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Review

Design of computer experiments: A review

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ABSTRACT

In this article, we present a detailed overview of the literature on the design of computer experiments. We classify the existing literature broadly into two categories, viz. static and adaptive design of experiments (DoE). We begin with the abundant literature available on static DoE, its chronological evolution, and its pros and cons. Our discussion naturally points to the challenges that are faced by the static techniques. The adaptive DoE techniques employ intelligent and iterative strategies to address these challenges by combining system knowledge with space-filling for sample placement. We critically analyze the adaptive DoE literature based on the key features of placement strategies. Our numerical and visual analyses of the static DoE techniques reveal the excellent performance of Sobol sampling (SOB3) for higher dimensions; and that of Hammersley (HAM) and Halton (HAL) sampling for lower dimensions. Finally, we provide several potential opportunities for the future modern DoE research.

Contents

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Abbreviations

Abbreviations

AES	adaptive exploratory sampling
AHS	adaptive hybrid sampling
AMPSO	adaptive memetic particle swarm optimization
ANN	artificial neural networks
BB	branch and bound
CAMM	continuous and multi-modal
CC	clustering constraint
CDM	crowding distance metric
CP	columnwise–pairwise
CV	cross validation
CVE	cross validation error
DF	departure function
DHASD	Delaunay hybrid adaptive sequential design
DoE	design of experiments
DT	Delaunay triangulation
EE	expected error
ESE	enhanced stochastic evolutionary
FLOLA	fuzzy local linear approximation
GLS	good lattice sampling
HAL	Halton sampling
HAM	Hammersley sampling
ILS	iterative local search
IMSE	integrated mean squared error
JK	Jackknifing
KL	Kullback–Leibler
LHD	Latin hypercube designs
LHS	Latin hypercube sampling
LOLA	local linear approximation
MCS	Monte Carlo sampling
MD	Mahalanobis distance
ME	maximum entropy
Mm	maximin distance
mM	minimax distance
MMSE	maximum mean squared error
MSD	maximin scaled distance
MSE	mean squared error
MSE	maximum sampling error
MST	minimum spanning tree
NLP	nonlinear programming
NN	nearest neighbor
OA	optimization algorithms
OAS	orthogonal array sampling
PerGA	permuted genetic algorithm
PE	potential energy
PSO	particle swarm optimization
QLHD	quasi-Latin hypercube Design
QMCS	quasi-Monte carlo sampling
QNS	quasi-Newton search
QRLD	quasi-random low discrepancy
RBF	radial basis functions
RCE	row column exchange
SA	simulated annealing
SFC	space-filling criteria
SMCS	stratified Monte Carlo sampling
SOB1	Sobol sampling in Matlab (based on Joe and Kuo, 2003)
SOB2	Sobol sampling in MoDS (based on Joe and Kuo, 2003)
SOB3	Sobol sampling in MoDS (based on Joe and Kuo, 2008)
SOBSA	sequencing optimization based on simulated annealing
SVM	support vector machines
TA	threshold accepting based global search
TP	translational propagation
UD	uniform designs
VT	Voronoi tessellation

Notation

Subscripts

n	index for elements of design/input variables' vector
s	index for elements of response/output variables' vector
R	radix or base

Superscripts

j	index for elements of set
k	index for elements of set
t	index for elements in set of sampling techniques
L	lower bound
U	upper bound

Parameters

m	moment of x
p	ordering parameter in ϕ_p
B	number of bins in orthogonal array
K	total number of sample points in a sample set
N	total number of input domain dimensions
S	total number of output domain dimensions
T	strength of orthogonal array
λ	orthogonal array index

Continuous variables

x	vector of input/design variables
y	vector of output/response variables

Symbols

d	Euclidean distance
DT	Delaunay triangulation
$\tilde{f}$	surrogate model form
H	entropy
$\boldsymbol{L}$	$K \times N$ matrix
$\mathbb{1}_{[0,1]^N}$	indicator function
$\mathcal{D}$	real bounded domain
$\mathbb{E}$	expectation
$\mathbb{N}$	set of natural numbers