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Improved Formulation Of Audze–Eglājs Criterion For Space-Filling Designs

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ABSTRACT: The Audze–Eglājs (AE) criterion was developed to achieve uniform distribution of experimental points in a hypercube. However, the paper shows that the AE criterion provides strongly nonuniform designs due to the effect of boundaries of the hypercube. We propose a simple remedy that lies in the assumption of periodic boundary conditions. The biased behavior of the original AE criterion and excellent performance of the modified criterion is demonstrated using simple numerical examples focused on (i) uniformity of the samples density over the design space and, (ii) statistical sampling efficiency measured through the ability to correctly estimate statistics of functions of random variables.

1. INTRODUCTION

This article, which is a promotion of a recent article by Eliáš and Vořechovský (2015), considers the choice of an experimental design for computer experiments. The choice of experimental points is an important issue in planning an efficient computer experiment. The methods used for formulating the plan/experimental points are collectively known as Design of Experiments (DoE). DoE is a crucial process in many engineering tasks. Its purpose is to provide a set of points lying inside a chosen *design domain* that are optimally distributed; the optimality of the experimental points depends on the nature of the problem. Various authors have suggested intuitive goals for good designs, including "good coverage", the ability to fit complex models, many levels for each factor, and good projection properties. At the same time, a number of different mathematical criteria have been put forth for comparing designs.

The selection of the sampling points is important when evaluating approximations to integrals as is performed in Monte Carlo simulations (numerical integration), where equal sampling probabilities inside the design domain are required. Such a design of experiments for Monte Carlo Sampling is typically performed in a hyper-cubical domain of N_{var} dimensions, where each dimension/variable, U_v, ranges between zero and one ($v = 1, \ldots, N_{\text{var}}$). In this paper, the *design domain* is a classical N_{var}-dimensional unit hypercube. This *design domain* is to be covered by N_{sim} points as evenly as possible.

The process of finding the experimental points can be understood as an optimization problem: we are searching for a design that minimizes an objective function, E. After an initial set of experimental points have been generated (typically via a pseudo-random generator), some modifications of them are performed in sequential steps to find the minimum of the objective function. The quality of the design is controlled by a chosen objective function (or design criterion).

Several criteria (objective functions) have been developed and used, e.g. the Audze-Eglājs (AE) criterion (Audze and Eglājs, 1977), the Euclidean MaxiMin and MinMax distance between points, Modified L2 discrepancy, Wrap-Around L_2-Discrepancy, Centered L_2-discrepancy, the $D-$optimality criterion, criteria based on correlation (orthogonality), Voronoi tessellation, the ϕ criterion, dynamic modeling of an expanding lattice, designs maximizing entropy, integrated mean-squared error, and many others. Some authors be-

lieve that in order to obtain a versatile (robust) design, several criteria should be used simultaneously.

Several authors have proposed a combination of uniformity criteria with Latin Hypercube Sampling (LHS) as a representative of variance reduction techniques (these designs are sometimes named optimal LHS). When optimizing an existing LH sample, the coordinates for each variable have already been selected, so the remaining task is to perform pairing (changing mutual orderings = shuffling) in order to minimize the DoE criterion. LHS is a type of stratified sampling technique; the coordinates of N_{sim} experimental points (simulations) are sampled from N_{sim} equidistant subintervals of length $1/N_{\text{sim}}$ so that every subinterval contains one and only one point. LHS guarantees the uniform distribution of experimental points along each dimension where it is used, typically along all N_{var} dimensions. The strongest LHS requirement samples only in an a priory chosen set of coordinates, most often the centers of the intervals (called LHS-median by Vořechovský and Novák (2009)) with coordinates $(i-0.5)/N_{\text{sim}}$ for $i \in \langle 1, 2, \ldots, N_{\text{sim}} \rangle$. Such a type of LHS will be used in this paper.

This paper is focused on the performance of the widely used Audze-Eglājs (AE) criterion and its improvement. It is shown that the original AE criterion provides designs that are not *uniform*. A simple explanation for this bias that arises from the presence of hypercube boundaries. Therefore, a remedy leading to uniform designs that involve the assumption of periodicity is introduced. The remedy does not increase computational complexity and is extremely easy to implement in source codes that already contain an evaluation of the original AE criterion. Three simple numerical examples are performed to show that (i) the sampling bias in the original AE criterion leads to errors in the estimation of moments of statistical models and (ii) the improved periodic criterion provides correct values with low variance.

2. Review of the original AE criterion

The AE criterion was developed by Audze and Eglājs (1977). The authors claimed that the criterion may be understood to express the potential energy of a system of particles with repulsive forces between each pair of them; minimization of this potential energy optimizes the spatial arrangement of the points. The repulsive forces between pairs of points are functions of their distance. The Euclidean distance, L_{ij}, between points (realizations) $u_i = (u_{i,1}, u_{i,2}, \ldots, u_{i,N_{\text{var}}})$ and u_j in N_{var}-dimensional space can be expressed as a function of their coordinates

$$L_{ij}^2 = L^2\left(u_i, u_j\right) = \sum_{v=1}^{N_{\text{var}}} \left(\Delta_{ij,v}\right)^2 \tag{1}$$

where $\Delta_{ij,v} = |u_{i,v} - u_{j,v}|$ is the distance between two points measured along (or projected onto) axis/dimension v (difference in variable U_v); $|X|$ stands for the absolute value of X. Each variable U_v ranges between zero and one, therefore $\Delta_{ij,v}$ has the same limits: $\Delta_{ij,v} \in \langle 0, 1 \rangle$. The Audze-Eglājs criterion is defined using the squared Euclidean distances between all pairs of experimental points as

$$E^{\text{AE}} = \sum_{i=1}^{N_{\text{sim}}} \sum_{j=i+1}^{N_{\text{sim}}} \frac{1}{L_{ij}^2} \tag{2}$$

3. Optimization of a sample using the AE criterion

One of the possible applications of the AE criterion is in the optimization of samples used in Monte Carlo numerical integration, e.g. statistical analyses of functions involving random variables. It is well recognized that simple random sampling of the Monte Carlo type does not perform well when it comes to uniformly spreading out the sample points with respect to the target density function. This is a pronounced issue especially for small sample sizes. An improvement in reducing the variance of estimated statistics can be achieved by LHS. The AE criterion can then be employed in combination with the LHS strategy, the concept for which appeared in (Bates et al., 2003).

In sampling analyses, the preparation of a sample is, in fact, the preparation of a sampling plan, i.e. a matrix of size $N_{\text{sim}} \times N_{\text{var}}$. Fig. 1 left shows a sampling plan for two variables and six simulations in the form of a table. When combining sampling strategies with given coordinates for each separate variable (as in the case of LHS), the only way

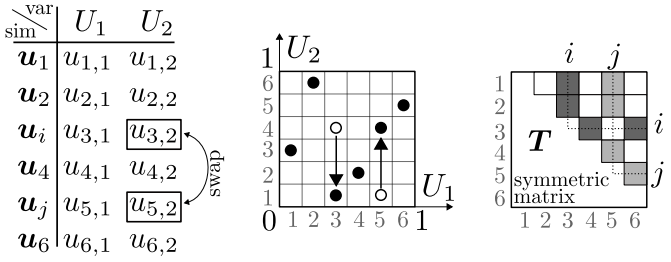

Figure 1: Swap (exchange) of coordinates i and j of variable U_2 in the sampling plan (left); in a bivariate scatterplot (middle); affected elements in a square symmetrical matrix of inverted squared pair distances between the points (right).

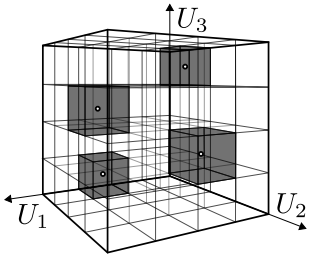

Figure 2: The considered design domain *– a unit hypercube ($N_{\text{var}} = 3$) divided into bins of equal volumes. Boxes with $N_{\text{sim}} = 4$ experimental points are highlighted.*

to optimize the sample with respect to a particular criterion (correlation, AE criterion) is to change the mutual ordering of these samples. In this paper, we focus on LHS, in which each variable (dimension) has N_{sim} fixed coordinates (e.g. centers of N_{sim} equidistant intervals). To minimize E^{AE}, one can search among all $(N_{\text{sim}}!)^{N_{\text{var}}-1}$ possible mutual orderings of these fixed coordinates. As shown by Bates et al. (2003), genetic algorithms can be effectively utilized. However, we use simulated annealing optimization (Vořechovský and Novák, 2009) to search for a good solution instead. It involves the subsequent swapping of the coordinates of a pair of points (see the exchange of coordinates in Fig. 1 middle). Details regarding this heuristic optimization algorithm can be found in (Vořechovský and Novák, 2009).

At this point, we should mention that the AE criterion can also be used when optimizing samples obtained by crude Monte Carlo Sampling (independent sampling on the $\langle 0, 1\rangle$ interval).

4. BIASED DESIGN

The *supposed uniformity* of the original AE design is critically evaluated in this section. The uniformity of point distribution can be measured as follows. The probability that the i-th experimental point will be located inside some chosen subset of the domain must be equal to V_S/V_D, with V_S being the subset volume and V_D the volume of the whole domain (for unconstrained design $V_D = 1$).

Since we are using LHS, the coordinates of the points are known and the whole unit hypercube of volume $V_D = 1^{N_{\text{var}}} = 1$ can be divided into ${N_{\text{sim}}}^{N_{\text{var}}}$ bins of the same volume using the grid of equidistant coordinates along each dimension, see Fig. 2. A uniform design is achieved if the probability of filling each of these bins is identical. In order to perform a numerical test of AE-optimized LHS designs, N_{run} designs (sampling plans of dimensions $N_{\text{var}} \times N_{\text{sim}}$) have been simulated and optimized. After generating the N_{run} designs, the total number of sampled points is $N_{\text{sim}}N_{\text{run}}$. The average number of points inside one bin should be for *uniform* design $f_a = N_{\text{sim}}N_{\text{run}}/{N_{\text{sim}}}^{N_{\text{var}}} = N_{\text{run}}/{N_{\text{sim}}}^{N_{\text{var}}-1}$. For each bin, we now count the actual frequency of occurrence of the points inside that bin, f. Finally, we define a variable $\bar{f}$ (a normalized frequency) that can be calculated for each bin using the ratio

$$\bar{f} = f\frac{1}{f_a} = f\frac{{N_{\text{sim}}}^{N_{\text{var}}-1}}{N_{\text{run}}} \tag{3}$$

An ideal design criterion should produce $\bar{f} = 1$ for every possible bin.

The results of the numerical study are shown in Fig. 3 for various numbers of samples N_{sim} and dimensions N_{var} in 2D images. The number of repetitive optimized designs used, $N_{\text{run}} = 10^7$, is high enough to reveal unwanted patterns. The gray color represents the $\bar{f}$ value at individual LHS points (bins). The first dimension (variable) is associated with the horizontal axis, the second variable with the vertical axis, and the third variable (if present) is captured by repetitive 2D images (slices) produced for different values of the third coordinate. Similarly, the fourth dimension (if present) is shown by repetitive views of 3D plots made for different values of the fourth coordinate.

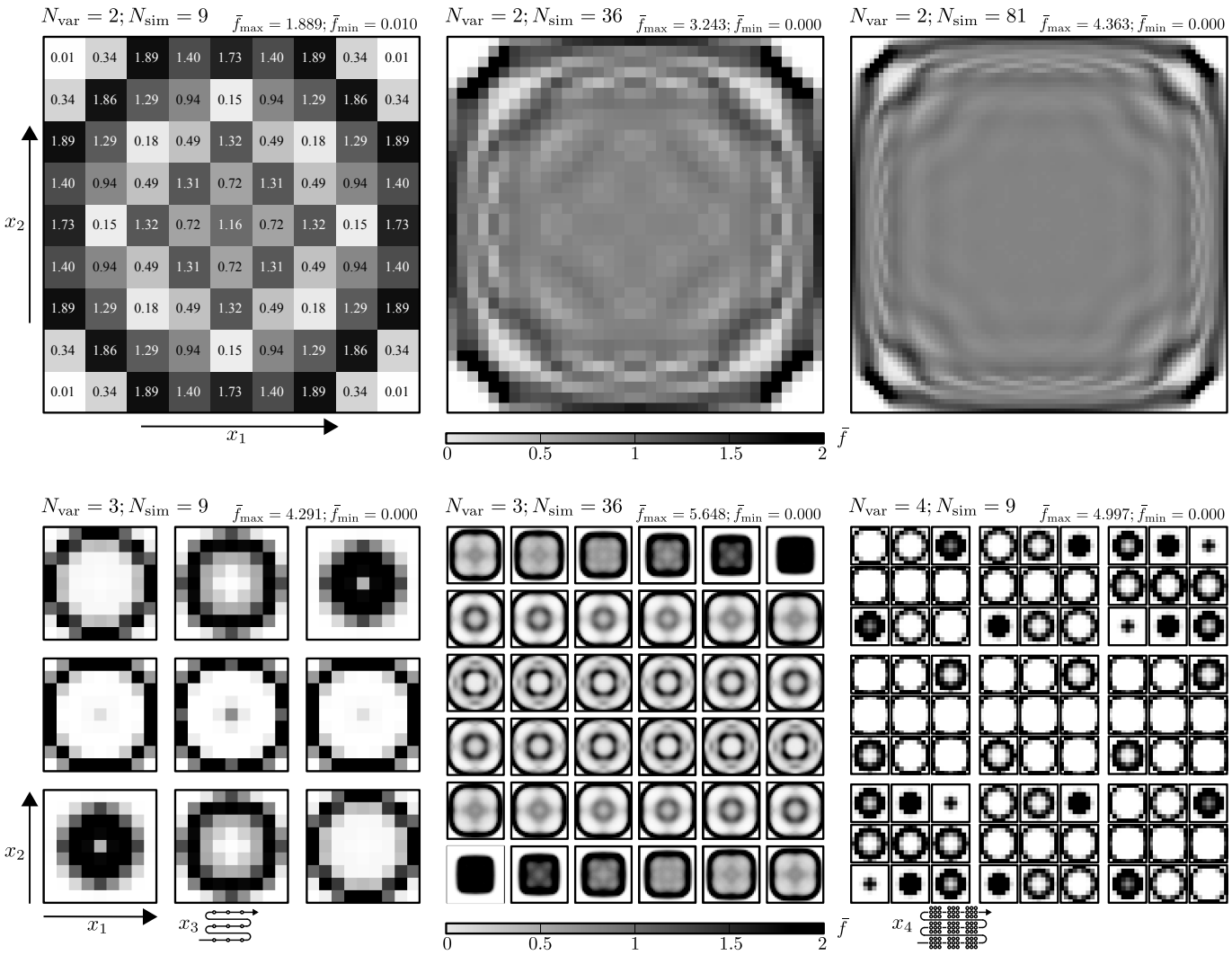

Figure 3: LHS designs using the original Audze–Eglājs (AE) criterion. Relative frequencies $\bar{f}$ calculated from $N_{\text{run}} = 10^7$ designs with various numbers of simulations N_{sim}. Top row: $N_{\text{var}} = 2$ variables. Bottom row: $N_{\text{var}} = 3$ and 4. The proposed PAE criterion leads to uniform gray color in all cases.

The figures clearly show the *non-uniformity* of point density in the design domain when the original AE criterion is used for optimization. In 2D space, the corners are not sampled at all, but there is an area of highly probable points close to them followed again by an improbable region. A similar behavior is observed in 3D and 4D spaces, where the corners of the domain are always sampled poorly. The plot for $N_{\text{var}} = 3$ shows a formation resembling a sphere with an empty interior (low N_{sim}) or with a less-accentuated second interior sphere (higher N_{sim}). For $N_{\text{var}} = 4$, a similar hypersphere forms. Generally, the tendency to avoid the corners of the hypercube is apparent. The more coordinates that reach its extremes (0 or 1) at the corner/edge, the more pronounced the effect, i.e. in 3D, corners are more "repellent" than edges. Appendix A of the paper by Eliáš and Vořechovský (2015) provides proof that the original AE criterion delivers a non-uniform distribution of points over the design space, and thus explains the source of the bias.

After the above demonstration of the undesired non-uniformity of the AE criterion, we continue with a description of a simple and computationally cheap remedy that provides *uniform* designs while keeping the concept of the AE criterion (the analogy between the point distribution and minimizing the energy of a system of particles) unchanged.

5. AE CRITERION IN PERIODIC SPACE

The remedy proposed by Eliáš and Vořechovský (2015), that leads to *uniform* designs, is based on periodic repetition of the unit hypercube (see Fig. 2) containing the experimental points, along all directions/variables of the design domain. In order to simplify the situation with a large number of (or even infinitely many) periodic images of each point, the authors shown in (Eliáš and Vořechovský, 2015) that it suffices to take only the nearest image of point. The proposed simplification lies in considering only the *shortest* distance, $\overline{L}_{ij}$, among all these pairs, see the very thick line in Fig. 4 for the case of $N_{\text{var}} = 2$. The squared *shortest* distance $\overline{L}_{ij}$ between

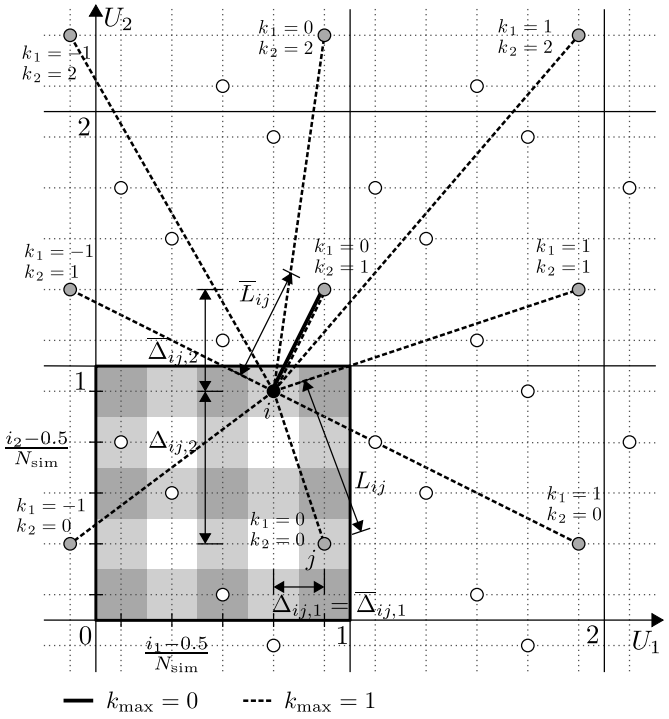

Figure 4: Periodic space, the shortest distance $\overline{L}_{ij}$ and all pairs in the first layer around point u_i.

two points i and all its periodic images is given by expression

$$\overline{L}_{ij}^2 = \sum_{v=1}^{N_{\text{var}}} \left[\min\left(\Delta_{ij,v}, 1-\Delta_{ij,v}\right)\right]^2 \qquad (4)$$

6. UNIFORMITY OF THE PROPOSED PERIODIC AUDZE-EGLĀJS CRITERION

Motivated by the observation described in the previous section, an improvement of the AE criterion is proposed. To distinguish between the original AE formulation (Audze and Eglājs, 1977) and the proposed one based on periodic space, we will call the new formulation the Periodic Audze-Eglājs (PAE) criterion. The proposed PAE criterion has the following form

$$E^{\text{PAE}} = \sum_{i=1}^{N_{\text{sim}}} \sum_{j=i+1}^{N_{\text{sim}}} \frac{1}{\overline{L}_{ij}^2}, \qquad (5)$$

By comparing Eq. (5) with the original formulation in Eq. (2) one can see that the only difference between them lies in selecting the minima between $(\Delta_{ij,v})$ and $(1-\Delta_{ij,v})$ along each coordinate $v \in \langle 1, N_{\text{var}} \rangle$ instead of using the coordinate difference $(\Delta_{ij,v})$ directly. Technically, this improvement is very easy to implement in computer programs and the additional computer time necessary to perform the comparison and selection of the minima is inconsiderable. Fig. 3 calculated with the proposed PAE criterion is just a uniformly gray rectangle clearly demonstrating that the new formulation provides truly *uniform* designs.

The source of uniformity actually lies in the *invariance of PAE with respect to translation*. If all the points in periodic space are shifted by an arbitrary vector, the PAE value remains unchanged. The invariance with respect to translation is simple to show (Eliáš and Vořechovský, 2015).

7. APPLICATION TO STATISTICAL ANALYSES OF FUNCTIONS OF RANDOM VARIABLES

As mentioned above, one of the frequent uses of DoE is in *statistical sampling* for Monte Carlo integration. We present the application of statistical sampling to the problem of estimating statistical moments of a function of random variables. In particular, a deterministic function, $Z = g(\boldsymbol{X})$, is considered, which can be a computational model or a physical experiment. Z is the uncertain response variable (or generally a vector of the outputs). The vector $\boldsymbol{X} \in \mathbb{R}^{N_{\text{var}}}$ is considered to be a random vector of N_{var} continuous marginals (input random variables describing uncertainties/randomness) with a given joint probability density function (PDF).

Estimation of the statistical moments of variable $Z = g(\boldsymbol{X})$ is, in fact, an estimation of integrals over

domains of random variables weighted by a given joint PDF of the input random vector $f_{\boldsymbol{X}}(\boldsymbol{x})$. We seek the statistical parameters of $Z = g(\boldsymbol{X})$ in the form of the following integral:

$$\mathrm{E}[S[g(\boldsymbol{X})]] = \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} S[g(\boldsymbol{x})] \, \mathrm{d}F_{\boldsymbol{X}}(\boldsymbol{x}) \qquad (6)$$

where $\mathrm{d}F_{\boldsymbol{X}}(\boldsymbol{x}) = f_{\boldsymbol{X}}(\boldsymbol{x}) \cdot \mathrm{d}x_1 \, \mathrm{d}x_2 \cdots \mathrm{d}x_{N_{\mathrm{var}}}$ is the infinitesimal probability ($F_{\boldsymbol{X}}$ denotes the joint cumulative density function) and where the particular form of the function $S[g(\cdot)]$ depends on the statistical parameter of interest. For example, to gain the mean value, $S[g(\cdot)] = g(\cdot)$. Computation of the variance involves additionally the second power $S[g(\cdot)] = g^2(\cdot)$.

In Monte Carlo sampling, which is the most prevalent statistical sampling technique, the above integrals are numerically estimated via calculation of averages of functions of random variables obtained using N_{sim} sampled points (realizations, a sample) that are selected with the same probability of occurrence $1/N_{\mathrm{sim}}$. Practically, this can be achieved by reproducing a *uniform distribution* in the design space (unit hypercube) that represents the space of sampling probabilities. We now limit ourselves to independent random variables in vector $\boldsymbol{X}$.

We now assume an estimate of integral in Eq. (6) by the following statistic (the average computed using N_{sim} realizations of $\boldsymbol{U}$, namely the sampling points $\boldsymbol{u}_j$ $(j = 1, \dots, N_{\mathrm{sim}})$)

$$\mathrm{E}[S[g(\boldsymbol{X})]] \approx \frac{1}{N_{\mathrm{sim}}} \sum_{i=1}^{N_{\mathrm{sim}}} S[g(\boldsymbol{x}_i)] \qquad (7)$$

where the sampling points $\boldsymbol{x}_i = \{x_{i,1}, \dots, x_{i,v}, \dots, x_{i,N_{\mathrm{var}}}\}$ are selected using the transformation $x_{i,v} = F_v^{-1}(u_{i,v})$, in which we assume that each of the N_{sim} sampling points $\boldsymbol{u}_i$ $(i = 1, \dots, N_{\mathrm{sim}})$ were selected with the same probability of $1/N_{\mathrm{sim}}$. Violation of the uniformity of the distribution of points $\boldsymbol{u}_i$ in the unit hypercube may lead to erroneous estimations of the integrals. We will show that the original definition of the AE criterion suffers from this problem.

7.1. Numerical examples

This section continues with two numerical examples presenting transformations of standard independent Gaussian random variables X_v, $v = 1, \dots, N_{\mathrm{var}}$. The non-uniformity of the original AE criterion and also the improved performance of the proposed PAE criterion will be demonstrated by showing the ability of the optimized samples to estimate the mean value and standard deviation (denoted as μ_Z, σ_Z) of the transformed variable $Z = g(\boldsymbol{X})$.

We consider two functions (transformations of input random variables):

$$Z_{\mathrm{sum}} = g_{\mathrm{sum}}(\boldsymbol{X}) = \sum_{v=1}^{N_{\mathrm{var}}} X_v^2 \qquad (8)$$

$$Z_{\mathrm{exp}} = g_{\mathrm{exp}}(X) = \sum_{v=1}^{N_{\mathrm{var}}} \exp\left(-X_v^2\right) \qquad (9)$$

where the input variables X_v, $v = 1, \dots, N_{\mathrm{var}}$ are independent standard Gaussian variables.

The first random variable Z_{sum} has a chi-squared distribution (also chi-square or χ^2-distribution) with N_{var} degrees of freedom. The standard deviation of this distribution is well known: $\sigma_{\mathrm{sum}} = \sqrt{2N_{\mathrm{var}}}$. The chi-squared distribution slowly converges to a Gaussian distribution as $N_{\mathrm{var}} \to \infty$.

The second random variable Z_{exp} has the exact statistical moments derived in (Eliáš and Vořechovský, 2015). The approximate standard deviation is $\sigma_{\mathrm{exp}} \approx 0.337\,461\sqrt{N_{\mathrm{var}}}$.

The quality of sampling is measured through the difference between the theoretical and estimated statistical parameters of Z. Since the placement of N_{sim} design points into an N_{var}-dimensional hypercube is random (it depends on sequences generated by a pseudo-random number generator), the estimated statistical parameter can also be viewed as a realization of a random variable. The simulated annealing algorithm by Vořechovský and Novák (2009) has been used for the optimization of the mutual ordering of LHS samples for three DoE criteria: AE, PAE and COR (Pearson's correlation coefficient). A relatively high number of $N_{\mathrm{run}} = 10^3$ designs were optimized for the same settings (criterion, N_{sim} and N_{var}) and the mean value and stan-

dard deviation of the estimated statistical parameters have been plotted in the form of graphs – dependencies on the sample size N_{sim}; see Fig. 5. The graphs show the exact solution for each selected statistical parameter via a dashed line. The average result of its estimation is plotted by a full line surrounded by a scatter-band representing the average $\pm$ one standard deviation. Such graphs give an idea about the convergence of the average estimation and also the variance of the estimation. Crude Monte Carlo results are not presented as the estimates exhibit a large variance. In LHS, the variability of the estimate is never higher than in crude Monte Carlo sampling because the selection of sampling probabilities is deterministic and the only variability arises from random mutual pairing.

The ability to estimate the mean value is purposely not presented. The reason is that samples optimized with all three criteria (COR, AE and PAE) provide exactly the same estimates of μ_{sum} and μ_{exp}. These estimates have no variability as the functions are additive and, in the LHS method, the averages are independent of the mutual ordering of samples.

The general trends are as follows:

- The AE criterion yields, on average, erroneous estimates (with almost no variability) for the studied statistical characteristics of the investigated three g functions. The error becomes pronounced for higher N_{var}. Increasing the sample size N_{sim} does not help. Both the incorrect means and the low variance of estimates are consequences of *non-uniform* sampling: some regions are under-represented (such as corners) and others are over-represented (as documented in Fig. 3 where the AE samples occur only in hyper-spheres inside the hypercube).

- The PAE criterion yields a uniform distribution of sample points and therefore the estimators converge to the exact values.

- The COR criterion yields a uniform distribution of sample points for $N_{\text{sim}} \to \infty$; however, for small N_{sim} the algorithm selects from a limited number of optimal arrangements (Vořechovský, 2012) that are not uniform.

- Estimates obtained with PAE are, on average, never worse than with COR – in most of the cases they are better. Also, the variance of the estimates obtained with PAE is never higher than that gained from COR. In other words, the estimates converge faster with smaller variance.

The best of the three methods seems to be the PAE criterion.

More numerical examples showing also the ability to estimate higher statistical moments are available in the paper by Eliáš and Vořechovský (2015).

8. Conclusions

It has been shown that the original Audze-Eglājs criterion used for optimization of the design of experiments provides a *non-uniform* experimental point distribution. Though this feature is not important in several applications of Design of Experiments, it is the crucial property in numerical Monte-Carlo type integration. Similarly, the correlation criterion of optimization (COR) also yields nonuniform coverage of the design domain; however, the problem disappears when sample size N_{sim} increases. Since the widely used AE criterion samples more frequently in some subregions of the design domain while leaving other areas underrepresented, numerical integration using the AE criterion provides incorrect results.

A simple remedy based on considering the periodicity of the design space was proposed, and it was demonstrated that the modified version – the Periodic Audze-Eglājs (PAE) criterion – provides a truly uniform distribution of points in the design domain. The PAE and AE criteria have the same computational complexity, so no additional effort is associated with considering the proposed scheme. The proposed PAE criterion is invariant with respect to shifts of the whole sample in any direction.

The numerical studies presented in this paper were performed with Latin Hypercube Samples (optimized using three criteria). However, the criticism of the AE criterion and the remedy using the proposed PAE criterion also holds for crude

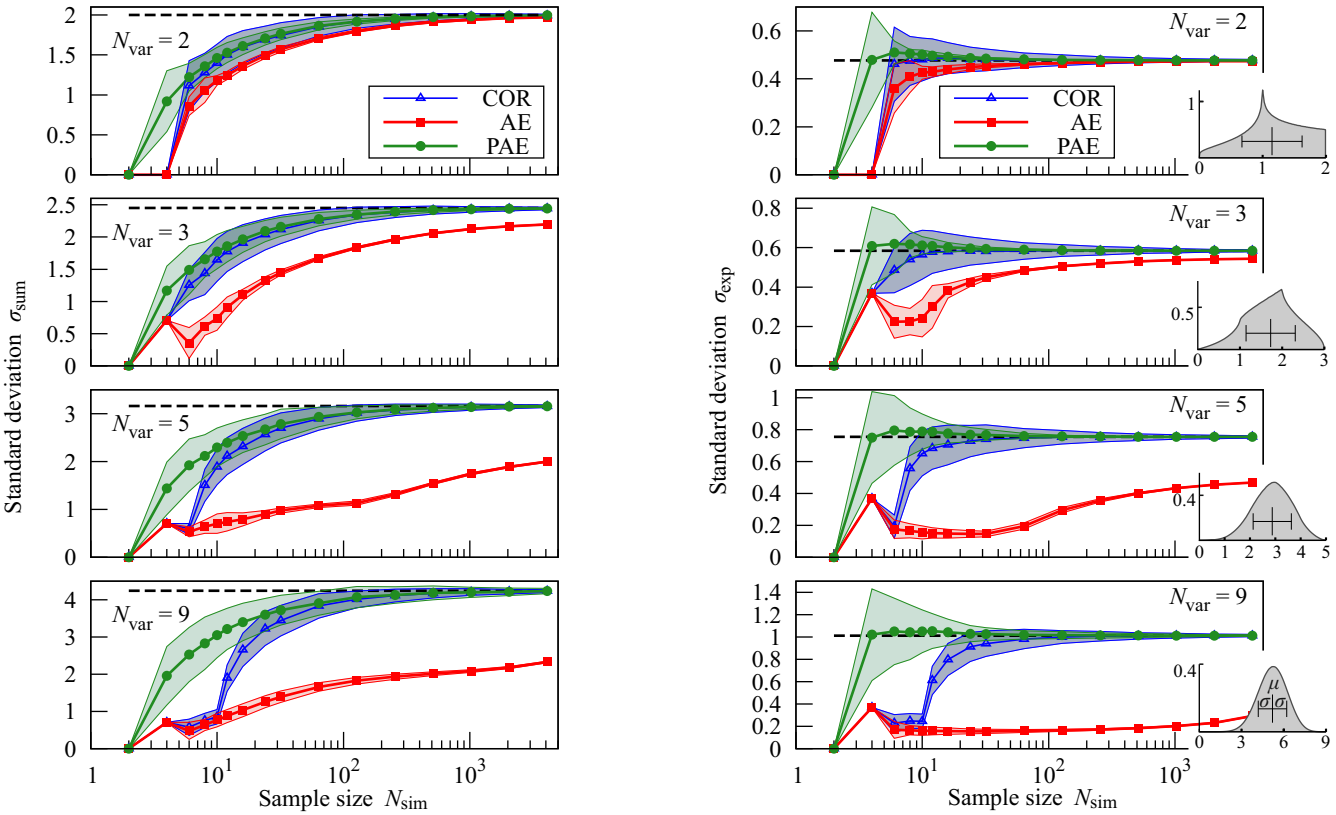

Figure 5: Convergence of estimated standard deviations σ_{sum} and σ_{exp} with increasing sample size N_{sim}. The insets visualize the PDF of Z_{exp}.

Monte Carlo Sampling (independent sampling on the $\langle 0, 1\rangle$ interval).

The proposed criterion is implemented in FReET software (Novák et al., 2014). It has also been implemented for the optimization of a sample in the sample size extension of an existing LH sample (a method proposed by Vořechovský (2015)).

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