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COMPARISON OF SPACE-FILLING DESIGNS IN DISCRETE DOMAINS

E. Janouchová*, A. Kučerová*

Abstract: *In order to properly explore response of a model, one needs to perform simulations for a set of design points. When dealing complex non-linear models, the simulations are usually very time-consuming, hence the number of simulations performed within a limited time is rather low. Randomly chosen design points do not ensure the observed properties will be captured properly. Therefore, the design points must be chosen carefully. The motivation of the presented contribution is to investigate methods, which are suitable for generating designs in discrete parameter space, where each parameter can attain different number of levels, because commonly used software based on Latin Hypercube Sampling fails in solving such a situation. Hence, we compare here several well-known metrics for assessing optimal designs as for instance the Euclidean maximin distance, the maximum pairwise correlation or the D-optimal criterion. The resulting optimal designs are consequently employed for the evaluation of the stochastic sensitivity analysis so as to investigate their ability in prediction of the 'parameter-response' correlations.*

Keywords: ***Design of experiments, discrete domains, space-filling, orthogonality, stochastic sensitivity analysis.***

1. Introduction

The increasing complexity of numerical models makes the exploration of a model response an important area of investigation. To minimize the number of time-exhaustive simulations, reliable meta-models are usually constructed (Simpson et al., 2001). The meta-models represent the approximation/interpolation of a model response over the domain of model parameters called the design space. They are usually obtained by minimization of their error in a set of design points. The predictability of the resulting meta-model is in such setting driven by the choice of the design points being often called as the design of experiments.

The following section reviews several common metrics for assessing optimal designs and explores their properties when applied to discrete design spaces. Each metric defines a different optimal design. It is shown that the design optimal with respect to one metric does not reach the optimum for other metrics. After introducing the space-filling algorithms, in Section 3, we present their mutual comparison with emphasis on discrete domains. This is complemented with the optimal LHS algorithm due to Iman & Conover (1980), which is available in many engineering software packages. The ability of the optimal designs to capture the impact of model parameters to model responses is then critically assessed in Section 4. Finally, Section 5 gives conclusions and suggests directions for future work.

2. Metrics for assessing optimal designs

Let us recall several metrics commonly used for the determination of a suitable design of experiments.

Audze-Eglais objective function (AE) proposed by Audze & Eglais (1977) is based on a potential energy among design points. The points are distributed as uniformly as possible when the potential energy proportional to the inverse of the squared distance between points is minimized, i.e.

* Eliška Janouchová and Ing. Anna Kučerová, Ph.D.: Faculty of Civil Engineering, Czech Technical University in Prague, Thákurova 7/2077; 166 29, Prague; CZ, e-mails: eliska.janouchova@fsv.cvut.cz, anicka@cml.fsv.cvut.cz

$$\min AE = \min \sum_{i=1}^{n} \sum_{j=i+1}^{n} \frac{1}{L_{ij}^2}\,, \tag{1}$$

where n is the number of points and L_{ij} is the Euclidean distance between points i and j.

Euclidean maximin distance (EMM) is another metric preferring uniform designs. For a given design, the Euclidean maximin distance is defined as a minimal distance among all distances L_{ij}. A larger value is better, so we minimize the negative value of the minimal distance.

Pearson product-moment correlation coefficient (PMCC) can be used as a metric, which does not prefer uniformity, but leads to orthogonal designs. A correlation among design points can induce spurious correlation among coefficients of linear meta-models and can affect other meta-model-based estimates (Cioppa & Lucas, 2007). The simplest metric computes the absolute value of a correlation for each pair of variables. The goal is then to minimize the obtained maximal correlation.

Spearman's rank correlation coefficient (SRCC) is considered to be more general than PMCC, because the PMCC reveals only the linear dependence between two variables. Here, the correlation is not computed between coordinates of points, but these coordinates are ordered and the correlation is computed between the resulting ranks.

D-optimality (Dopt) is a metric formulated for maximization of entropy. The goal is to maximize the determinant of the information matrix **A**. Here we employ a Bayesian modification to the information matrix proposed by Hofwing & Strömberg (2010) in order to eliminate duplicates in the final D-optimal design. As we assume a minimization process, we minimize $\mathrm{Dopt} = -\det \mathbf{A}$.

When determining the optimal design of experiments, the criteria described above are supposed to be minimized by an optimization algorithm. Therefore, one aspect is the difficulty of its minimization. As the first study, we considered two-dimensional square domain with the fixed position of three points placed into the corners (top-right, bottom-right and bottom-left). Then, we were searching for an optimal position of the fourth point. Fig. 1 shows the value of particular metrics as a function of the fourth point position.

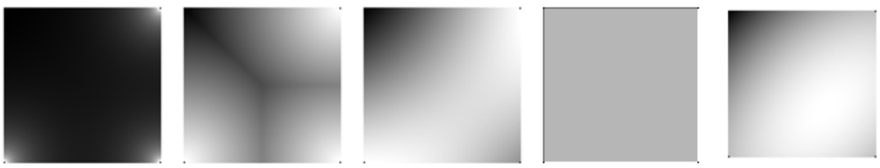

Fig. 1: Shape of different metrics for varying position of the 4th point. Black is the desired minimum, white is the maximum. From left: AE, EMM, PMCC, SRCC, Dopt.

Regarding the obtained shapes, we can conclude that the AE, EMM and SRCC metrics have one clear optimum in the fourth (top-left) corner. The value of the AE metric steeply decreases with increasing distance from the three occupied corners, but there is a large slowly decreasing valley towards the fourth corner. The EMM metric decreases more rapidly, but its shape is not smooth. The SRCC metric is constant over almost the whole domain except boundary, which can make the optimization unfeasible for gradient-based algorithms. Finally, the metrics PMCC and Dopt are smooth but have local extremes at occupied corners. Therefore, we conclude that the AE metric seems to be easiest for the minimization.

3. Tournaments of metrics

When generating large designs including a high number of points, the optimization of the described metrics becomes a complex task. Therefore, packages with the optimal Latin Hypercube Sampling method are often used for this purpose. LHS defines constraints to the designs which significantly reduce the design space and simplifies the following optimization. The main idea is to divide the interval of each variable to a number of levels equal the number of design points. Unfortunately, such an approach is not applicable for discrete variables as each may attain different number of values. Hence, we focus on the optimal designs not suffering the LHS restrictions.

To examine the quality of optimal designs with respect to different metrics, we have studied three different situations with 7, 10 and 13 design points to be placed into the two-dimensional square discrete domain with 10 levels in both dimensions. Since the designs are not excessively complex, a Simulated Annealing method with a sufficient number of iterations was applied to find the global optimum on each metric. While AE and Dopt metrics both define only one optimal design, other metrics lead to several designs with the same optimal value. Hence, the results in all following tables present the worst case scenario – the values correspond to the worst (optimal valued) design. In each row of Tabs. 1 – 3, one metric was optimized and the obtained optimal design was evaluated by other metrics. In Tab. 2, one row for optimal LHS is added, since only in such a scenario, the number of design points is equal to the number of levels in both dimensions. In particular, oLHS optimized with respect to SRCC were obtained by software SPERM 2.0 (Novák, www).

Tab. 1: Values and ranks (#) of metrics optimized for placing 7 points into the domain 10×10.

Metric	***AE***		***EMM***		***PMCC***		***SRCC***		***Dopt***		***Average #***
	value	***#***	***value***	***#***	***value***	***#***	***value***	***#***	***value***	***#***	
AE	*0.485*	*1*	*-4.00*	*2*	*0.018*	*2*	*0.000*	*1*	-2.10^{13}	*2*	***1.6***
EMM	*0.587*	*3*	*-4.47*	*1*	*0.271*	*4*	*0.198*	*3*	-5.10^{12}	*3*	***2.8***
PMCC	*4.609*	*4*	*-1.00*	*3*	*0.000*	*1*	*0.372*	*4*	-1.10^{7}	*4*	***3.2***
SRCC	*4.784*	*5*	*-1.00*	*3*	*0.474*	*5*	*0.000*	*1*	-1.10^{6}	*5*	***3.8***
Dopt	*0.514*	*2*	*-4.00*	*2*	*0.019*	*3*	*0.049*	*2*	-3.10^{13}	*1*	***2***

Tab. 2: Values and ranks (#) of metrics optimized for placing 10 points into the domain 10×10.

Metric	***AE***		***EMM***		***PMCC***		***SRCC***		***Dopt***		***Average #***
	value	***#***	***value***	***#***	***value***	***#***	***value***	***#***	***value***	***#***	
AE	*1.375*	*1*	*-3.00*	*2*	*0.015*	*3*	*0.020*	*3*	7.10^{15}	*6*	***3.0***
EMM	*1.801*	*3*	*-3.61*	*1*	*0.153*	*4*	*0.142*	*5*	-1.10^{27}	*2*	***3.0***
PMCC	*8.092*	*5*	*-1.00*	*5*	*0.000*	*1*	*0.227*	*6*	-1.10^{16}	*4*	***4.2***
SRCC	*9.408*	*6*	*-1.00*	*5*	*0.241*	*5*	*0.000*	*1*	-7.10^{15}	*5*	***4.4***
Dopt	*1.450*	*2*	*-2.83*	*3*	*0.015*	*3*	*0.026*	*4*	-7.10^{28}	*1*	***2.6***
oLHS	*3.555*	*4*	*-1.42*	*4*	*0.006*	*2*	*0.006*	*2*	-3.10^{20}	*3*	***3.0***

Tab. 3: Values and ranks (#) of metrics optimized for placing 13 points into the domain 10×10.

Metric	***AE***		***EMM***		***PMCC***		***SRCC***		***Dopt***		***Average #***
	value	***#***	***value***	***#***	***value***	***#***	***value***	***#***	***value***	***#***	
AE	*2.83*	*1*	*-3.00*	*1*	*0.015*	*2*	*0.017*	*2*	-1.10^{36}	*2*	***1.6***
EMM	*3.20*	*2*	*-3.00*	*1*	*0.153*	*3*	*0.186*	*5*	-6.10^{28}	*3*	***2.8***
PMCC	*16.04*	*5*	*-1.00*	*3*	*0.000*	*1*	*0.180*	*4*	-2.10^{21}	*5*	***3.6***
SRCC	*14.50*	*4*	*-1.00*	*3*	*0.241*	*4*	*0.000*	*1*	-2.10^{25}	*4*	***3.2***
Dopt	*3.42*	*3*	*-1.42*	*2*	*0.015*	*2*	*0.056*	*3*	-6.10^{42}	*1*	***2.2***

4. Prediction of correlation between model inputs and outputs: illustrative examples

Among the first steps of meta-model formulation is the determination of important model parameters with high impact on model response. This is usually done by stochastic sensitivity analysis.

Tab. 4: Prediction of input-output correlation for model z = x + y.

Design	***Full***	***AE***	***EMM***	***PMCC***	***SRCC***	***Dopt***	***oLHS***
corr (x, z)	*0.700*	*0.699*	*0.813*	*0.236*	*0.975*	*0.694*	*0.835*
corr (y, z)	*0.700*	*0.686*	*0.566*	*0.840*	*0.161*	*0.673*	*0.530*
Sum of errors		*0.016*	*0.247*	*0.604*	*0.814*	*0.033*	*0.305*
Rank (#)		***1***	***3***	***5***	***6***	***2***	***4***

Therefore, we studied the ability of optimal designs to predict the SRCC between each parameter and the model response. For the sake of clarity, we considered two simple models, linear and non-linear, both along with two discrete parameters x and y, each having 10 levels. The real parameter-response correlation can be obtained for a *full* design comprising all 100 samples. One design with 10 points was optimized for each metric and we evaluated the corresponding estimate of the parameter-response correlation. The results are summarized in Tabs. 4 and 5.

Tab. 5: Prediction of input-output correlation for model $z = x^2 + y^2$.

Design	***Full***	***AE***	***EMM***	***PMCC***	***SRCC***	***Dopt***	***oLHS***
corr (x, z)	*0.686*	*0.699*	*0.419*	*0.195*	*0.948*	*0.698*	*0.827*
corr (y, z)	*0.686*	*0.686*	*0.875*	*0.914*	*0.160*	*0.669*	*0.450*
Sum of errors		*0.013*	*0.456*	*0.719*	*0.788*	*0.029*	*0.377*
Rank (#)		***1***	***4***	***5***	***6***	***2***	***3***

5. Conclusions

The goal of this contribution was to compare different metrics determining design of experiments suitable for construction of a meta-model. In Section 2, it was shown that the AE metric is superior to other metrics from an optimization point of view. Section 3 then examines designs optimized for one metric with respect to other metrics. The results have shown that the AE metric defines nearly orthogonal designs with very good uniformity. Also the Dopt metric provide the nearly orthogonal designs with good uniformity, but their overall quality is a little bit worse than the quality of AE designs. Finally, Section 4 presents two examples of design-based estimation of the parameter-response correlation. Also here, the AE and Dopt metrics exceed the remaining ones. We should also point out that the commonly used oLHS generated by the SPERM software can produce an estimate with non-negligible error. Nevertheless, its widespread usage is driven by its uncontested ability to quickly generate reasonably good and very complex designs and especially designs for non-uniformly distributed parameters. Unfortunately, oLHS is useless in case of discrete domains with different number of parameter levels. Hence, we focus our future work on development of an optimization algorithm capable to minimize the AE metric even for more complex designs in discrete space.

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