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COMPUTATIONAL EXPERIMENT OF ITERATED LOCAL SEARCH FOR HIGHER DIMENSIONS ((k, N) = (4, 9)) FOR OPTIMIZING LATIN HYPERCUBE DESIGNS

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ABSTRACT

A k-dimensional Latin hypercube design (LHD) of n points, is a set of n points where $x_i = (x_{ij}, x_{i2}, \ldots, x_{ik}) \in \{0, \ldots, N-1\}^k$ such that for each factor j all x_{ij} are distinct. we assume that our design space is equal to the $[0, N-1]^k$ hypercube. However by scaling, we can use LHDs for any rectangular design space. One definition of LHD is to divide each axis into n equally sized bins and randomly select points such that each bin contains exactly one point. However, we refer to this technique as Latin hypercube sampling (LHS).We have compared the performance of ILS approach with other approaches regarding various characteristics of the optimal designs by considering a typical design namely (k, N) = (4, 9). The comparison study reveals that ILS approach is one of the best approaches for finding maximin LHDs.

KEYWORDS: Latin hypercube design (LHD), Iterated Local search, Optimal criteria.

1. INTRODUCTION

Computer simulation experiments [e.g., Santner et al (2003); Fang et al (2006)] have now become a popular substitute for real experiments when the physical experiment are infeasible or too costly. In these experiments, a deterministic computer code, the simulator, replaces the real (stochastic) data generating process. This practice has generated a wealth of statistical questions, such as how well the simulator is able to mimic reality or which estimators are most suitable to adequately represent a system. However, the foremost issue presents itself even before the experiment is started, namely how to determine the inputs for which the simulator is run? It has become standard practice to select these inputs such as to cover the available space as uniformly as possible, thus generating so called space-filling experimental designs. Naturally, in dimensions greater than one, there are alternative ways to produce such designs.

For the design of computer experiments Latin Hypercube Designs (LHDs), first introduced in [McKay et al. (1979)], fulfill the non-collapsing property. LHDs are important in the design of computer-simulated experiments (e.g., [Fang et al. (2006)]). Here LHD is defined a bit different than [McKay et al. (1979)] but similar to [Johnson et al. (1990); Husslage et al. (2006); Morris and Mitchell (1995); Grosso et al. (2008)]. Assume that we have to place N design points and that there are k distinct parameters. We would like to place the points so that they are uniformly spread when projected along each single parameter axis. We will assume that each parameter range is normalized to the interval [0, N-1]; Then, a LHD is made up by N points, each of which has k integer coordinates with values in 0,1, . . . , N-1 and such that there do not exist two points with one common coordinate value. This allows a non-collapsing design because points are evenly spread when projected along a single parameter axis.

A k-dimensional Latin hypercube design (LHD) of n points, is a set of n points where $x_i = (x_{ij}, x_{i2}, \ldots, x_{ik}) \in \{0, \ldots, N-1\}^k$ such that for each factor j all x_{ij} are distinct. In this definition, we assume that our design space is equal to the $[0, N-1]^k$ hypercube. However by scaling, we can use LHDs for any rectangular design space. Alternative definitions of LHDs also occur in the literature. One alternative definition is to divide each axis into n equally sized bins and randomly select points such that each bin contains exactly one point. However, we refer to this technique as Latin hypercube sampling (LHS). In this paper the term 'LHD' thus only refers to the first definition.

A configuration

$$\mathbf{X} = \begin{pmatrix} x_1 \\ \vdots \\ x_N \end{pmatrix} = \begin{pmatrix} x_{11} & \cdots & x_{1k} \\ \vdots & \cdots & \vdots \\ x_{N1} & \cdots & x_{Nk} \end{pmatrix}$$

with all $x_{ij} = \{0, 1, \cdots N-1\}$ is a LHD if each column has no duplicate entries. This one-dimensional projective property ensures that there is little redundancy of design points when some of the factors have a relatively negligible effect (sparsity principle).

Unfortunately, randomly generated LHDs almost always show poor space-filling properties or / and the factors are highly correlated. On the other hand, maximin distance objective based designs proposed by [Johnson et al. (1990)], have very good space-filling properties but often no good projection properties under the Euclidean (L^2), or the Rectangular (L^1), distance. To overcome this shortcoming, Morris and Mitchell [Morris and Mitchell (1995)] suggested for searching **maximin LHDs** which have both the important properties when looking for "optimal" designs. An LHD is called maximin when the separation distance $\min_{j \neq i} d(x_i, x_j)$ is maximal among all LHDs of given size n, where d is a certain distance measure. In this paper, we concentrate on the Euclidean (L^2) distance measure, i.e.,

$$d(x_i, x_j) = \sqrt{\sum_{l=1}^{k} (x_{il} - x_{jl})^2}$$

2. **Maximin Latin Hypercube Designs**

We will denote as follows the p-norm distance between two points x_i and x_j, $\forall\ i, j = 1, 2, \cdots, N$:

$$d_{ij} = \| x_i - x_j \|_p,$$

Unless otherwise mentioned, we will only consider the Euclidean distance measure ($p = 2$) and Manhattan distance (p = 1). In fact, we will usually consider the squared value of d_{ij} (in brief d), i.e. d^2 (saving the computation of the square root) in case of Euclidean distance. This has a noticeable effect on the execution speed since the distances d^2 will be evaluated many times.

3. COMPUTATIONAL EXPERIMENT OF ITERATED LOCAL SEARCH FOR HIGHER DIMENSIONS ((k, N) = (4, 9)):

Symbols	Meaning	Symbols	Meaning
ρ	Average correlation	D1(J1)(L1)	$D_1(J_1)$ value in L^1
ρmax	Maximum correlation	D1(J1)(L2)	$D_1(J_1)$ value in L^2
D1	Minimum pair-wise distance in a LHD	Φ_p(L1)	Φ_p value in L^1
(J_1)	Number of time D_1 occur in a LHD	Φ_p(L2)	Φ_p value in L^2
(L1)	Manhattan distance measure (L^1)	A-E((L1)	A-E value in in L^1
(L2)	Euclidean distance measure (L^2)	A-E(L2)	A-E value in in L^2
Φp	Φ_p optimal criterion	ω_1 and ω_2	(Weight average) constant
A-E	Audze-Eglais optimal criterion		

It is observed in the Table that each optimal LHD is best according to the corresponding optimal criteria. Anyway it is observe that the ρ of MLH-SA and **MLH-**

ILS are comparable in which both LHDs are optimized by same Φ_p criterion. Though ρ value **MLH- ILS** is worse compare to other LHDs but the multi-co-linearity of the LHD is negligible as ρ = 0. 5 .

It is also observed in the Table that though MLH-**SA** is best in $D_1(J_1)^{(1)}$ value (as it is optimized regarding L^1 measure) but the $D_1(J_1)^{(1)}$ value of **MLH- ILS** is comparable with that of MLH-**SA** and almost identical with other LHDs. Moreover the $\Phi_p^{(L1)}$ value of **MLH-ILS** is almost identical with that of MLH-**SA** and relatively better than other optimal LHDs. Again it is notice that A-$E^{((L1)}$ and A-$E^{((L2)}$ values of **MLH- ILS** are also comparable with the best one that is with the A-$E^{((L1)}$ and A-$E^{((L2)}$ values of MLH-ESE which is optimized by A-$E^{((L2)}$ optimal criterion. We observe that the $\Phi_p^{(L2)}$ value of **MLH- ILS** is better than that of other optimal LHDs as **MLH- ILS** is optimized by

$\Phi_p^{(L2)}$ optimal criteria along with tracking D_1 value. Now it is remarkable that the $D_1(J_1)^{(L2)}$ value of **MLH- ILS** is significantly better and ultimately the best among the other optimal LHDs according to $D_1(J_1)^{(L2)}$ value. It may conclude that tracking D_1 along with

$\Phi_p^{(L2)}$ optimal criteria ILS approach outperform compare to other approaches. Moreover **MLH-ILS** is good enough according to other experimental properties.

Comparison of MLH-SA, OMLH – MSA, OLH- Y, MLH-ESE and MLH-ILS for (N,k)=(9, 4) :

Method →	MLH-SA	OMLH – SA_M	OLH- Y	MLH-ESE	**MLH- ILS**
Optimal Criteria →	Φ_p	$\omega_1 \Phi_p + \omega_2 \rho^2$	$\rho = 0$	A-E	Φ_p, D_1
Distance measure →	L^1	L^1	L^1	L^2	L^2
Optimal LHD Design Matrix →	1 3 3 2 5 8 3 8 6 4 7 1 5 2 9 6 9 5 7 1 4 8 4 2 9 6 7	4 1 5 3 3 8 2 2 5 8 2 3 9 7 5 6 4 3 8 1 3 5 7 1 7 9 6 6 9 9 7 7 1 2 4 1 8 8 4 2 5 9 4 6 6	1 2 6 3 2 9 7 6 3 4 2 9 4 7 1 2 5 5 5 5 6 3 9 8 7 6 8 1 8 1 3 4 9 8 4 7	1 5 8 5 2 1 4 6 3 6 1 3 4 8 5 9 5 9 7 2 6 2 6 1 7 3 2 8 8 4 9 7 9 7 3 4	1 5 8 4 2 7 4 9 3 2 1 6 4 8 3 3 5 1 5 1 6 3 7 8 7 6 9 2 8 9 6 7 9 4 2 5
PROPERTIES ↓					
ρ →	0.108	0.063	**0.000**	0.083333	0.151
ρ_{max} →	0.217	0.117	**0.000**	0.052264	0.233
$D_1(J_1)^{(L1)}$ →	**11(3)**	11(4)	10(8)	10 (4)	10(4)
$\Phi_p^{(L1)}$ →	**0.105**	**0.105**	0.115	0.116	0.108
$D_1(J_1)^{(L2)}$ →	33(2)	31(1)	30(8)	34 (1)	**42(6)**
$\Phi_p^{(L2)}$ →	0.031	0.033	0.037	0.036	**0.026**
A-E$^{((L2)}$ →	0.668	0.669	0.7	**0.660**	0.667
A-E$^{(L1)}$ →	2.772	**2.764**	2.8102	2.785	2.791

CONCLUSION

Regarding correlation criterion and some other criteria we have performed another experiment in the Chapter V. For this experiment we have considered several optimal LHDS with $(N,k)=(9, 4)$. We again observe in this experiment that maximin LHD obtained by ILS approach is significantly better than all other optimal LHDs regarding D_1 value. Though according to the ρ (correlation coefficient) value maximin LHD obtained by ILS approach is worse compare to OMLH – SA_M and OLH- Y in which DoE are optimized by ρ^2 optimal criterion, the value of ρ in maximin LHD are enough small.

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