Advances in Engineering Software 100 (2016) 82–96

Contents lists available at ScienceDirect

Advances in Engineering Software

journal homepage: www.elsevier.com/locate/advengsoft

Research Paper

Modification of the Audze–Eglājs criterion to achieve a uniform distribution of sampling points

Jan Eliáš*, Miroslav Vořechovský

Institute of Structural Mechanics, Faculty of Civil Engineering, Brno University of Technology, Czech Republic

ARTICLE INFO

Article history:
Received 2 December 2015
Revised 14 June 2016
Accepted 13 July 2016

Keywords:
Design of experiments
Periodic boundary conditions
Latin Hypercube sampling
Uniform distribution
Combinatorial optimization
Audze–Eglājs criterion
Audze-Eglais criterion

ABSTRACT

The Audze–Eglājs (AE) criterion was developed to achieve a 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 the 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 are demonstrated using simple numerical examples focused on (i) the uniformity of sampling density over the design space and, (ii) statistical sampling efficiency measured through the ability to correctly estimate the statistical parameters of functions of random variables. An engineering example of reliability calculation is presented, too.

1. Introduction

This article 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 of 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 N_{sim} points (a sample) 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.

There are two main application areas for DoE methods in the area of computer experiments. First, DoE is often used for evaluating the effects of different parameters of a function while searching for a response surface. The choice of location for the evaluation points or plan points is important in order to obtain a good approximation of the response surface. A surrogate model that approximates the original, complex, model, can be e.g. a response surface [32], a support vector regression or a neural network [25]. The surrogate model is based on a set of carefully selected points in the domain of variables. The process of finding optimal experimental points might be performed adaptively, i.e. in several sequential steps, where the location of the additional points in every step are based on result achieved so far [49].

Second, the selection of the sampling points is even more 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. These integrals may, for example, represent variables being estimated in uncertainty analyses. The evaluation of the uncertainty associated with analysis outcomes is now widely recognized as an important part of any modeling effort. A number of approaches to such evaluation are in use, including neural networks [6], variance decomposition procedures [27,42], and Monte Carlo (i.e. sampling-based) procedures [16,46].

In both applications mentioned above, it is convenient when the probability that the ith experimental point is located inside some chosen subset of the domain equals to V_S/V_D, with V_S being the subset volume and V_D the volume of the whole domain (for unconstrained design $V_D = 1$). Whenever this is valid, the design criterion will be called *uniform*. Even though such uniformity is conceptually simple and intuitive on a qualitative level, it is somewhat complicated to describe and characterize it mathematically. Although some problems do not require this uniformity, it is the crucial assumption in Monte-Carlo integration and its violation may (as will be demonstrated below) lead to significant errors.

* Corresponding author. Tel.: +420541147132.
E-mail address: elias.j@fce.vutbr.cz (J. Eliáš).

http://dx.doi.org/10.1016/j.advengsoft.2016.07.004
0965-9978/

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. Several optimization algorithms can be utilized; simulated annealing [57] will be employed in this paper. The chosen optimization algorithms may strongly affect the number of optimization steps and therefore the time to achieve the minimum, as well as the ability to find the global minimum among many extremes (local minima). However, the quality of the design is controlled by a chosen objective function (or design criterion).

Several criteria (objective functions) have been developed and used [21], e.g. the Audze-Eglājs (AE) criterion [1], the Euclidean MaxiMin and MiniMax distance between points [22], Modified L2 discrepancy [8], Wrap-Around L_2-Discrepancy [7], Centered L_2-discrepancy [9], the $D-$optimality criterion [50], criteria based on correlation (orthogonality) [54,55,57], Voronoi tessellation [45], the ϕ criterion introduced in [31], dynamic modeling of an expanding lattice, designs maximizing entropy [48], integrated mean-squared error [47], and many others. Some authors believe that in order to obtain a versatile (robust) design, several criteria should be used simultaneously [13].

It should be also noted that an experimental design can be also obtained via so-called "quasi-random" low-discrepancy sequences (deterministic versions of MC analysis) that can often achieve reasonably uniform point placement in hypercubes. One such example is the Niederreiter sequence [37]. Actually, fairly uniform point distributions can be produced by Halton [15] and Sobol' [51] sequences despite the flexibility of sample size selection: the points are added one-at-a-time to the design space. For resolving response probabilities, the Hammersley and modified-Halton methods were found in [44] using several test problems to perform only slightly better than Latin Hypercube Sampling. However, when the hyperspace dimension N_{var} becomes moderate to large and/or N_{sim} becomes high, usually these sequences suffer from spurious sample correlation [10,19]. These deterministic techniques are not further exploited in the paper.

Several authors have proposed a combination of uniformity criteria with Latin Hypercube Sampling (LHS) [5,20,30] as a representative of variance reduction techniques (these designs are sometimes named optimal LHS). Tang [53] has introduced orthogonal-array-based Latin hypercubes to improve projections on higher dimensional subspaces, the space-filling properties of which were *supposedly* improved in [26] by using the Audze-Eglājs criterion (without explicitly citing [1]). 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 frequently used version of LHS limits the selection of coordinates along each variable to fixed set of values, most often the centers of the intervals (called LHS-median in [57]) 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. When optimizing an existing LH sample, discrete domain consisting of interval centers is prescribed for each variable, so the remaining task is to perform pairing (changing mutual orderings = shuffling) in order to minimize the DoE criterion.

The design of experiments is typically performed in a hypercubical domain of N_{var} dimensions, where each dimension/variable, U_v, ranges between zero and one ($v = 1, \ldots, N_{\text{var}}$). Sometimes, additional constraints are required and the design of experiments is performed in a constrained domain and becomes more complicated [33,41]. 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.

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*. The appendix provides 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. Finally, a finite element model with a nonlinear constitutive law for concrete beam loaded in bending, featuring four random variables, shows the bias in calculation of probability of failure when the original AE criterion is used.

2. Review of the original AE criterion

The AE criterion was developed by Audze and Eglājs [1]. 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) $\boldsymbol{u}_i = \left(u_{i,1}, u_{i,2}, \ldots, u_{i,N_{\text{var}}}\right)$ and $\boldsymbol{u}_j$ in N_{var}-dimensional space can be expressed as a function of their coordinates

$$L_{ij} = L\left(\boldsymbol{u}_i, \boldsymbol{u}_j\right) = \sqrt{\sum_{v=1}^{N_{\text{var}}} \left(u_{i,v} - u_{j,v}\right)^2} = \sqrt{\sum_{v=1}^{N_{\text{var}}} \left(\Delta_{ij,v}\right)^2} \tag{1}$$

where

$$\Delta_{ij,v} = |u_{i,v} - u_{j,v}| \tag{2}$$

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

$$E^{\text{AE}} = \sum_{i=1}^{N_{\text{sim}}} \sum_{j=i+1}^{N_{\text{sim}}} \frac{1}{L_{ij}^2} \tag{3}$$

Several authors claim that the force interactions mimic gravitational forces. For example, Bates et al. [3] claim that "if the magnitude of the repulsive forces is inversely proportional to the distance squared between the points" then Eq. (3) represents potential energy. Similar statements are to be found in [11,18,58,59]. In [24], the authors, in contrast, claim that the AE criterion "is equal to the minimum of potential energy of repulsive forces for the points with unity mass if the magnitude of these repulsive forces is inversely proportional to the distance between the points". We disagree with both these explanations. If the criterion quantifies the potential energy of a system of particles, the repulsive force between pairs of particles must be equal to the negative derivative of the contact potential energy with respect to distance

$$F_{ij} = -\frac{\mathrm{d}\, E_{ij}^{\text{AE}}}{\mathrm{d}\, L_{ij}} = -\frac{\mathrm{d}\, \frac{1}{L_{ij}^2}}{\mathrm{d}\, L_{ij}} = \frac{2}{L_{ij}^3} \tag{4}$$