9.

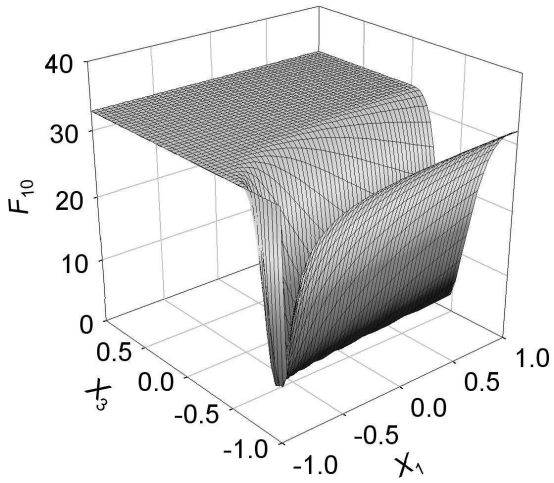


Fig. 7. Exact function $F_{10}$ ($x_2$ fixed to zero)

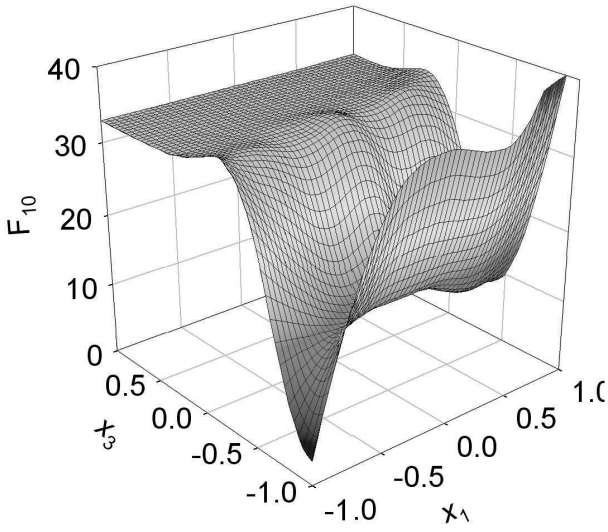


Fig. 8. Local quadratic approximation of $F_{10}$

Results for Multivariate Adaptive Regression Splines (MARS), Radial Basis Functions (RBF) and Kriging are taken from work [19]. In all cases 125-runs 3 factors designs were

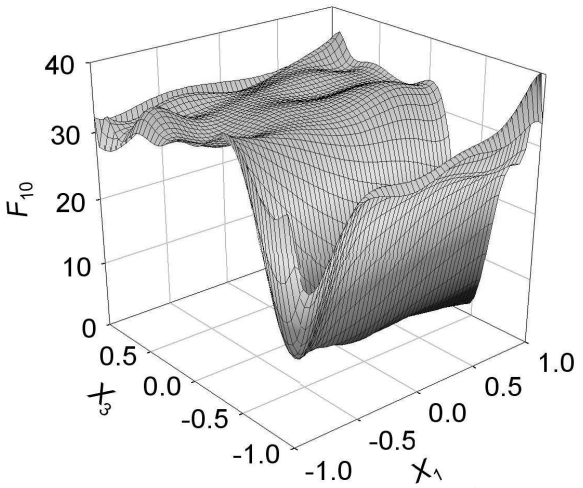


Fig. 9. Ortogonal polynomial approximation of $F_{10}$

used. For the third order polynomial (PR), Orthogonal Polynomial [22] (OP) and Local quadratic methods *MSE*-optimized design was used. In this case the Orthogonal Polynomial approximation method gives the best result. This function seems to be too complex for approximation with only 125-runs experimental design.

## IV. CONCLUSIONS

Comparing results of many test problems of metamodeling, it was concluded that in the case of second order local polynomial approximation the use of Mean Square Error criterion is preferable, because this gives good accuracy of metamodels and the finding of optimal designs using the proposed algorithm is less difficult than optimization according to other criteria. The experimental designs, found by the developed program *Relax*, are placed at the address http://213.175.94.108/designDB/search.php of Riga Technial University page http://www.mmd.rtu.lv/ for common use for approximation and optimization tasks

TABLE 9
THE ACCURACY OF METAMODELS FOR FUNCTION $F_{10}$

| | MARS* | RBF* | Kriging* | PR | OP | Local quadratic |
|---|---|---|---|---|---|---|
| R2 | 0.7434 | 0.7441 | 0.7628 | 0.586 | 0.9175 | 0.819 |

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**Janis Auzins**, Leading Researcher, Dr.sc.ing.,Machine and Mechanism Dynamics Research Laboratory, Riga Technical University. Address: Ezermalas iela 6, Rīga, LV-1006, Latvia. Phone: +371 7089396, Fax: +371 7089746. E - mail: auzinsjp@latnet.lv

**Alexander Janushevskis**, Head of Laboratory, Dr.sc.ing.,Machine and Mechanism Dynamics Research Laboratory, Riga Technical University. Address: Ezermalas iela 6, Rīga, LV-1006, Latvia. Phone: +371 7089396, Fax: +371 7089746. E - mail: janush@latnet.lv

**Janis Janushevskis**, Researcher, Dr.sc.ing., Machine and Mechanism Dynamics Research Laboratory, Riga Technical University. Address: Ezermalas iela 6, Rīga, LV-1006, Latvia. Phone: +371 7089396, Fax: +371 7089746. E - Mail: janisj@latnet.lv

**Jānis Auziņš, Aleksandrs Januševskis, Jānis Januševskis. Optimizētie eksperimentu plāni metamodelēšanai: Skaitliskais salīdzinājums**
Šajā darbā tiek apskatīta viendimensijas relaksācijas un koordinātu apmaiņas ar uzlabotu multistartu algoritmu efektivitāte. Tā tiek demonstrēta meklējot D-optimālos plānus ar nepārtrauktiem un 3 līmeņu diskrētiem parametriem 3 līdz 15 dimensijās ar 10 līdz 300 eksperimentu punktiem (45 līdz 4500 optimizācijas parametri) un veicot Latīņu hiperkubu plānu optimizāciju atbilstoši vairākiem kritērijiem. Optimizētie plāni tiek salīdzināti, risinot daudzus metamodelēšanas testa uzdevumus. Gadījumā ar otrās pakāpes lokālu polinomiālu aproksimāciju tiek piedāvāti vidējās kvadrātiskās kļūdas optimālie Latīņu hiperkubu plāni un Gausa modificētā svara funkcija. Optimizētie eksperimentu plāni ir publiski pieejami Internetā.

**Янис Аузиньш, Александр Янушевскис, Янис Янушевскис. Оптимизированные планы экспериментов для метамоделирования: Численное сравнение**
В работе исследуются алгоритмы одномерной релаксации и обмена координат с улучшенным мультистартом. Эффективность алгоритмов показана при поиске D-оптимальных планов для непрерывных и дискретных на 3 уровнях переменных начиная с 3 до 15 мерного пространства с числом экспериментов от 10 до 300 (число оптимизируемых параметров от 45 до 4500) и при оптимизации по нескольким критериям планов латинских гиперкубов. Оптимизированные планы сравниваются на многих тестовых примерах метамоделирования. Для случая локальной аппроксимации квадратичным полиномом предлагается использование СКО оптимальных планов латинских гиперкубов и модифицированной весовой функции Гаусса. Оптимизированные планы экспериментов опубликованы в интернете.