21st International Conference ENGINEERING MECHANICS 2015
Svratka, Czech Republic, May 11 –14, 2015
Paper #066, pp. 284–285

Evaluation of Audze-Eglājs Criterion for Orthogonal and Regular Triangular Grids

Magdalena Šmídová[a*], Václav Sadílek[b],
Jan Eliáš[c], Miroslav Vořechovský[d]

Institute of Structural Mechanics, Faculty of Civil Engineering, Brno University of Technology, Veveří 331/95, 602 00 Brno, Czech Republic

[a]smidova.m@fce.vutbr.cz, [b]sadilek.v@fce.vutbr.cz, [c]elias.j@fce.vutbr.cz,
[d]vorechovsky.m@fce.vutbr.cz

Keywords: Audze-Eglājs criterion, optimization, design of experiments, full factorial design (orthogonal grid), regular triangular design

Abstract: This article describes two deterministic designs that optimally fill a unit hypercube. The motivation is to estimate the lower bound of the Audze-Eglājs (AE) criterion – a criterion for optimization of designs of experiments or for a sample for statistical analyses when uniform filling of sampling space is required.
The construction of the two deterministic designs is described and the analysis of mutual distances of sample points in the designs (the distances are featured in the formula for the AE criterion) is performed. A closed form for evaluation of the AE criterion on these deterministic designs is developed.

Introduction

These days, physical experiments realized in research to get deeper insight into the examined issue are often replaced by computer experiments in order to decrease cost and time necessary for the modelling and realization of the experiment. The principle of the computer experimenting is the evaluation of a certain number of simulations (N_s) of the problem and estimation of an unknown quantity using statistical methods.

As an evaluation of a single simulation may be inadequately time-consuming in case of complex engineering problems, further approximation can be used to decrease the computational time, e.g. the response surface method as described in [1, 2]. Response surface is derived based on limited number of simulations of the real problem. Various requirements may be demanded from such a set of simulations. One of the usual requirements is uniform probability of the simulations evaluated.

To ensure uniform probability, the space of input random variables of the original problem is transformed into a sampling space where all the inputs are mutually independent and are represented by their probabilities. The sampling space is, therefore, a unit hypercube $[0, 1]^{N_v}$, where N_v is the number of input random variables of the original problem. This hypercube should then be filled uniformly with the points that represent individual simulations.

The problem of optimal filling of a space with respect to a predefined criteria is often solved by Monte Carlo type stochastic methods (crude Monte Carlo, Latin Hypercube Sampling) optimized by some heuristic algorithm (simulated annealing [3], genetic algorithms [4], etc.). The aim of optimization is to maximize or minimize the selected criterion, thereby the optimality with respect to this criterion is ensured.

For certain optimization algorithms the knowledge of the lower bound is crucial. As Audze-Eglājs (AE) criterion is said to prioritize uniform space-filling [5, 6] and its lower bound for arbitrary N_s is not known, the authors investigate deterministic designs that fill the unit hypercube uniformly, in order to estimate the lower bound of the criterion for stochastic designs.

AE Criterion

The AE criterion is based on the analogy with system of mass points interacting by repulsive forces. It is defined [5] using the distances between all pairs of points $L_{i,j}$ as

$$E^{\mathrm{AE}} = \sum_{i=1}^{N_{\mathrm{s}}} \sum_{j=i+1}^{N_{\mathrm{s}}} \frac{1}{L_{ij}^2} \,. \tag{1}$$

Investigated deterministic designs

In order to estimate the lower bound of AE, we test two different types of design (arrangement of points in N_{v}-dimensional unit hypercube). The two types of design are the full factorial design (FFD) and a new type of design called regular triangular design (RTD).

FFD. This design places $N_{\mathrm{s}} = N^{N_{\mathrm{v}}}$ points in an N_{v}-dimensional hypercube arranged in a perfect orthogonal grid (N is a natural integer here selected identical for all marginal variables). The computation of AE criterion may become very time-consuming for large N_{s}, therefore we present an analysis of distances between all pairs of points. This combinatorial analysis allows for fast evaluation of AE criterion using closed form expressions.

RTD. The other type of design – regular triangular grid – arranges the points into repeated units formed by triangles ($N_{\mathrm{v}} = 2$), tetrahedrons ($N_{\mathrm{v}} = 3$) etc. in N_{v}-dimensional space while fulfilling the requirement of periodicity. We present an algorithm for construction of such a design, limited to $N_{\mathrm{s}} = N^{N_{\mathrm{v}}}$ and the analysis of lengths among all pairs of points and AE criterion.

These two designs are compared with respect to the histograms of lengths between points and also their AE criteria. It is believed that these perfect arrangements lead to lower bounds of the AE criterion.

Acknowledgement: The authors acknowledge financial support provided by the Czech Ministry of Education, Youth and Sports under Specific University Research project No. FAST-J-13-1922, and also support provided by the Czech Science Foundation under projects Nos. GC13-19416J and GA14-10930S (SPADD).

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