

**OPTIMALITY ANALYSIS OF MAXIMIN LHDs OBTAINING BY
ITERATED LOCAL SEARCH HEURISTICS APPROACH
REGARDING AUDZE-EGLAIs CRITERION.**

By

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Declaration

This is to certify that the thesis work entitled “*Optimality Analysis of Maximin LHDs Obtaining by Iterated Local Search Heuristics Approach Regarding Audze-Eglais Criterion*” has been carried out by *Debasish Bokshi* in the Department of Mathematics, Khulna University of Engineering & Technology, Khulna, Bangladesh. The above thesis work or any part of thesis work has not been submitted anywhere for the award of any degree or diploma.

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Dedication

To
my mother **Charubala Bokshi**
&
my wife **Athoy Bokshi**
who always helped and inspired me to complete this degree.

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Abstract

The design of experiments (DoEs) have much recent interest and this is likely to grow as more and more simulation models are used to carry out research. A good experimental design should have at least two important properties namely projective property (non-collapsing) and Space-filling (design points should be evenly spread over the entire design space) property. Any Latin Hyper-cube design (LHD) is inherently preserve projective property. But randomly generated LHDs have poor space-filling property. In consequence, in sense of space-filling, Optimal LHDs are required for good DoEs. Several optimal LHDs are available in the literature; Maximin LHD is one of the most frequently used among such optimal LHDs. It is also noted that researchers implement different type of methods to find out maximin LHDs. But the performances of the approaches are not same. In this study, we consider maximin LHDs obtained by Iterated Local search (ILS) heuristic approach in which inter-site distances are measured in Euclidean distance measure. We have compared the performance and effectiveness of ILS approach with some well-known approaches available in the literature regarding maximin LHDs in Euclidean distance measure. The experimental study agrees that ILS approach outperforms regarding maximin LHDs measured in Euclidean distance measure. We perform further extensive experiments in perspective of Audze-Eglais values. We compare Audze-Eglais values of maximin LHDs, which are optimized regarding ϕ_p optimal criterion and obtained by ILS approach, with Audze-Eglais value of Audze-Eglais LHDs, which are optimized regarding Audze-Eglais optimal criterion and obtained by Enhanced Stochastic Evolutionary (ESE) algorithm. In the experimental results show that the Audze-Eglais value of Maximin LHDs are comparable. We have also 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.

Publication

The following paper has been extracted from this thesis work:

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CHAPTER I

INTRODUCTION

1.1 Background

Design of experiments (DOE) or experimental design is the design of any information-gathering exercises where variation is present, whether under the full control of the experimenter or not. However, in statistics, these terms are usually used for controlled experiments. Formal planned experimentation is often used in evaluating physical objects, chemical formulations, structures, components, and materials. Other types of study, and their design, are discussed in the articles on computer experiments, opinion polls and statistical surveys (which are types of observational study), natural experiments and quasi-experiments (for example, quasi-experimental design).

In the design of experiments, the experimenter is often interested in the effect of some process or intervention (the "treatment") on some objects (the "experimental units"), which may be people, parts of people, groups of people, plants, animals, etc. Design of experiments is thus a discipline that has very broad application across all the natural and social sciences and engineering.

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..

The design of computer experiments has much recent interest and this is likely to grow as more and more simulation models are used to carry out research. Computer simulation experiments are used in a wide range of application to learn about the effect of input variables x on a response of interest y [Butler (2001)]. In computer experiments, instead of physically doing an experiment on the product, mathematical models describing the performance of the product are developed using engineering/physics laws and solved on computers through numerical methods. As simulation programs are usually deterministic so the output of a computer experiment is not subject to random variations, which makes the design of computer experiments different from that of physical experiments [(Fang et al. (2006)]. Many simulation models involve several hundred factors or even more. It is desirable to avoid replicates when projecting the design on to a subset of factors. This is because a few, out of the numerous factors in the system, usually dominate the performance of the product. Thus a good model can be fitted using only these few important factors. Therefore, when we project the design on to these factors, replication is not required.

As is recognized by several authors, the choice of the design points for computer experiments should at least fulfill two requirements (for details see [Johnson et al. (1990); Morris and Mitchell (1995)]). First of all, the design should be space- filling in some sense. When no details on the functional behavior of the response parameters are available, it is important to be able to obtain information from the entire design space. Therefore, design points should be evenly spread over the entire region. Secondly, the design should be non-collapsing. When one of the design parameters has (almost) no influence on the function value, two design points that differ only in this parameter will collapse, i.e., they can be considered as the same point that is evaluated twice. For deterministic functions this is not a desirable situation. Therefore, two design points should not share any coordinate value when it is not known a priori which parameters are important.

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 $0, 1, \dots, N-1$ 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 $x_i = (x_{i1}, x_{i2}, \dots, x_{ik}) \in \{0, \dots, N-1\}^k$ 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 $x_{ij} \in \{0, 1, \dots, N-1\}$ 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.,

$$d(x_i, x_j) = \sqrt{\sum_{l=1}^k (x_{il} - x_{jl})^2} \quad (1.1)$$

since this measure is often the first choice in practice. The definition of optimal LHDs through the maximin criterion has been proposed in [Johnson et al. (1990)] : given a point-to-point distance metric $d(x_i, x_j); i, j \in I$ (I is the index set) ; then the maximin LHD problem is to find a LHD such that the minimum point-to-point distance occurring in such configuration is maximized (as large as possible). In the literature the optimal criterion for maximin LHD are defined in several ways [Grosso et al. (2009)] but the main objective is identical i.e. searching the LHD with the maximizing the minimum pair-wise distance. Also different definitions for the distance $d(x_i, x_j)$ are considered in literature; in this work d is to be the Euclidean distance, which is one of the most frequently used distance-measure in the applications.

For the presents of combinatorial nature, the number of possible LHDs is very high - $(N!)^k$. For example, to optimize the location of 20 samples in two dimensions, the algorithm has to select the best design from more than 10^{36} $(20!)^2$ possible designs. If the number of variables is increased to 3, the number of possible designs is more than 10^{55} . Consequently, when number of factors and/ or number of design points are large then it requires hundreds of hours by the *brute-force* approach to find out the optimal design. So researchers choose heuristic approaches to find out optimal designs. Here, we choose Iterated Local search (ILS) heuristic approaches to find the optimal (maximin) LHD [Grosso et al. (2009)]. For the optimal criterion they considered the following maximin optimal criteria in Euclidean distance measure which is similar to [Johnson et al. (1990)] but a quite different regarding computational effort:

$$\Phi_p(X) = \sum_{i=1}^N \sum_{j=i+1}^N \left[\frac{1}{d_{ij}^p} \right]^{\frac{1}{p}} \quad (1.2)$$

where $d_{ij} = d(x_i, x_j)$ be the Euclidian distance between points x_i and x_j and p is a positive integer parameter and which can be computed without the need of detecting and ordering all D_i (pair-wise inter side distance) values which is required in [Johnson et al. (1990)]. They denotes this optimal criterion as $\text{Opt}(\varphi)$. Under this criterion, LHD Y is better than X if

$$\Phi_p(Y) < \Phi_p(X) \quad (1.3)$$

Note that in [Johnson et al. (1990)] the definition of maximin optimal criterion is as follows :

$$\Phi_p(X) = \sum_{r=1}^R \left[\frac{J_r(X)}{D_r(X)^p} \right]^{\frac{1}{p}}, \quad (1.4)$$

where $D_1(X) < D_2(X), \dots, D_R(X)$ (pair-wise inter side distances), R is the number of different distances in X . Also note that authors in [Grosso et al. (2008); Grosso et al. (2009)] considered another maximin optimal criterion denoted as $\text{Opt}(D1)$, which is also considered in [Johnson et al. (1990)], is given below.

max $D_1(X)$ such that

$$D_1 = D_1(X) = \min d(x_i, x_j) \quad i \neq j; X \in LHD \quad (1.5)$$

with min $J = |(i, j)| : d(x_i, x_j) = D_1(X)$

Under this criteria, LHD Y is better than X if

$$\begin{aligned} D_1(Y) > D_1(X) & \quad \text{or} \\ D_1(Y) > D_1(X) \text{ and } J_1(Y) < J_1(X) & \quad (1.6) \end{aligned}$$

and so on.

There is also a set of maximin-distance designs (when there exist several), a maximin-optimal design ξ^*_{Mm} is such that the number of pairs of points (x_i, x_j) at the distance $d_{ij} =$

$\phi_p(\xi^*_{mM})$ is minimum (several such designs can exist, and measures can be taken to remove draws, Morris and Mitchell (1995), but this is not important for our purpose). Consider now designs ξ that attempt to make the maximum distance from all the points in X to their closest point in ξ as small as possible. This is achieved by minimizing the minimax-distance criterion $\phi_{mM}(\xi) = \max \text{Min} \|x_i - x_j\|$. We call a design that minimizes $\phi_{mM}(\xi)$ a minimax distance design, Johnson et al (1990). These designs can be motivated by a table allocation problem in a restaurant, such that a waiter is as close as possible to a table wherever he is in the restaurant. In other terms, one wishes to cover X with n balls of minimum radius. Among the set of minimax-distance designs (in case several exist), a minimax-optimal design ξ^*_{mM} maximizes the minimum number of x_i 's such that $\min_i \|x_i - x_j\| = \phi_{mM}(\xi^*_{mM})$ over all points x having this property.

Besides maximin LHDs, and minimax LHDs we also treat Audze-Eglais LHDs. Audze-Eglais designs are obtained by minimizing the following objective:

$$\sum_{i=1}^n \sum_{j=i+1}^n \frac{1}{d(x_i, x_j)^2} \quad (1.7)$$

here $d(x_i, x_j)$ is again the Euclidean distance between points x_i and x_j . By minimizing this objective, we can also obtain LHDs with “evenly spread” points (Bates et al. 2004). The problem of finding Audze Eglais LHD is formulated and a permutation genetic algorithm is used to generate them by [Liefvendahl and Stocki (2006)]. They compared maximin and Audze Eglais LHDs and recommend on Audze Eglais criterion over the maximin criterion.

For all the classes of LHDs, our aim is to construct a database of the best designs known in literature. We do this by generating new designs and comparing them with existing results. These designs are often approximate maximin or Audze-Eglais designs in the sense that optimality of the objective is not guaranteed. The reason for this is that optimization over the total set of LHDs can be very time-consuming for larger values of k and N . Therefore, in order to find good designs, optimization is often done over a certain class of LHDs or heuristics are used which do not guarantee optimality. The periodic LHDs [Hussluge et al. (2006)] are a good example of the first case. Examples of the second case are simulated annealing used by Morris and Mitchell (1995), the permutation

genetic algorithm of Bates et al. (2004) and the Enhanced Stochastic Evolutionary (ESE) algorithm of Jin et al. (2005).

1.2 Literature Review

1.2.1 Experimental Designs

Since physical experiments are inevitably very expensive and time consuming, computer experiments are widely used for simulating physical characteristics and for the design and development of products [Fang et al. (2006)]. A computer experiment is modeled as a realization of a stochastic process, often in the presence of nonlinearity and high dimensional inputs [Sacks et al. (1989a)]. In order to perform efficient data analysis and prediction and in order to determine the best settings for a number of design parameters that have an impact on the response variable(s) of interest and which influence the critical quality characteristics of the product or process, it is often necessary to set a good design as well as to optimize the product or process design. In computer experiments, instead of physically doing an experiment on the product, mathematical models describing the performance of the product are developed using engineering/physics laws. Then the mathematical models are solved on computers through numerical methods such as the finite element method. A computer simulation of the mathematical models is usually time consuming and there is a great variety of possible input combinations. For these reasons, meta-models [Barthelemy and Haftka (1993); Sobieski and Haftka (1997)] that model the quality characteristics as explicit functions of the design parameters are constructed. Such a meta-model, also called a (global) approximation model or surrogate model, is obtained by simulating a number of design points. Since a meta-model evaluation is much faster than a simulation run, in practice such a meta-model is used, instead of the simulation model, to gain insight into the characteristics of the product or process and to optimize it. Therefore, a careful choice of the design points at which performing simulations in order to build the meta-model is of primary importance.

In [Jurecka et al. (2005)], the concept of robust design is presented and the need for meta-models within this framework is elaborated. They also introduced a method to sequentially

update the meta-models during the robust design optimization process through strategies typically used in global optimization. Bates et al. [Bates et al. (1996)] obtains designs for computer experiments by exploring so-called lattice points and using results from number theory.

Fang [Fang et al. (2000a); Fang et al. (2000b)] defined a uniform design as a design that allocates experimental points uniformly scattered on the domain. Uniform designs do not require orthogonal. They consider projection uniformity over all sub dimensions. In [Fang et al. (2000b)] they classify uniform designs as space-filling designs.

Lee and Jung (2000) proposed maximin Eigen value sampling, that maximizes minimum Eigen value, for Kriging model where maximin Eigen value sampling uses Eigen values of the correlation matrix. The Kriging model is obtained from sampled points generated by the proposed method. Note that the Kriging model [Krige (1951)] is used to compare the characteristics of proposed sampling design with those of maximum entropy sampling.

The maximin design problem has also been studied in location theory. In this area of research, the problem is usually referred to as the max-min facility dispersion problem [Erkut (1990)]; facilities are placed such that the minimal distance to any other facility is maximal. Again, the resulting solution is certainly space-filling, but not necessarily non-collapsing.

In statistical environments Latin Hypercube sampling is often used. In such an approach, points on the grid are sampled without replacement, thereby deriving a random permutation for each dimension ([McKay et al. (1979)]).

Giunta [Giunta et al. (2003)] gives an overview of pseudo- and quasi-Monte Carlo sampling, Latin hypercube sampling, orthogonal array sampling, and Hammersley sequence sampling.

Lin, in [Lin and Steinberg (2006)], proposed several methods for extending the uniform sampling to higher dimensions. The method has also been used to construct LHDs with low correlation of first-order and second-order terms. It generates orthogonal LHDs that can include many more factors than those proposed by [Ye (1998)].

Cioppa, in his dissertation [Cioppa (2002)], developed a set of experimental designs by considering orthogonal Latin hypercube and uniform designs to create designs having near orthogonality and excellent space-filling properties. Multiple measures were used to assess the quality of candidate designs and to identify the best one.

Morris (1991) and Kleijnen (1997) make it clear that many simulation models involve several hundred factors or even more. Consequently, factor screening is useful in computer experiments for reducing the dimension of the factor space before carrying out more detailed experiments. Butler (2001) proposed optimal and orthogonal LHDs which is suitable for factor screening. Olsson (2003) suggested Latin Hypercube sampling as a tool to improve the efficiency of different importance sampling methods for structural reliability analysis.

1.2.2. Optimal Criteria

McKay et al. (1979), Stein (1987) and Owen (1994b) had shown that Latin Hyper Cube Designs (LHDs) perform much better than completely randomized designs. More recently, algorithms have been used to construct systematic LHDs under various optimality criteria. In particular, as already remarked, randomly generated LHDs often show poor space-filling properties. Therefore, the search for “optimal” LHDs has attracted attention (e.g., [Morris and Mitchell (1995); Park (1994); Tang (1994); Ye (1998); Ye et al. (2000)]). Different optimality criteria for LHDs have been proposed, including maximum entropy designs [Shewry and Wynn (1987); Currin et al. (1991)], Integrated Mean Squared Error (IMSE) of prediction [Sacks et al. (1989a)] and minimax and maximin distance designs [Johnson et al. (1990)].

Here some literature reviews regarding optimal criteria regarding experimental design are discussed briefly. So several heuristics approaches (rather than exact optimization methods) have been proposed in the literature to detect optimal experimental designs. van Dam [Dam et al. (2007b)] proposed some bounds, for the separation distance of certain classes of maximin LHDs, which are useful for assessing the quality of approximate maximin LHDs. By using some of the special properties of LHDs, they were able to find new and tighter bounds for maximin LHDs. Besides these bounds, they presented a method to obtain a bound for three-dimensional LHDs that is better than Baer's bound for many values of N . They also constructed maximin LHDs attaining Baer's bound for infinitely many values of N in all dimensions.

Johnson (1990) and Morris and Mitchell (1995) proposed the maximin distance criterion which maximizes the minimum distance between design points. Morris and Mitchell (1995) adopted a simulated annealing [Aarts and Lenstra (1997)] to find approximate maximin LHDs for up to five dimensions and up to 12 design points and a few larger values, with respect to the ℓ^1 - [Manhattan distance] and L^2 - [Euclidian distance] measure. In Morris and Mitchell's algorithm, a search begins with a randomly chosen LHD, and proceeds through examination of a sequence of designs, each generated as a perturbation of the preceding one. A perturbation D_{try} of a design D is generated by interchanging two randomly chosen elements within a randomly chosen column in D . The perturbation D_{try} replaces D if it leads to an improvement. Otherwise, it will replace D with probability $\pi = \exp[-\{\phi(D_{try}) - \phi(D)\} / t]$, where t is the preset parameter known as the "temperature" and ϕ is some measure of the quality of the design. Li and Wu [Li and Wu (1997)] considered a class of Column-wise Pair-wise (CP) algorithms in the context of the construction of optimal supersaturated designs. A CP algorithm makes exchanges on the columns in a design and can be particularly useful for designs that have structure requirements on the columns. Note that each column in a LHD is a permutation of $\{0, \dots, N - 1\}$. At each step, another permutation of $\{0, \dots, N - 1\}$ is chosen to replace a column so that the LHD structure is retained.

Husslage et al. [Husslage et al. (2005)] constructed nested maximin designs in two dimensions. They showed that different types of grids should be considered when constructing nested designs and discussed how to determine which grid is the best for a specific computer experiment. Santner [Santner et al. (2003)], Bursztyn and Steinberg [Bursztyn and Steinberg (2006)] and Simpson [Simpson et al. (2001)] showed that maximin optimal LHDs generally speaking yield the best approximations. van Dam [Dam et al. (2007a)] derive general formulas for two-dimensional maximin LHDs, when the distance measure is L^∞ or L^1 , while for the L^2 -distance measure (approximate) maximin LHDs up to 1000 design points are obtained by using a branch-and-bound algorithm and constructing (adapted) periodic designs.

We remark that the maximin criterion is not the only one used in the literature. Other criteria are the maximum entropy [Shewry and Wynn (1987)], the integrated mean squared error [Crary (2002)], the minimum correlation between components [Owen (1994b)] and a mixed criterion involving both maximin distance and correlation [Joseph and Hung (2008)]. For more details we also refer to the book [Santner et al. (2003)] but for the completeness, in the following literature review, we will mention some articles in which several optimal criteria are considered.

Iman and Conover in [Iman and Conover (1982a)] proposed a design by minimizing a linear correlation criterion for pairwise factors. This is modified into a polynomial canonical correlation criterion by [Tang (1998)]. Tang [Tang (1998)] proposed a LHD by the extension of the concept of Iman and Conover [Iman and Conover (1982a)], namely minimizing a polynomial canonical correlation criterion for pair-wise factors.

Ye [Ye (1998)] constructed orthogonal LHDs in order to enhance the utility of LHDs for regression analysis. Ye defines an Orthogonal Latin Hypercube (OLHC) as a Latin Hypercube for which every pair of columns has zero correlation. Furthermore, in Ye's OLHC construction, the element-wise square of each column has zero correlation with all other columns, and the element-wise product of every two columns has zero correlation

with all other columns. These properties ensure the independence of estimates of linear effects of each variable and the estimates of the quadratic effects and bilinear interaction effects are uncorrelated with the estimates of the linear effects.

Joseph and Hung in [Joseph and Hung (2008)] proposed a multi-objective optimization approach to find good LHDs by combining correlation and distance performance measure. In [Sebastiani and Wynn (2000)] Sebastiani and Wynn considered maximum entropy sampling criterion for the optimal Bayesian experimental design. The main contribution of this paper is the extension of the MES principle for the estimation of the problems. Currin [Currin et al. (1991)] also considered an entropy-based design criterion for Bayesian prediction of deterministic functions. Crombecq et al. [Crombecq et al. (2011)] consider space-filling and non-collapsing sequential design strategies for simulation based modeling.

Hongquan Xu in [Hongquan Xu (1999)] introduced the concept of universal optimality from optimum design theory into computer experiments, and then exhibited some universally optimal designs with respect to different distance measures. He showed that Latin Hypercube and saturated orthogonal arrays are universally optimal with respect to Hamming distance [Hamming (1950)], and that universally optimal designs with respect to Lee distance [Lee (1958)] are also derived from Latin Hypercubes and saturated orthogonal arrays.

Recently Jourdan and Franco [Jourdan and Franco (2010)] proposed a space-filling LHD design, where they consider a new optimal criterion called Kullback–Leibler criterion. This Kullback–Leibler criterion is relatively very new proposed by Jourdan and Franco [Jourdan and Franco (2009)]. The new designs are compared with several traditional optimal Latin hypercube designs. Leary et al. [Leary et al. (2003)] proposed orthogonal-array-based LHDs for obtaining better space-filling property. As an optimal criterion, they consider the sum of (square of) reverse inter-site distances i.e potential energy criterion.

In [Steinberg and Dennis (2006)] Steinberg and Dennis constructed LHDs in which all main effects are orthogonal. Their method can also be used to construct LHDs with low correlation of first-order and second-order terms. It also generates orthogonal LHDs that can include many more factors than those proposed by Ye [Ye (1998)]. Butler [Butler (2001)] proposed optimal and orthogonal LHDs which are suitable for factor screening .

A lot of improved values (maximin LHD values) are obtained by the ILS approaches proposed by Grosso et. al. (2009) where LHDs are optimized in Euclidean distance measure. The improved values are available in the well known web portal <http://www.spacefillingdesigns.nl>. Jamali et al. (2010) analyzed the multicollinearity of the maximin LHD obtained by the ILS approach. In this article it is shown that the ILS approach not only able to obtain good LHD in the sense maximin property but the multicollinearity among the factors of the designs are negligible i.e. the average coefficient of correlations are low.

From the point of view of computational complexity the problem is, to the authors' knowledge, open (but suspected to be NP-complete). For the presence of combinatorial nature, the number of possible LHDs is very high - $(N!)^k$ (where N is number of design points and k is number of factors). Consequently, when number of factors and/ or number of design points are large then it requires hundreds of hours by the brute-force approach to find out the optimal design. So when numbers of factors as well as number of experimental points are large, the algorithm requires a couple of hours or even more to find out a simulated optimal design. So time complexity is an important issue for a good algorithm, especially when we need a real time solution. Anyway Parimal [2012] performed several experiments for analyzing the time complexity of the ILS approach. Experimentally, he showed that the time complexity of the ILS algorithm is of polynomial time with order four ($O(N^4)$) when consider $\text{Opt}(\Phi, D1)$ criterion and $O(N^3)$ when consider $\text{Opt}(D_1, J_1)$ criterion [Jamali (2009)]. Recently Isahaque (2014) study the maximin LHDs obtained by ILS approach regarding Manhattan distance measure.

Anyway there is another important optimal criterion which is called Audze-Eglais optimal criterion. Audze-Eglais designs are obtained by minimizing the following criterion which is indeed analog with potential energy among the charged particles:

$$\sum_{i=1}^n \sum_{j=i+1}^n \frac{1}{d(x_i, x_j)^2}$$

where $d(x_i; x_j)$ is the distance between points x_i and x_j and N is the number of design points. The criterion was first introduced by Audze and Eglais (1977) and is based on the analogy of minimizing forces between charged particles. The principle of the Audze–Eglais DoE is to distribute experiment points as uniformly as possible within the design variable domain. This is achieved by minimizing the potential energy of the points of a DoE. The generation of the Audze–Eglais DoE is time consuming and requires optimization to solve the minimization problem. In Bates et al. (2003) , the problem of finding Audze-Eglais LHDs is formulated and a permutation genetic algorithm is used to generate them. Liefvendahl and Stocki (2006) compare maximin and Audze-Eglais LHDs and recommend the Audze-Eglais criterion over the maximin criterion. Examples of practical applications of Audze-Eglais LHDs can be found in Rikards et al. (2001), Bulik et al. (2004).

1.2.3 Methods

By using the Latin Hypercube sampling method Hwan Yang [Hwan (2007)] performed the uncertainty and sensitivity analysis for the time-dependent effects in concrete structure. The results of the Latin Hypercube simulations were used to determine which of the model parameters are most significant in affecting the uncertainty of the design [Iman and Helton (1985)]. For each sample, a time-dependent structural analysis was performed to produce response data, which were then analyzed statistically.

Stocki [Stocki (2005)] and Liefvendahl and Stocki [Liefvendahl and Stocki (2006)] proposed probabilistic search algorithm, namely Column-wise Pair-wise (CP) search algorithms and Genetic algorithms to construct optimal LHDs. For the optimal criterion they considered energy function (the sum of the norms of the repulsive forces if the

samples are considered as electrically charged particles) as proposed in [Audze and Eglais (1977)]. To improve the reliability, Stocki (2005) considered the pairwise correlation. Liefvendahl and Stocki (2006) also compared the performance of the CP and genetic algorithms for optimal LHDs.

Wang [Wang (2003)] used the Latin Hypercube Design (LHD) instead of the Central Composite Designs (CCD), for improvement of Adaptive Response Surface Method (ARSM). Note that ARSM was developed to search for the global design optimum for computation-intensive design problems. Also note that Response Surface Method (RSM) plans a group of design alternatives and performs the design analysis and simulation simultaneously on these design alternatives. Then an approximation model, called a response surface, is constructed.

Fang et al. (2000) considered Simulated Annealing approach to detect maximin LHD. In [Li and Wu (1997)] a class of algorithms based on column pair-wise exchange has been proposed to build supersaturated designs. In [Ye et al. (2000)] an exchange algorithm for finding approximate maximin LHDs has been proposed with the further restriction to Symmetric LHDs (SLHDs). In [Dam et al. (2007a)], general formulae for maximin LHDs with $k = 2$ are given for the 1-norm (L^1) and infinite norm (L^∞) distances, while for the Euclidean distance (approximate) maximin LHDs up to $N = 1000$ design points are obtained by (adapted) periodic designs, while, using a branch-and-bound algorithm, exact solutions have been obtained for N up to 70. Inspired by Dam et al. (2007a), Husslage (2006) proposed (adapted) periodic designs and simulated annealing to extend the known results and construct approximate maximin latin hypercube designs for k up to 10 and N up to 100. All these designs are available in the website <http://www.spacefillingdesigns.nl>. In [Husslage et al. (2006)], it has been shown that the periodic heuristic tends to work when the number N of design points gets above some threshold which depends on the dimension k of the design (more precisely), such threshold increases with k . Viana [Viana et al. (2010)] proposed the translational propagation algorithm, a new method for obtaining optimal or near optimal Latin hypercube designs (LHDs) without using formal optimization. For the optimal criterion they also considered $\text{Opt}(\phi)$ to maximin LHD.

Monte Carlo simulations were used to evaluate the performance of the algorithm for different design configurations where both the dimensionality and the point density were studied. In [Gross et al. (2008)] Gross et al. successfully implements Iterated local search (ILS) approach for finding maximin LHDs for $k = 3, 4, \dots, 10$, and $N = 3, 100$. For the optimal criterion they considered maximin LHDs with $\text{Opt}(D_1, J_1)$ and $\text{Opt}(\phi)$ optimal criteria with Euclidian distance measure (Eq. (1.1) to Eq. (1.4)).

Using (adapted) periodic designs and simulated annealing, Husslage et al. in [Husslage et al. (2006)] extended the known results and construct approximate maximin Latin hypercube designs for up to ten dimensions and for up to 100 design points. All these designs can be downloaded from <http://www.spacefillingdesigns.nl>. Inspired by the paper [Morris and Mitchell (1995)], in which authors show that LHDs often have a nice periodic structure, Husslage et al. (2006) developed adapted periodic designs. By considering periodic and adapted periodic designs, approximate maximin LHDs for up to seven dimensions and for up to 100 design points are constructed. They have shown that the periodic heuristic tends to work well even for a small number N of design points at low values of the dimension k , but as k increases the periodic heuristic tends to get better than other approaches like simulated annealing only at large N values.

Jin [Jin et al. (2005)] proposed an enhanced stochastic evolutionary algorithm for finding maximin LHDs. They also apply their method to other space-filling criteria, namely the optimal entropy and centered L_2 discrepancy criteria. Stinstra et al. [Stinstra et al. (2003)] proposed sequential heuristic algorithms for constrained maximin designs by considering high number of design sites with small volume of feasible design space and other constraints. They also used their methods in many practical situations.

Park (1994) and Sacks et al. (1989a) constructed optimal LHDs in which IMSE and entropy optimization criteria were considered. To construct optimal LHDs, Park [Park 1994] presented an approach based on the exchanges of several pairs of elements in two rows. His algorithm first selects some active pairs which minimize the objective criterion value by excluding that pair from the design. Then, for each chosen pair of two points i_1

and i_2 , the algorithm considers all possible exchanges and find the best exchange among them.

Joseph and Hung (2008) proposed a modified simulated annealing algorithm with respect to [Morris and Mitchell (1995)]. Instead of randomly choosing a column and two elements within that column, as in [Morris and Mitchell (1995)], they choose them judiciously in order to achieve improvement in their multi-objective function. Ye et al. (2000) and Li and Kenny (2009) proposed an exchange algorithm for finding approximate optimal LHDs, but they consider symmetric Latin hypercube designs (SLHDs). The symmetry property is used as a compromise between computing effort and design optimality. However, one important change had made to accommodate the special structure of SLHD. For a SLHD two simultaneous pair exchanges were made in each column to retain the symmetry. Ye et al. (2000) considered maximin as an optimal criterion, whereas Li and Kenny (2009) considered both the maximin and the entropy optimal criterion.

Fang. (2000a) proposed threshold accepting heuristic approaches for optimal LHDs to produce low discrepancy designs compared to theoretic expectation and variance. They considered centered L_2 -discrepancy for optimizing the designs. Different methods have been presented in the literature to detect maximin LHDs. For example, the book of Santner et al. (2003) and the article of Li and Kenny (2009) considered both the maximin and the entropy optimal criterion. Bates et al. (2004) proposed a permutation genetic algorithm to find optimal Audze- Eglais LHDs. Recently Husslage et al. (2011) obtained optimal maximin LHDs as well as optimal Audze-Eglais LHDs by implement Enhanced Stochastic Evolutionary (ESE) algorithm.

1.3 Goals of the Thesis

Many simulation models involve several hundred factors or even more. But few, out of the numerous factors in the system, usually dominate the performance of the product. Thus a good model can be fitted using only these few important factors. To identify the effect of

each factors, it is disable to avoid the replication when projection the design on to a subset of factors. The experimental design should fulfill three important properties – Non-collapsing, Space-filling and non-multicollinearity. Though Latin Hypercube Designs (LHDs) inherently non-collapsing but randomly generated LHDs are poor regarding space-filling property. So researchers seek LHD with good space-filling property. Many researchers have shown that optimal LHD mainly maximin LHD has good space-filling including non-collapsing property. There are several approaches as well as optimal criteria exist in literature to find out the optimal LHD such as Simulated annealing, Tabu search, Iterated Local Search (ILS) etc. In the paper [Grosso et al. (2008)], authors have shown that ILS approach able to find out a remarkable improved optimal experimental design regarding available one in the literature. They considered ϕ_p optimal criterion and find maximin optimal LHD. Recently several author consider Audze- Eglais optimal criterion for optimized maximin LHD. For this reason we will investigate maximin LHD obtained by ILS regarding Audze-Eglais value. The main goal of the study is pointed out as follows:

- (a) The comparison of ILS approach with some well-known approaches regarding maximin LHDs measured in Euclidian distance measure with available ones in the literature.
- (b) The comparison of maximin LHDs obtained by ILS approach with Audze-Eglais LHDs obtained by ESE algorithm regarding Audze-Eglais values.
- (c) The comparison of several characteristics of maximin LHDs obtained by ILS approach with that of some other optimal LHDs.

1.4 Structure of the Thesis

After the introduction and literature review which are represent in this **Chapter**, the remaining thesis is organized as follows:

Chapter II discusses the overview of optimal criteria regarding experimental design. Mainly this chapter points out of some frequently use optimal criteria regarding LHD. **Chapter III** discusses and presents the heuristic approach mainly Iterated Local Search (ILS) approach. In **Chapter IV** several experiments are performed for analysis the ILS approach regarding Euclidian distance measure.. At first the performance of the algorithm is compared with available one in the literature regarding inter-site Euclidian distance measure. From the experimental design it is shown that the algorithm is state-of-arts regarding maximin LHD. In **Chapter V** several experiments have been performed extensively regarding Audze-Eglais value. For this investigation we first consider those maximin LHDs obtained by ILS approach. Then the designs are compared with Audze-Eglais based Optimal LHDs obtained by ESE algorithm regarding Audze-Eglais value. Moreover in this chapter several optimal LHDs are compared in perspective several characteristics. Finally a brief discussion and concluding remarks are given in Chapter 6. References are included in the last of the thesis as well and publications are mentioned before the index of the thesis.

CHAPTER II

OPTIMALITY CRITERION

2.1 Introduction

In the design of experiments, optimal designs are a class of experimental designs that are optimal with respect to some statistical criterion. The creation of this field of statistics has been credited to Danish statistician Kirstine Smith (1918). Experimental designs are evaluated using statistical criteria. In the design of experiments for estimating statistical models, optimal designs allow parameters to be estimated without bias and with minimum-variance. A non-optimal design requires a greater number of experimental runs to estimate the parameters with the same precision as an optimal design. In practical terms, optimal experiments can reduce the costs of experimentation. The optimality of a design depends on the statistical model and is assessed with respect to a statistical criterion, which is related to the variance-matrix of the estimator. Specifying an appropriate model and specifying a suitable criterion function both require understanding of statistical theory and practical knowledge with designing experiments. Optimal designs offer three advantages over suboptimal experimental designs:

1. Optimal designs reduce the costs of experimentation by allowing statistical models to be estimated with fewer experimental runs.
2. Optimal designs can accommodate multiple types of factors, such as process, mixture, and discrete factors.
3. Designs can be optimized when the design-space is constrained, for example, when the mathematical process-space contains factor-settings that are practically infeasible (e.g. due to safety concerns).

2.2 Distance measure

Since in the experimental design the optimality is based on distance of the design points so before discuss several type of optimality criteria we will introduce two measure namely Euclidean Distance measure and Manhattan distance measure among several type of distance measure existing in the literature.

(a) Euclidean Distance measure: In mathematics, the Euclidean distance or Euclidean metric is the "ordinary" distance between two points that one would measure with a ruler, and is given by the Pythagorean formula. By using this formula as distance, Euclidean space (or even any inner product space) becomes a metric space. The associated norm is called the Euclidean norm.

The Euclidean distance between points \mathbf{p} and \mathbf{q} is the length of the line segment connecting them (\mathbf{p}, \mathbf{q}). In Cartesian coordinates, if $\mathbf{p} = (p_1, p_2, \dots, p_n)$ and $\mathbf{q} = (q_1, q_2, \dots, q_n)$ are two points in Euclidean n -space, then the distance from \mathbf{p} to \mathbf{q} , or from \mathbf{q} to \mathbf{p} is given by:

$$d_2 = d(\mathbf{p}, \mathbf{q}) = \sqrt{\sum_{i=1}^n (q_i - p_i)^2} \quad (2.1)$$

The position of a point in a Euclidean n -space is a Euclidean vector. So, \mathbf{p} and \mathbf{q} are Euclidean vectors, starting from the origin of the space, and their tips indicate two points. The Euclidean norm (L^2), or Euclidean length, or magnitude of a vector measures the length of the vector:

$$\|\mathbf{p}, \mathbf{q}\| = \sqrt{\sum_{i=1}^n (q_i - p_i)^2}$$

The standard Euclidean distance can be squared in order to place progressively greater weight on objects that are farther apart. Squared Euclidean Distance is not a metric as it does not satisfy the triangle inequality, however it is frequently used in optimization problems in which distances only have to be compared. Note that Euclidean distance is also called L^2 -norm. Note that in the following study we always consider square value of $d(\mathbf{p}, \mathbf{q})$.

(b) Manhattan Distance measure: Manhattan distance also a special case of Minkowski distance. Taxicab geometry, considered by Hermann Minkowski in the 19th

century, is a form of geometry in which the usual metric of Euclidean geometry is replaced by the taxicab metric. The taxicab distance, d_1 , between two vectors \mathbf{x} , \mathbf{y} in an n -dimensional real vector space with fixed Cartesian coordinate system, is the sum of the lengths of the projections of the line segment between the points onto the coordinate axes. More formally,

$$d_1 = d(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|_1 = \sum_{i=1}^n |x_i - y_i| \quad (2.2)$$

where $\mathbf{x} = (x_1, x_2, \dots, x_n)$ and $\mathbf{y} = (y_1, y_2, \dots, y_n)$ are vectors.

2.3 Definition of some important optimality criteria

In Experimental design, an optimality criterion is a criterion which summarizes how good a design is, and it is maximized or minimized by an optimal design. There are several optimal criteria available in the literature regarding experimental design. But we will present some frequently used optimal criteria regarding experimental design.

2.3.1 Maximin distance designs

Maximin distance design, or brief maximin design, was first proposed and studied by Johnson et al. (1990). A maximin distance design is a design in that the minimum distance between any two points is maximized. The idea of maximin design is that how well all design points fill the space of a design. Maximin distance is to select a design in which the minimum distance between any two sites (design points) in the subset is reached as large as possible. The design is selected based on its distance only and does not require the assumption of a particular model. For a Gaussian process with correlation depending on distance, a maximin distance design minimizes the maximum correlation if the correlation function is a decreasing function. Johnson et al. (1990) showed that maximin distance designs are asymptotically D-optimal for a Gaussian process when the correlation between sites decreases as the distance increases. An Latin Hypercube Design (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. Below we present some optimal criteria based on maximin distance design.

(a) Opt(D₁, J₁) Optimality Criterion

In order to drive the search through LHDs we need some criterion to compare them. Below we will describe some of the criteria employed in the literature. Opt(D₁, J₁) Optimality Criterion : Under this criterion a LHD Y can be considered better than another one X if a lexicographic ordering holds:

$$\begin{aligned} &D_1(Y) > D_1(X) \text{ or} \\ &D_1(Y) = D_1(X) \text{ and } J_1(Y) < J_1(X). \end{aligned} \quad (2.3)$$

By generalizing this approach, we can consider the problem like a multiobjective problem with priorities: maximize the objective with highest priority D₁; within the set of optimal solutions with respect to D₁, minimize the objective with second highest priority J₁. Note that Johnson et. al. [1990] first proposed this optimality criterion.

(b) Opt(φ) Optimality Criterion

As previously remarked, if there exist different LHDs with equal D₁ and J₁ values, i.e. in case there exist at least two LHDs X,Y such that D₁(X) = D₁(Y) = D₁ and J₁(X) = J₁(Y) = J₁, we could further consider the objective D₂ and maximize D₂(X), the second smallest distance in X, and, if equality still holds, minimize J₂(X), the number of occurrence of D₂(X), and so on. Then an optimal design X sequentially maximizes D_i's and minimizes J_i's in the following order: D₁, J₁; D₂, J₂; · · · ; D_m, J_m. Morris and Mitchell (1995) have used all the above measures to define a family of scalar-valued functions (to be minimized), which can be used to rank competing designs in such a way that a maximin design receives the highest ranking. This family of functions, indexed by p, is given by

$$\phi_p(x) = \sum_{r=1}^m \left[\frac{J_r(X)}{(D_r(X))^p} \right]^{1/p} \quad (2.4)$$

where p is a positive integer parameter. Under this criterion, LHD Y is better than X if

$$\phi_p(\mathbf{Y}) < \phi_p(\mathbf{X}).$$

Note that for large enough p , each term in the sum in (2.4) dominates all subsequent terms. Through p we can control the impact of the different D_r relevant. In the form (2.4), the evaluation of ϕ_p would be computationally costly. However, it has a computationally cheaper form [122]). Indeed, (2.1) can be simplified as

$$\phi_p(X) = \left[\sum_{i=1}^N \sum_{j=i+1}^N \frac{1}{d_{ij}^p} \right]^{\frac{1}{p}} \quad (2.5)$$

which can be computed without the need of detecting and ordering all the D_i values.

(c) **Opt(ϕ , D_1) Optimality Criterion**

An apparent drawback of the Opt(ϕ) criterion, if we are interested in maximum values (maximum D_1 value), is that LHDs with smaller (better) ϕ_p can have a worse (smaller) D_1 , i.e. we can have X and Y such that $\phi_p(X) < \phi_p(Y)$ and $D_1(X) < D_1(Y)$. This phenomenon has been frequently observed in the computational experiments [Jamali (2009)]. Nevertheless, a profitable choice is to work in order to minimize the ϕ_p function but, at the same time, keep track of the best (D_1 , J_1) values observed during such minimization. This way the search in the solution space is guided by a kind of heuristic function. Such a mixed approach might appear strange but it is extremely effective [Jamali (2009)]. This heuristic based criterion is denoted as **Opt(ϕ , D_1)** optimal criterion.

2.4 Audze –Eglais design and optimal criteria

The Audze-Eglais Design of Experiment (DoE) is based on the following physical analogy: a system consisting of points of unit mass exert repulsive forces on each other causing the system to have potential energy. When the points are released from an initial state, they move. If the magnitude of the repulsive forces is inversely proportional to the distance square between the points, mathematically for unit mass, it can be written as follow:

$$U = \sum_{i=1}^n \sum_{j=i+1}^n \frac{1}{d(\mathbf{x}_i, \mathbf{x}_j)^2} \quad (2.6)$$

where U is the potential energy and $d(\mathbf{x}_i, \mathbf{y}_j)$ be the Euclidean distance between points \mathbf{x}_i and \mathbf{y}_j . They will reach equilibrium when the potential energy U of the repulsive forces between the masses is at a minimum i.e. the minimizing Eq. (2.6) will produce a system of points distributed as uniformly as possible

$$\min U = \min \sum_{i=1}^n \sum_{j=i+1}^n \frac{1}{d(\mathbf{x}_i, \mathbf{x}_j)^2} \quad (2.7)$$

The Audze and Eglais criterion was first introduced by Audze and Eglais (1977) and is based on the analogy of minimizing forces between charged particles. If $d(\mathbf{x}_i, \mathbf{y}_j)_s$ be the distance between two points \mathbf{x}_i and \mathbf{y}_j $i, j = 1, 2, \dots, N$ of any DoE in some distance measure s , then Audze-Eglais designs are obtained by minimizing the following Audze-Eglais optimal criterion is :

$$\text{Opt(A-E)} = \sum_{i=1}^n \sum_{j=i+1}^n \frac{1}{d(\mathbf{x}_i, \mathbf{x}_j)^2} \quad (2.8)$$

The principle of the Audze-Eglais DoE is to distribute experiment points as uniformly as possible within the design variable domain. This is achieved by minimizing the potential energy of the points (A-E criteriion) of a DoE. The DoE for k variables and N experiments is independent of the application under consideration, so once the design is formulated for N points and k design variables, it is stored in a matrix and need not be formulated again.

2.5 Orthogonality-based criteria

Besides space-filling and no-collapse criteria another important criterion frequently need in DoE is orthogonality criterion. If the design points are correlated then the individual effect of the parameter can not be identified. So the data of the parameters (coordinates) should be as much as possible uncorrelated. In this aspect several optimal criteria are proposed in the literature in which the correlations among the parameters are minimized.

Correlation criteria seek to analyze the similarity and difference between two sets of results. Usual applications are the correlation of test and analysis results and the comparison of various analysis results. Ideally correlation criteria should quantify the

ability of two models to make the same predictions. Since the predictions of interest is for a particular model can really be pin pointed precisely one has to use general quality and select from a list of possible criterion, the ones that can be computed and do a good enough job for the interest. Correlation is widely used statistical technique. Correlation coefficients are the index of the measurement of the relationship among the sets of variables. There are several kinds of correlation coefficients regarding the number of the variables considered. They are (i) Simple correlation (ii) Multiple correlation and(iii) Partial correlation. There are several ways are available in the literature to measure the correlations. There are two well-know approaches to evaluate the orthogonality of a DoE. The most popular one is based on correlation among the samples' coordinates, the other one is a condition number.

(a) Pair-wise correlation of sample coordinates based criteria

There are well known approaches to measure correlation of sample coordinates namely (i) Kerl Pearson coefficient of correlation or coefficient of correlation by product-moment formula (KPCC) (ii) Spearman's rank correlation coefficient (SRCC) and (iii) Kendall tau rank correlation coefficient (KRCC)

(i) **Kerl Pearson coefficient of correlation or coefficient of correlation by product-moment formula (KPCC):** Let there are two coordinates x and y $\{(x_i, y_j) : j = 1, 2, \dots, N\}$ with dimension k of any DoE. Then product-moment coefficient of correlation ρ_{ij} of the coordinates is defined as follow:

$$\rho_{ij} = \frac{N \sum x_i x_j - \sum x_i \sum x_j}{\sqrt{\{N \sum x_i^2 - (\sum x_i)^2\} \{N \sum x_j^2 - (\sum x_j)^2\}}} \quad (2.9)$$

To overcome the sign of correlation we square each ρ_{ij} . Then calculating all pair-wise correlation among the factors of a DoE, we have following average pair-wise correlations:

$$\rho^2 = \frac{\sum_{i=2}^k \sum_{j=1}^{i-1} \rho_{ij}^2}{k(k-1)/2} \quad (2.10)$$

Therefore the **KPCC** based criterion will be the minimization of the equation (2.10).

(ii) **Spearman's rank correlation coefficient (SRCC):** Spearman's rank correlation coefficient (SRCC) can be used to capture a nonlinear but monotonic relationship between two variables and therefore, it can be efficiently applied for estimation of correlations in sampling-based SA [J.C. Helton et al. (2006)]. The idea is to replace the values of x_{ai} and x_{aj} by their corresponding ranks $r(x_{ai})$ and $r(x_{aj})$ and then the SRCC can be computed as follow:

$$\rho_{ij} = 1 - \frac{6 \sum_{a=1}^n (r(x_{ai}) - r(x_{aj}))^2}{n(n^2 - 1)} \quad (2.11)$$

In case of a multi-dimensional design space, the orthogonality of the DoE can be achieved by minimizing

$$E^{SRCC} = \sqrt{\sum_{i=1}^k \sum_{j=i+1}^k \rho_{ij}^2} \quad (2.12)$$

(iii) **Kendall tau rank correlation coefficient (KRCC)** is an alternative measure of a nonlinear dependence between two variables. In particular, it is based on the number of concordant ($T_{c,ij}$) and discordant ($T_{d,ij}$) pairs of samples according to

$$\tau_{ij} = \frac{T_{c,ij} - T_{d,ij}}{n(n-1)/2}, \quad (2.13)$$

and again, the orthogonal DoE can be obtained by minimizing the following objective function

$$E^{KRCC} = \sqrt{\sum_{i=1}^k \sum_{j=i+1}^k \tau^2} \quad (2.14)$$

(b) **Condition number base optimal criterion**

Condition number (CN) is commonly used in numerical linear algebra to examine the sensitivities of a linear system. Here, we use condition number of $\mathbf{X}^T \mathbf{X}$, where \mathbf{X} is a matrix of the design points' coordinates, so called design matrix

$$\mathbf{X} = \begin{pmatrix} x_0 \\ \vdots \\ x_{N-1} \end{pmatrix} = \begin{pmatrix} x_{01} & \cdots & x_{0k} \\ \vdots & \cdots & \vdots \\ x_{(N-1)1} & \cdots & x_{(N-1)k} \end{pmatrix} \quad (2.15)$$

where N is the number of the design points and k is the dimension of the design space. The condition number is then defined as

$$E^{CN} = \text{cond}(\mathbf{X}^T \mathbf{X}) = \frac{\lambda_1}{\lambda_n} \quad (2.16)$$

where λ_1 and λ_n are the largest and smallest eigen values of $\mathbf{X}^T \mathbf{X}$, respectively, therefore

the *ECN* is greater or equal to 1. Values closer to 1 correspond to more orthogonal DoE, therefore the condition number should be minimized.

Now some well known approaches with optimal criteria are summarized in the Table 2.1.

Table 2.1 : Some well known approaches as well as optimal criterion for optimal experimental designs

Researchers	Year	Algorithm	Objective
Audze and Eglajs	1977	Coordinates Exchange Algorithm	Opt (A-E) criterion (Potential Energy)
Park	1994	A 2-stage(exchange-and Newton-type) algorithm	Integrated mean squared error and
Morris &	1995	Simulated annealing (SA)	Φ_p criterion
Ye et al.	2000	Column-wise-pair-wise	Φ_p and entropy
Fang et al.	2002	Threshold accepting algorithm	Centered L_2 discrepancy
Bates et al.	2004	Genetic algorithm	Potential energy
Jin et al.	2005	Enhanced stochastic evolutionary algorithms	Φ_p criteria, entropy and L_2 discrepancy
Liefvendahl and Stocki	2006	Columnwise-pairwise and genetic algorithms	Opt (A-E) criterion (Potential Energy)
Van Dam et al.	2007	Branch-and-bound algorithm	1-norm and infinite norm distances
Grosso et al.	2008	Iterated local search and	Opt (Φ_p, D_1) criterion

CHAPTER III

REVIEW OF ITERATED LOCAL SEARCH AND LATIN HYPERCUBE DESIGN

3.1 Introduction

Iterated local search (ILS) approaches are frequently used to solve the problems here. The general form of Iterated Local Search (ILS) approaches are briefly discussed. In the case of combinatorial optimization problem where the search space is discrete and highly multimodal.

3.2 ILS approach

Iterated Local Search (ILS) is a meta-heuristic designed to embed another, problem specific, local search as if it were a black box. This allows ILS to keep a more general structure than other meta-heuristics currently in practice. This simple type of search has been reinvented numerous times in the literature, with one of its earliest incarnations appearing in [Lin and Kernighan (1973)]. This simple idea [Baxter et al. (1981)] has a long history, and its rediscovery by many authors has lead to many different names for iterated local search like iterated descent [Baum et al. (1986)], large-step Markov chains [Martin et al. (1991)], iterated Lin-Kernighan [Johnson D. S. (1990)], chained local optimization [Martin Otto (1996)], or combinations of these [Applegate et al. (1999)]. ILS has many of the desirable features of a meta-heuristic: it is simple, easy to implement, robust and highly effective. The essence of the iterated local search meta-heuristic can be given in a nut-shell: one iteratively builds a sequence of solutions generated by the embedded heuristic, leading to far better solutions than if one were to use repeated random trials of that heuristic. Two main points in ILS are the following: (i) there must be a single chain that is being followed (this then excludes population-based algorithms); (ii) the search for

better solutions occurs in a reduced space defined by the output of a black box heuristic. In practice, local search has been the most frequently used embedded heuristic, but in fact any optimizer can be used, be it deterministic or not. The essential idea of ILS lies in focusing the search not on the full space of solutions but on a smaller subspace defined by the solutions that are locally optimal for a given optimization engine. The purpose of this review is to give a detailed description of iterated local search and to show where it stands in terms of performance. So far, in spite of its conceptual simplicity, it has led to a number of state-of-the-art results without the use of too much problem-specific knowledge; perhaps this is because iterated local search is very malleable, many implementation choices being left to the developer. In what follows we will give a formal description of ILS and comment on its main components.

Procedure *Iterated Local Search*

s_0 = Generate Initial Solution

s^* = Local Search(s_0)

repeat

s' = Perturbation(s^*)

$s^{*'} = \text{Local Search}(s')$

$s^* = \text{Acceptance Criterion}(s^*, s^{*'})$

until termination condition met

end

ILS involves four main components:

1. Creating an initial solution;
2. A black-box heuristic that acts as a local search on the set S ;
3. The perturbation operator, which modifies a local solution;
4. The acceptance criterion, which determines whether or not a perturbed solution will become the starting point of the next iteration.

Local search applied to the initial solution s_0 gives the starting point s^* of the walk in the set S . Starting with a good s^* can be important if high-quality solutions are to be reached as fast as possible. The initial solution s_0 used in the ILS is typically found one of two

ways: a random starting solution is generated or a greedy construction heuristic is applied. A “random restart” approach with independent samplings is sometimes a useful strategy (in particular when all other options fail), it breaks down as the instance size grows because in that time the tail of the distribution of costs collapses. A greedy initial solution s_0 has two main advantages over random starting solutions: (i) when combined with local search, greedy initial solutions often result in better quality solutions s^* ; (ii) a local search from greedy solutions takes, on average, less improvement steps and therefore the local search requires less CPU time.

The current s^* , we first apply a change or perturbation that leads to an intermediate state s' (which belongs to S where S is set of all local optimum). Then Local Search is applied to s' and we reach a solution s'^* in S^* . If s'^* passes an acceptance test, it becomes the next element of the walk in S^* ; otherwise, one returns to s^* . The resulting walk is a case of a stochastic search in S^* , but where neighborhoods are never explicitly introduced. This iterated local search procedure should lead to good biased sampling as long as the perturbations are neither too small nor too large. If they are too small, one will often fall back to s^* and few new solutions of S^* will be explored. If on the contrary the perturbations are too large, s' will be random, there will be no bias in the sampling, and we will recover a random restart type algorithm will be recovered. In practice, much of the potential complexity of ILS is hidden in the history dependence. If there happens to be no such dependence, the walk has no memory: the perturbation and acceptance criterion do not depend on any of the solutions visited previously during the walk, and one accepts or not s'^* with a fixed rule. This leads to random walk dynamics on S^* that are “Markovian”, the probability of making a particular step from s_1^* to s_2^* depending only on s_1^* and s_2^* . Most of the work using ILS has been of this type, though the studies show unambiguously that incorporating memory enhances performance [Stutzle (1998)].

The main drawback of any local search algorithm is that, by definition, it gets trapped in local optima that might be significantly worse than the global optimum. The strategy employed by ILS to escape from local optima is represented by perturbations to the current local optima. The perturbation scheme takes a locally optimal solution, s^* , and produces another solution from which a local search is started at the next iteration. Hopefully, the perturbation will return a solution outside the basins of attraction of

previously visited local minima. That is, it will be “near” a previously unvisited local optimum. Choice of the correct perturbation scheme is of primary importance, because it has a great influence on the intensification/diversification characteristics of the overall algorithm. Generally, the local search should not be able to undo the perturbation; otherwise one will fall back into the local optimum just visited. Perturbation schemes are commonly referred to as “strong” and “weak”, depending on how much they affect the solution that they change. A perturbation scheme that is too strong has too much diversity and will reduce the ILS to an iterated random restart heuristic. A perturbation scheme that is too weak has too little diversity and will result in the ILS not searching enough of the search space. The perturbation scheme should be chosen in such a way that it is as weak as possible while still maintaining the following condition: the likelihood of revisiting the perturbed solution on the next execution of Local Search should be low [Lourenco et al. (2002)]. The strength should remain as low as possible to speed up execution time. The desired perturbation scheme will return a solution near a locally optimal value. If this is the case, the local search algorithm should take less time to reach the next locally optimal value. Components from other meta-heuristics can sometimes be incorporated into the perturbation phase. Battiti and Protasi (1997) proposed memory structures to control the perturbation. In doing so, one can force intensification when globally good values are reached and force diversification when the search stagnates in an area of the search space. Borrowing from Simulated Annealing [Kirkpatrick et al. (1983)], temperature controlled techniques have been used to force the perturbation to change in a deterministic manner. Basic variable neighborhood search employs a deterministic perturbation scheme. Just as perturbation can range from too much intensification (no perturbations) to too much diversification (perturb all elements of the solution), acceptance criterion choices affect the search in a similar way. The most dramatic acceptance criterion on the side of diversification is to accept all perturbed solutions. This type of practice can undermine the foundations of ILS, since it encourages a “random-walk” type search. Contrasting with this, the algorithm accepts only solutions that are improvements to the globally optimal value (a sort of greedy strategy). Many implementations of ILS employ this type of acceptance strategy [Rossi-Doria et al. (2002)]. This type of criterion, especially with a weak perturbation scheme, can restrict the search from escaping the current basin of attraction. Moreover, with this type of scheme the probability of reaching the same locally optimal value increases a trait that reduces the algorithm’s overall effectiveness. When the

search stagnated, the random restart is a good way to ensure some diversification and to counterbalance the (possible) negative effects of too greedy a search. Large perturbations are only useful if they can be accepted. This only occurs if the acceptance criterion is not too biased toward better solutions [Lourenco et al. (2001)]. Stutzle (1998) showed that acceptance criteria that accept some worse solutions outperform their best-only counterparts.

For what concerns the stopping rule, generally the algorithm executes until one of the following conditions is met:

- A fix number of cycle have finished ;
- The best solution has not changed for a predefined number of cycles;
- a solution has been found that is beyond some predefined threshold.

ILS has many of the desirable features of a meta heuristic: it is simple, easy to implement, robust, and highly effective. The essential idea of ILS lies in focusing the search not on the full space of solutions but on a smaller subspace defined by the solutions that are locally optimal for a given optimization engine. The success of ILS lies in the biased sampling of this set of local optima. How effective this approach turns out to be depends mainly on the choice of the local search, the perturbations, and the acceptance criterion. Interestingly, even when using the most naive implementations of these parts, ILS can do much better than random restart. But with further work so that the different modules are well adapted to the problem at hand, ILS can often become a competitive or even state of the art algorithm. This dichotomy is important because the optimization of the algorithm can be done progressively, and so ILS can be kept at any desired level of simplicity. This, plus the modular nature of iterated local search, leads to short development times and gives ILS an edge over more complex metaheuristics in the world of industrial applications. As an example of this, recall that ILS essentially treats the embedded heuristic as a black box; then upgrading an ILS to take advantage of a new and better local search algorithm is nearly immediate. Because of all these features, we believe that ILS is a promising and powerful algorithm to solve real world complex problems in industry and services, in areas ranging from finance to production management and logistics. Finally, notice that although all of the present review is given in the context of tackling combinatorial optimization problems, in reality much of what is covered can be extended in a straightforward manner to continuous optimization problems.

3.3 Maximin Latin Hypercube Designs:

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

$$d_{ij} = \|x_i - x_j\|_p, \quad (3.1)$$

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.

3.4 Definition of LHD:

A Latin Hypercube Design (LHD) is a statistical design of experiments, which was first defined in 1979 [McKay et al. (1979)]. An LHD of k -factors (dimensions) with N design points, $x_i = (x_{i1}, x_{i2}, \dots, x_{ik}) : i = 0, 1, \dots, N-1$, is given by a $N \times k$ -matrix (i.e. a matrix with N rows and k columns) \mathbf{X} , where each column of \mathbf{X} consists of a permutation of integers $0, 1, \dots, N-1$ (note that each factor range is normalized to the interval $[0, N-1]$) so that for each dimension j all $x_{ij}, i = 0, 1, \dots, N-1$ are distinct. We will refer to each row of \mathbf{X} as a (discrete) design point and each column of \mathbf{X} as a factor (parameter) of the design points. We can represent \mathbf{X} as follows:

$$\mathbf{X} = \begin{pmatrix} x_0 \\ \vdots \\ x_{N-1} \end{pmatrix} = \begin{pmatrix} x_{01} & \cdots & x_{0k} \\ \vdots & \cdots & \vdots \\ x_{(N-1)1} & \cdots & x_{(N-1)k} \end{pmatrix} \quad (3.2)$$

such that for each $j \in \{1, 2, \dots, k\}$ and for all $p, q \in \{0, 1, \dots, N-1\}$ with $p \neq q$: $x_{pj} \neq x_{qj}$ holds.

Given a LHD \mathbf{X} and a distance d ,

let $D = \{d(x_i, x_j) : 1 \leq i < j \leq N\}$.

Note that $|D| \leq \binom{n}{2}$. We define $D_r(\mathbf{X})$ as the r -th minimum distance in D , and $J_r(\mathbf{X})$ as the

number of pairs $\{x_i, x_j\}$ having $d(x_i, x_j) = D_r(\mathbf{X})$ in \mathbf{X} .

The maximin LHD problem aims at finding a LHD \mathbf{X}^* such that $D_1(\mathbf{X})$ is as large as possible. However, a search which only takes into account the D_1 values is certainly not efficient. Indeed, the landscape defined by the D_1 values is “too flat”. For this reason the search should be driven by other optimality criteria, which take into account also other values besides D_1 .

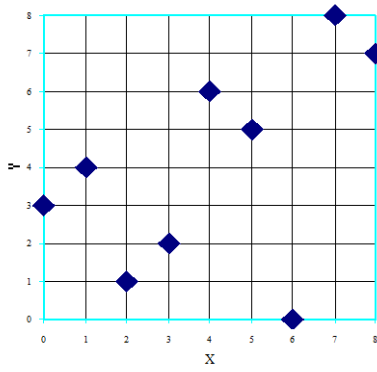


Fig: (a) $D_1^{(2)}(\mathbf{X}_r)=2, J_1^{(2)}(\mathbf{X}_r)=4$

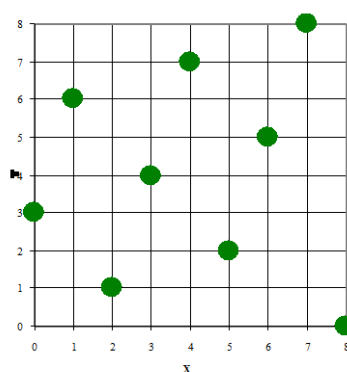


Fig: (b) $D_1^{(2)}(\mathbf{X}_{sm})=8, J_1^{(2)}(\mathbf{X}_{sm})=4$

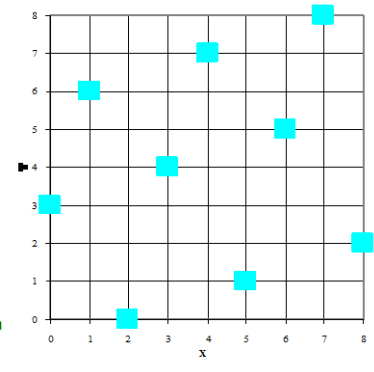


Fig (c) $D_1^{(2)}(\mathbf{X}_{sm})=11, J_1^{(2)}(\mathbf{X}_{sm})=10$

Figure 3.1: Some LHDs and their corresponding (D_1, J_1) values

3.5 Optimality Criteria for LHD

In order to optimized LHD an optimal criterion need to set for searching through LHDs. We consider the $\mathbf{Opt}(\phi, \mathbf{D}_1)$ criterion [Jamali (2009)] which is already shown in Chapter II.

3.6 ILS Approach for Maximin LHD

In Section 3.2 we have discussed a general scheme for ILS-based algorithms. Now we present the ILS based procedure for maximin Latin hypercube design. As we have stated earlier, the main components of ILS heuristic approaches are Initialization (I_S), LocalSearch (L_M), Perturbation Move (P_M), and the Stopping Rule (S_R).

The pseudo-code of the proposed ILS heuristic for maximin LHD problems is given below:

```

Step 1. Initialization :  $X = I_S(\{0, 1, \dots, N-1\})$ 
Step 2. Local Search :  $X^* = L_M(X)$ 
while  $S_R$  not satisfied do
Step 3. Perturbation Move :  $X' = P_M(X)$ 
Step 4. Local Search :  $X^* = L_M(X')$ 
Step 5. Improvement test : if  $X^*$  is better than  $X$ ,
set  $X = X^*$ 
end while
Return  $X$ 

```

Below we detail the components in order to fully specify the algorithm.

3.6.1 Initialization (I_S)

The initialization (I_S) procedure embedded in our algorithm is extremely simple: the first initial solution is randomly generated. In particular, the first initial solution generation is built as follows. For each component $h \in \{1, \dots, k\}$ a random permutation v_0, \dots, v_{N-1} of the integers $0, 1, \dots, N-1$ is generated and we set

$$x_{rh} = v_r \quad \text{for all } r \in \{0, \dots, N-1\}.$$

Although more aggressive procedures could be designed, we chose random generation because it is fast and unbiased.

3.6.2 Local Search Procedure (L_S)

In order to define a local search procedure (L_S), we need to define a concept of neighborhood of a solution. Given a LHD $\mathbf{X} = (x_1, \dots, x_N)$, its neighborhood is made of all other LHDs obtained by applying local moves to X . Before introducing some local moves, we first introduce the notion of critical point.

Critical point: We say that x_i is a critical point for \mathbf{X} , if

$$\min_{j \neq i} d(x_i, x_j) = D_1(X),$$

i.e., the minimum distance from x_i to all other points is also the minimum one among all the distances in \mathbf{X} . We denote by $I(\mathbf{X}) \subseteq \{1, \dots, N\}$ the set of indices of the critical points in X .

3.6.3 Local Moves (L_M):

A local move is an operator that applies some form of slight perturbation to a solution \mathbf{X} , in order to obtain a different solution. Different local moves define different

neighborhoods for local search. In the literature two different local moves are available: Rowwise-Pairwise (RP) exchange [Park (1994)] and Columnwise-Pairwise (CP) exchange [Morris and Mitchell (1995)]. In Park's algorithm [Park (1994)] some active pairs (pairs of critical points, in our terminology) are selected. Then, for each chosen pair of two active rows, say i_1 and i_2 , the RP exchange algorithm considers all the possible exchanges of corresponding elements as follows:

$$x_{i_1,p} \leftrightarrow x_{i_2,q} \quad \forall \quad p, q = 1, 2, \dots, k : p \neq q,$$

and finds the best exchange among them. The CP algorithm proposed by Morris and Mithchell (1995) exchanges two randomly selected elements within a randomly chosen column. But in [Li and Wu (1997)], Li and Wu defined the CP algorithm in a bit different way: they randomly choose a column and replace it by its random permutations if a better LHD is obtained.

It is observed that the effect of CP based local search and RP based local search is not significance [Jamali (2009)]. So, here, RP based local move is considered as defined in [Jamali (2009)] which is a bit different than that of [Park (1994)]. For optimal criteria we consider $\text{Opt}(\phi)$ optimal criteria.

The definition of Rowwise-Pairwise Critical Local Moves (we call it LM_{RPD_1}) as follows. The algorithm sequentially chooses two points (rows) such that at least one of them is a critical point, then exchanges two corresponding elements (factors) of the selected pair. If $i \in I(\mathbf{X})$, $r, j \in \{1, \dots, N\}$, $h, \ell \in \{1, \dots, k\}$, swapping the ℓ -th component gives the neighbor Y defined by

$$y_{rh} = \begin{cases} x_{rh} & \text{if } r \neq i \text{ or } h \neq \ell \\ x_{ih} & \text{if } r = j \text{ and } h = \ell \\ x_{jh} & \text{if } r = i \text{ and } h = \ell \end{cases} \quad (3.3)$$

It is remarked that, if $\text{Opt}(D_1, J_1)$ be the optimality criterion, it perfectly makes sense to avoid considering pairs x_i and x_j such that $I(X) \cap \{x_i, x_j\} = \emptyset$ since any swap involving two non-critical points cannot improve the D_1 value of the current LHD. When $\text{Opt}(\phi)$ is adopted as optimality criterion, any exchange can, in general, lead to an improved value of ϕ . The RP local move for $\text{Opt}(\phi)$ optimality criterion is denoted by $LM_{RP}\phi$ and is also defined as Eq. (3.8), the only difference being that we drop the requirement that at least one point must be critical.

We now illustrate the RP based local moves by considering a randomly generated initial design $A : (N ,k) = (7,2)$ (Figure 3.2(a)). Then a neighborhood solution of A , by considering points $(0,2)$, $(4,4)$ (here both are critical points), is LHD B , obtained after swapping the second coordinate of the points $(0, 2)$ and $(4,4)$ (Figure 3.2 (b)).

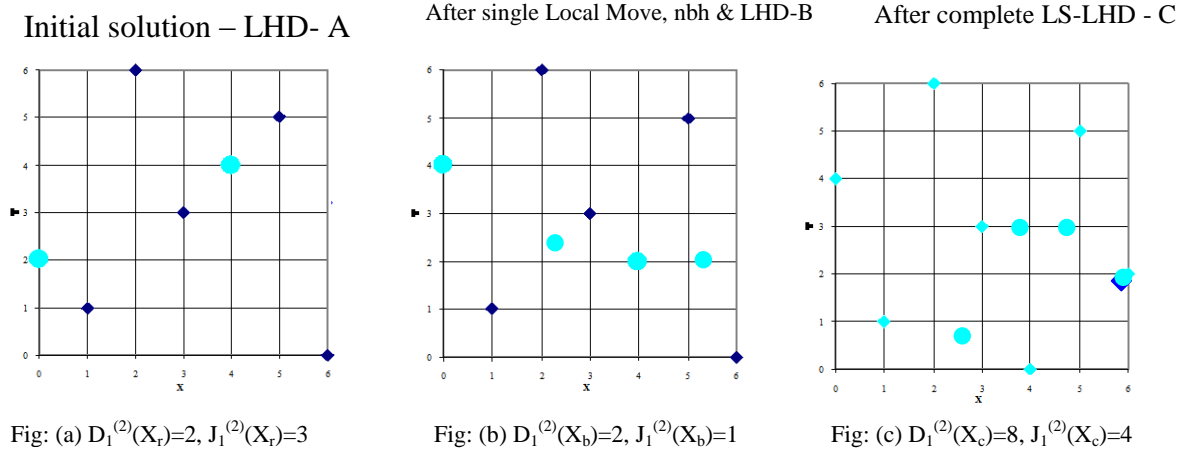


Figure 3.2: Illustration of Neighborhood solutions for Local search procedure of ILS approach

Also note that LHD B is an improving neighbor of LHD A , since $(D_1, J_1)(B) = (2,1)$ whereas $(D_1, J_1)(A) = (2,3)$. Finally Figure 3.2 (c) shows the maximin LHD produced by the Local search procedure. Though by considering Euclidean Distance the algorithm has optimized the LHD, but the LHD is improved regarding Manhattan distance too (see in the figures).

3.6.4 Acceptance Rule:

Among the two type of local moves [Jamali (2009)], we considered Best Improve (BI) acceptance rule as there are no significant difference regarding output [Jamali (2009)]. For the BI acceptance rule, the whole neighborhood of the current solution is searched for the best improving neighbor. We warn again the reader that the meaning of “ Y is better than X ” can be defined accordingly with the $Opt(D_1, J_1)$ or $Opt(\phi)$ optimality criterion. So for the $Opt(D_1, J_1)$ optimality criterion: “ Y is better than X ” if

$$D_1(Y) > D_1(X) \text{ or } (D_1(X) = D_1(Y) \text{ and } J_1(X) > J_1(Y)).$$

On the other hand for $Opt(\phi)$ optimality criterion : “ Y is better than X ” if

$$\phi_p(\mathbf{Y}) < \phi_p(\mathbf{X}),$$

where ϕ_p is defined by (2.5).

3.6.5 Perturbation Move (P_M)

Perturbation is the key operator in ILS, allowing the algorithm to explore the search space by jumping from one local optimum to another. Basically, a perturbation is similar to a local move, but it must be somehow less local, or, more precisely, it is a move within a neighborhood larger than the one employed in the local search. Actually the perturbation operator produces the initial solutions for all the local searches after the first one. Among the two types of perturbation operators, say, (i) Cyclic Order Exchange (COE) and (ii) Pairwise Crossover (PC) proposed in [Jamali (2009)], we consider here COE.

(i) **Cyclic Order Exchange (COE):** Our first perturbation move procedure is Cyclic Order Exchange (COE). The operator COE produce a cyclic order exchange upon a randomly selected single component (column) of a randomly selected portion of the design points (rows). Among the three variant of COE perturbation move techniques: Single Cyclic Order Exchange (SCOE) perturbation operation, Multiple Components Cyclic Order Exchange (MCCOE), and Multiple Single Cyclic Order Exchange (MSCOE) [Jamali (2009)], we consider here only SCOE technique.

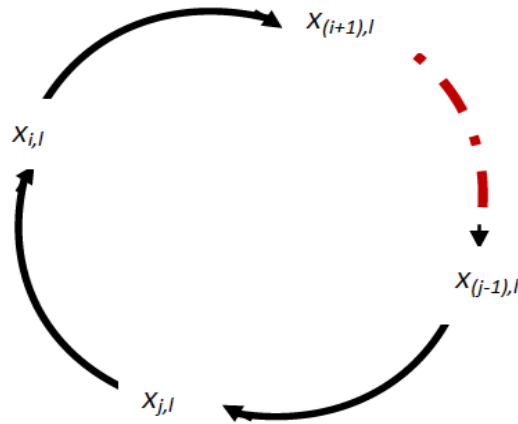


Fig. 3.3: Illustration of Cyclic Order Exchange perturbation technique

(ia) **Single Cyclic Order Exchange (SCOE):** For SCOE, we randomly choose two different rows (points), say x_i and x_j , such that $i < j$ and $j - i \geq 2$, in the current LHD \mathbf{X}^* .

Then, we randomly choose a column (component), say ℓ . Finally, we swap in cyclic order the value of component ℓ from point x_i to point x_j . See Fig -3.3. The pseudo-code structure for SCOE is the following.

- Step 1: randomly select two different points x_i and x_j
such that $i < j$ and $j - i \geq 2$
- Step 2: Randomly choose a component ℓ
- Step 3a: set temporarily $x_j^\ell = x_i^\ell$
for $t = j, j - 1, \dots, i + 1$ **do**
- Step 3b: Replace the component $x(t)\ell$ by $x(t-1)\ell$
end for
- Step 3c: and replace x_i^ℓ by x_j^ℓ

Note that we require $j - i \geq 2$ because otherwise the perturbation would be a special case of the local move employed in the local search procedure. We illustrate the SCOE perturbation by an example. Assume we have the current LHD \mathbf{X}^* with $N = 7$ and $k = 8$

$$\mathbf{X}^* = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 2 & 3 & 4 & 5 & 6 & 2 \\ 1 & 2 & 3 & 4 & 5 & 6 & 0 & 1 \\ 2 & 3 & 4 & 5 & 6 & 0 & 1 & 3 \\ 3 & 4 & 5 & 6 & 0 & 1 & 2 & 4 \\ 4 & 5 & 6 & 0 & 1 & 2 & 3 & 0 \\ 5 & 6 & 0 & 1 & 2 & 3 & 4 & 5 \\ 6 & 0 & 1 & 2 & 3 & 4 & 5 & 6 \end{pmatrix} \quad (3.4)$$

Now we randomly choose two rows (points), say x_2 and x_6 and we randomly choose the column (component) $\ell = 4$. Then, after the SCOE perturbation we get the following LHD \mathbf{X}' (bold faces denote the values modified with respect to \mathbf{X}^*),

$$\mathbf{X}' = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 2 & 3 & 4 & 5 & 6 & 2 \\ 1 & 2 & 3 & \mathbf{1} & 5 & 6 & 0 & 1 \\ 2 & 3 & 4 & \mathbf{4} & 6 & 0 & 1 & 3 \\ 3 & 4 & 5 & \mathbf{5} & 0 & 1 & 2 & 4 \\ 4 & 5 & 6 & \mathbf{6} & 1 & 2 & 3 & 0 \\ 5 & 6 & 0 & \mathbf{0} & 2 & 3 & 4 & 5 \\ 6 & 0 & 1 & 2 & 3 & 4 & 5 & 6 \end{pmatrix} \quad (3.5)$$

Note that SCOE only slightly modifies the current LHD \mathbf{X}^* but this exactly follows the spirit of ILS, where the perturbation should keep unchanged large portions of the current solution and should not completely disrupt its structure.

(ii) Pairwise Crossover: The second type of perturbation move that we consider is the Pairwise Crossover (PC). It is similar to biological crossover. we randomly select two points (rows) and then randomly selected portions of them which are interchanged. Here we propose three variant of PC namely Single Pair Crossover (SPC) and Multiple Pair Crossover (MPC) and Critical-point Far-most Pair crossover (CFPC).

(ii.a) Single Pair Crossover (SPC): For SPC, we first randomly select two rows, say, x_i and x_j , $i \neq j$, in the current LHD \mathbf{X}^* ; then we randomly select a component, say $l \geq 2$. Finally all the components $1, \dots, l$ of x_i are swapped with the corresponding components of x_j —refer to Figure 3.4. Note that we require $l \geq 2$, since otherwise it would be a single local move. It is also worthwhile to remark that the PC perturbation is meaningful only when number of factors of the LHD is greater than three. The pseudo code structure of SPC is as follows:

```

Step 1: randomly select two different points  $x_i$  and  $x_j$  such that  $i \neq j$ 
Step 2: Randomly choose a component  $l$  such that  $l \geq 2$ 
for  $k = 1, \dots, l$  do
Step 3: swap  $(x_{ik}, x_{jk})$ 
end for

```

$$\mathbf{X}^* = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 2 & 3 & 4 & 5 & 6 & 2 \\ 1 & 2 & 3 & 4 & 5 & 6 & 0 & 1 \\ 2 & 3 & 4 & 5 & 6 & 0 & 1 & 3 \\ 3 & 4 & 5 & 6 & 0 & 1 & 2 & 4 \\ 4 & 5 & 6 & 0 & 1 & 2 & 3 & 0 \\ 5 & 6 & 0 & 1 & 2 & 3 & 4 & 5 \\ 6 & 0 & 1 & 2 & 3 & 4 & 5 & 6 \end{pmatrix}$$

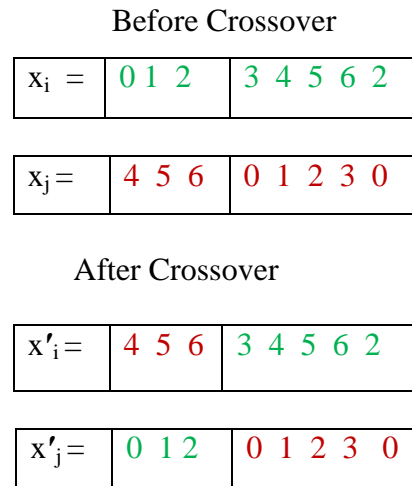


Fig. 3.4: Illustration of Single Pair Crossover perturbation technique

3.6.6 Stopping Rule (S_R)

We use a very simple stopping Rule (S_R). We introduce an integer parameter called Max Non-Imp (MNI) and the algorithm will stop if the currently best local optimizer \mathbf{X}^* cannot be improved for Max Non-Imp consecutive perturbations.

CHAPTER IV

EXPERIMENTS ON OPTIMAL LHDS REGARDING EUCLIDEAN MEASURE

4.1 Introduction

In this chapter we will discuss about the optimal maximin LHDS obtained by ILS approach in Euclidean distance measure and comparison with existence literatures. At first we will display the optimal LHDS to show the performance of ILS approach regarding Euclidean distance measure.

4.2 Experimental Results and Discussion for Euclidean Measure

At first we will compare the performance of several approaches available in the literature regarding maximin LHDS namely maximin LHDS obtained by ILS approach [Grosso et al. (2009)] and denoted by MLH-ILS; maximin LHDS obtained by Periodic design (PD) approach [Husslage et al. (2006)] and denoted by MLH-PD; maximin LHDS obtained by Simulated Annealing (SA) approach [Husslage et al. (2006)] and denoted by MLH-SA, maximin LHDS obtained by Simulated Annealing (SA_M) approach [Morris and Mitchel (1995)] and denoted by MLH-SA_M and maximin LHDS obtained by Enhanced Stochastic Evolutionary (ESE) algorithm [Husslage et al. (2011)] which is first proposed by Jin et al. (2005) and the designs are denoted by MLH_ESE.

It is noted that the best maximin LHDS are frequently update in the website <https://spacefillingdesigns.nl/> (2008) and we denote it as Best-Web. It will be worthwhile to mention here that we compare maximin LHDS of website during 2009 rather than recent update value (like 2016). We do so because at 2009 the website is updated by taking the values obtained by ILS approach [Grosso et al. (2009)] and accept few values MLH_ILS values reveal best till to date. For the comparison study we consider all designs with $\{(k, N) : k = 3, \dots, 10 ; N = 2, \dots, 100\}$. In the tables the head line of each design is shorted as MLH_ESE to ESE and so on. The experimental results are reputed in the Table 4.1 and Table 4.2.

Table 4.1: Comparison among PD, SA, ESE and ILS approaches regarding maximin LHDs in Euclidean distance measure for $k=3-6$

N	k=3				k=4				k=5				k=6			
	PD	SA	ESE	ILS	PD	SA	ESE	ILS	PD	SA	ESE	ILS	PD	SA	ESE	ILS
2	3	3	3	3	4	4	4	4	5	5	5	5	6	6	6	6
3	3	6	6	6	4	7	7	7	5	8	8	8	6	12	12	12
4	6	6	6	6	12	12	12	12	11	14	14	14	15	20	20	20
5	6	11	11	11	12	15	15	15	11	24	24	24	15	27	27	27
6	14	14	14	14	16	22	22	22	23	32	32	32	28	40	40	40
7	14	17	17	17	16	28	28	28	23	40	40	40	28	52	52	52
8	21	21	21	21	25	42	42	42	32	50	50	50	42	66	66	66
9	21	22	22	22	25	42	42	42	39	61	61	61	45	76	76	76
10	21	27	27	27	36	50	47	50	55	82	82	82	62	91	91	92
11	24	30	30	30	39	55	55	55	55	80	80	80	62	108	108	110
12	30	36	36	36	46	63	63	63	62	91	91	93	91	136	136	139
13	35	41	41	41	51	68	70	70	64	101	103	104	91	136	138	140
14	35	42	42	42	70	75	77	79	86	112	114	116	104	152	154	160
15	42	48	48	48	71	83	87	89	88	124	129	131	111	167	171	175
16	42	50	50	50	85	90	93	94	101	136	151	154	130	186	190	194
17	42	53	53	53	85	97	99	103	113	150	158	159	131	203	208	214
18	50	56	56	57	94	103	108	111	123	162	170	172	155	223	231	241
19	57	59	59	62	94	113	119	122	136	174	184	189	169	241	256	263
20	57	62	65	66	106	123	130	137	139	184	206	206	210	260	279	285
21	65	66	68	69	116	127	145	149	165	201	223	229	210	283	302	306
22	69	69	72	76	117	137	150	151	174	215	235	242	223	304	325	338
23	72	74	75	77	130	146	159	161	178	224	250	251	236	324	348	358
24	76	78	81	83	138	154	170	170	201	242	266	269	258	343	374	378
25	91	81	86	86	156	162	178	181	205	255	285	286	286	368	400	408
26	91	86	86	86	156	171	188	189	226	269	302	306	296	387	426	439
27	91	90	90	90	157	178	198	198	238	287	310	326	310	410	447	474
28	94	94	94	94	174	188	210	212	258	302	331	349	339	427	479	494
29	94	98	101	101	174	196	221	219	269	322	349	373	346	452	507	517
30	105	102	105	105	194	209	233	230	310	335	367	403	390	473	531	545
31	107	106	110	110	212	215	244	240	310	347	405	406	390	504	563	569
32	114	110	110	116	212	228	253	252	341	371	413	418	419	529	587	599
33	114	113	117	120	215	234	264	267	341	379	426	446	430	548	622	634
34	133	117	125	126	230	244	273	274	358	403	445	460	470	586	648	668
35	133	122	126	129	234	255	286	289	366	418	467	482	495	601	683	697
36	133	129	131	136	250	261	297	298	400	427	486	502	518	631	719	739
37	152	131	138	140	266	275	309	308	408	454	520	530	528	648	744	775
38	152	134	142	142	283	279	321	322	415	464	541	557	561	681	788	813
39	152	139	146	149	283	290	330	330	439	486	566	575	561	706	816	846
40	155	146	152	152	291	301	342	345	492	505	575	590	632	739	876	886
41	162	147	158	155	293	309	355	354	492	525	596	618	632	776	882	938
42	168	152	161	162	319	325	367	371	496	543	626	641	670	791	907	988
43	168	157	171	169	323	329	383	378	520	558	666	664	670	830	947	996
44	186	161	179	178	331	349	396	393	548	582	680	688	696	862	992	1041
45	186	166	182	179	347	362	407	405	565	615	698	706	737	891	996	1065
46	186	169	189	185	366	370	421	421	592	615	723	728	797	918	1064	1107
47	186	173	189	189	378	378	438	426	611	634	754	762	797	940	1088	1113
48	189	178	201	194	413	385	450	451	632	673	763	782	857	976	1119	1159
49	196	180	203	201	415	399	464	463	634	680	803	799	893	1015	1167	1181
50	213	185	206	206	415	414	478	473	663	699	830	830	893	1042	1203	1218
51	213	189	206	209	421	426	490	487	692	727	850	857	917	1067	1230	1258
52	213	198	217	214	455	429	504	501	709	742	883	874	1003	1100	1274	1292
53	216	200	219	221	455	447	515	516	716	765	894	901	1003	1136	1340	1340
54	233	213	209	227	477	454	534	526	760	783	932	935	1019	1171	1359	1392
55	243	214	230	233	483	477	546	541	760	805	956	966	1082	1198	1421	1432
56	243	216	230	235	515	479	558	565	784	830	982	992	1104	1236	1431	1484
57	261	221	249	241	515	490	574	570	846	854	1007	1018	1136	1265	1488	1523
58	261	227	245	246	539	500	594	591	846	878	1035	1046	1166	1303	1554	1559
59	266	229	254	254	544	519	609	607	849	905	1063	1064	1223	1328	1564	1615
60	273	237	261	258	568	530	618	622	904	928	1094	1101	1242	1381	1631	1647
61	274	244	266	262	620	538	630	640	941	939	1128	1134	1258	1413	1667	1703
62	283	245	269	269	620	554	657	645	934	991	1150	1156	1306	1450	1715	1756
63	297	249	281	276	620	575	670	666	967	989	1178	1187	1380	1497	1781	1781
64	297	258	278	281	625	579	684	678	985	1009	1206	1223	1430	1526	1804	1834
65	314	260	290	286	630	582	694	701	997	1035	1216	1239	1430	1565	1868	1884
66	314	269	299	294	666	602	718	706	1050	1051	1261	1272	1476	1590	1874	1926
67	314	270	294	297	666	614	735	726	1072	1085	1299	1283	1482	1646	1954	1977
68	314	278	306	306	685	623	746	738	1087	1119	1330	1360	1538	1664	1983	2014
69	324	280	306	310	698	650	765	754	1112	1114	1351	1399	1588	1704	2028	2070
70	325	285	314	313	716	658	779	773	1150	1135	1378	1439	1633	1759	2094	2116
71	325	289	314	325	716	665	793	795	1150	1187	1413	1416	1644	1783	2141	2168
72	341	296	314	326	750	678	810	810	1203	1197	1430	1454	1768	1862	2136	2215
73	350	299	329	329	759	688	834	818	1229	1242	1462	1549	1768	1872	2197	2252
74	350	306	341	341	767	703	842	845	1229	1269	1512	1562	1774	1910	2291	2299
75	350	310	341	345	771	714	867	854	1274	1282	1530	1571	1862	1963	2303	2365
76	363	324	341	349	813	750	882	877	1300	1318	1569	1597	1935	2024	2387	2415
77	363	325	341	355	823	762	894	890	1308	1331	1591	1631	1947	2051	2433	2456
78	387	337	371	362	844	761	910	906	1382	1360	1621	1654	2014	2079	2479	2502
79	387	333	374	376	848	788	927	921	1382	1399	1639	1668	2037	2120	2498	2550
80	403	344	374	371	873	786	949	943	1395	1430	1691	1690	2037	2152	2554	2597
81	406	338	381	381	916	782	963	972	1406	1431	1730	1731	2064	2217	2648	2665
82	406	353	374	389	938	825	989	979	1475	1482	1742	1773	2141	2239	2680	2715
83	417	369	374	401	940	829	1002	1006	1501	1509	1762	1804	2141	2290	2696	2752
84	426	363	406	401	967	838	1021	1015	1534	1510	1818	1825	2229	2325	2790	2803
85	426	369	413	406	967	877	1043	1032	1552	1566	1866	1871	2232	2399	2819	2877
86	428	376	413	422	967	867	1053	1047	1573	1578	1882	1890	2375	2437	2875	2929
87	428	374	413	419	976	877	1073	1062	1598	1589	1934	1922	2375	2476	2913	2988
88	437	374	434	426	1050	890										

Table 4.2: Comparison among PD, SA, ESE and ILS approaches regarding maximin LHDs in Euclidean distance measure for $k=7-10$

N	PD	$k=7$			$k=8$			$k=9$			$k=10$		
		SA	ESE	ILS	SA	ESE	ILS	SA	ESE	ILS	SA	ESE	ILS
2	7	7	7	7	8	8	8	9	9	9	10	10	10
3	7	13	13	13	14	14	14	18	18	18	19	19	19
4	16	21	21	21	26	26	26	28	28	28	33	33	33
5	16	32	32	32	40	40	40	43	43	43	50	50	50
6	29	47	47	47	54	53	54	61	61	61	68	68	68
7	31	61	61	61	70	70	71	80	80	81	89	89	90
8	46	79	79	79	91	90	91	101	101	102	114	114	114
9	47	92	92	93	112	112	113	126	126	128	141	142	143
10	68	110	109	111	130	131	133	154	154	157	172	171	174
11	69	128	129	132	152	152	154	178	178	181	206	206	209
12	95	150	152	155	176	177	181	204	204	209	235	235	240
13	95	174	178	181	202	205	210	232	235	242	267	268	275
14	119	204	215	217	228	236	243	265	268	278	298	305	313
15	129	211	220	223	257	273	280	296	309	318	337	347	358
16	155	238	241	249	286	317	326	330	352	358	378	393	406
17	161	256	266	272	312	332	332	367	396	405	415	442	458
18	186	281	291	298	344	361	368	398	451	466	458	496	509
19	195	305	323	326	370	390	398	438	469	472	498	554	569
20	226	332	349	360	403	425	434	472	506	517	542	625	641
21	236	361	380	393	438	463	471	517	548	559	592	650	650
22	270	384	418	425	467	501	508	555	595	614	643	691	704
23	273	410	448	454	501	542	549	596	640	651	685	747	750
24	308	444	481	492	538	585	595	639	690	699	739	800	818
25	350	467	520	531	583	626	637	688	739	752	792	857	875
26	365	499	548	570	612	664	688	726	791	810	854	910	931
27	382	526	585	599	648	712	738	780	840	859	896	976	1002
28	406	561	620	634	693	766	785	826	898	919	953	1041	1061
29	417	593	654	675	733	817	837	876	956	986	1015	1100	1132
30	458	620	691	714	787	849	897	925	1019	1041	1086	1173	1207
31	482	657	728	764	812	900	931	976	1104	1104	1138	1241	1275
32	518	695	778	803	866	966	976	1026	1139	1176	1194	1318	1351
33	537	723	814	844	900	1010	1037	1084	1201	1244	1253	1396	1436
34	561	751	851	891	945	1072	1089	1135	1270	1316	1329	1478	1514
35	586	811	914	934	1002	1113	1151	1190	1326	1398	1398	1555	1595
36	636	831	939	968	1042	1181	1205	1257	1405	1444	1459	1647	1679
37	668	863	976	1012	1079	1236	1272	1300	1477	1505	1516	1721	1761
38	709	923	1028	1055	1127	1286	1328	1367	1534	1577	1597	1790	1852
39	726	938	1084	1094	1192	1344	1397	1434	1609	1640	1665	1870	1987
40	786	970	1122	1148	1224	1416	1459	1489	1675	1728	1742	1946	2101
41	802	1016	1156	1197	1271	1496	1535	1562	1765	1793	1820	2058	2135
42	903	1064	1209	1249	1333	1526	1584	1639	1843	1871	1920	2149	2191
43	903	1112	1256	1301	1377	1597	1635	1683	1905	1957	1973	2224	2279
44	903	1140	1336	1340	1463	1653	1698	1752	1994	2042	2072	2319	2373
45	926	1192	1366	1408	1480	1723	1755	1820	2079	2126	2130	2415	2466
46	985	1243	1408	1448	1548	1794	1819	1906	2155	2220	2208	2507	2568
47	985	1268	1459	1521	1616	1847	1883	1958	2244	2312	2331	2600	2663
48	1054	1325	1531	1578	1658	1924	1957	2017	2336	2383	2387	2732	2760
49	1074	1356	1592	1649	1729	1989	2018	2103	2397	2470	2470	2828	2880
50	1113	1397	1639	1699	1772	2041	2089	2179	2492	2569	2556	2893	2991
51	1161	1450	1662	1744	1855	2132	2152	2243	2566	2637	2639	3006	3090
52	1231	1486	1734	1804	1888	2203	2218	2325	2686	2716	2745	3134	3202
53	1241	1537	1808	1886	1949	2234	2288	2429	2713	2798	2825	3261	3306
54	1288	1577	1856	1932	2006	2356	2383	2473	2805	2884	2892	3339	3412
55	1325	1639	1896	2000	2084	2429	2462	2570	2935	2996	3054	3452	3530
56	1358	1701	2003	2073	2162	2444	2533	2623	3021	3060	3100	3551	3643
57	1479	1721	2024	2098	2194	2554	2620	2704	3119	3162	3215	3651	3767
58	1479	1795	2043	2156	2258	2650	2679	2796	3187	3268	3305	3795	3843
59	1509	1821	2136	2187	2356	2733	2793	2881	3297	3350	3399	3889	3977
60	1577	1899	2232	2277	2393	2796	2873	2939	3420	3446	3500	4090	4109
61	1615	1928	2266	2316	2488	2868	2966	3021	3525	3565	3588	4158	4202
62	1680	2023	2345	2367	2541	2977	3048	3132	3636	3651	3700	4313	4322
63	1680	2035	2376	2417	2607	3056	3160	3215	3690	3760	3767	4355	4445
64	1769	2093	2452	2484	2734	3097	3207	3292	3820	3868	3955	4514	4560
65	1786	2132	2492	2547	2723	3219	3286	3357	3932	3991	4034	4581	4695
66	1857	2180	2543	2606	2841	3279	3418	3474	4004	4088	4143	4769	4818
67	1868	2238	2638	2672	2868	3399	3488	3543	4081	4200	4224	4942	4981
68	1940	2295	2693	2714	2956	3453	3600	3647	4212	4317	4360	4995	5077
69	1965	2351	2746	2794	3075	3520	3704	3716	4317	4400	4455	5127	5221
70	2130	2417	2838	2856	3130	3588	3779	3841	4464	4516	4539	5276	5366
71	2130	2451	2871	2939	3161	3749	3877	3936	4548	4666	4689	5437	5479
72	2177	2503	2960	2992	3220	3810	3962	4027	4666	4758	4812	5556	5625
73	2206	2598	3042	3077	3305	3932	4009	4134	4776	4858	4873	5661	5746
74	2244	2614	3120	3117	3432	3941	4127	4224	4915	4997	5038	5817	5879
75	2295	2703	3157	3230	3513	4073	4213	4298	5006	5141	5171	5937	6015
76	2375	2756	3218	3289	3559	4178	4326	4395	5179	5261	5254	6111	6163
77	2403	2819	3323	3359	3617	4266	4384	4492	5222	5364	5399	6272	6305
78	2505	2870	3387	3432	3684	4390	4491	4577	5385	5543	5489	6384	6449
79	2525	2950	3474	3488	3775	4465	4585	4705	5535	5631	5633	6466	6580
80	2590	2979	3550	3564	3877	4565	4695	4807	5577	5792	5773	6653	6733
81	2642	3086	3619	3638	4001	4679	4721	4888	5748	5922	5901	6780	6842
82	2753	3118	3669	3727	3998	4719	4809	5030	5859	6041	6013	6935	7041
83	2767	3195	3723	3800	4076	4848	4906	5102	5976	6196	6097	7094	7258
84	2838	3227	3870	3883	4183	4920	5006	5222	6119	6357	6273	7256	7362
85	2874	3299	3919	3954	4324	5032	5110	5340	6212	6479	6397	7357	7508
86	3103	3335	3958	4032	4397	5164	5205	5423	6346	6606	6491	7532	7687
87	3103	3450	4095	4119	4474	5225	5302	5538	6469	6761	6622	7639	7837
88	3183	3500	4166	4199	4524	5340	5426	5667	6660	6873	6803	7877	8022
89	3183	3541	4176	4290	4578	5450	5515	5774	6750	7004	6872	7950	8151
90	3190	3661	4308	4362	4699	5576	5608	5832	6901	7152	7040	8128	8325
91	3234	3677	4379	4423	4850	5626	5696	5969	6950	7296	7163	8330	8464
92	3277	3760	4428	4526	4873	5758	5822	6081	7067	7396	7286	8442	8681
93	3361	3811	4512	4574	4984	5832	5925	6231	7342	7446	7488	8601	8828
94	3474	3888	4581	4675	5067	6007	6032	6329	7436	7642	7536	8774	9066
95	3531	3940	4703	4758	5154	6064	6148	6396	7469	7748	7741	8877	9252
96	3639	4070	4808	4862	5220	6222	6277	6516	7645	7926	7777	9146	9445
97	3639	4069	4848	4919	5316	6304	6364	6649	7781	8011	8038	9379	9550
98	3690	4147	4936	5007	5445	6376	6467	6776	7896	8152	8242	9381	9820
99	3731	4214	4999	5117	5477	6448	6571	6912	8023				

To see the performance of each approaches at a glance, we summarized the above results in Table 4.3. In the Table 4.3, identical means the maximin LHDs obtained by ILS approach is identical compare to the best known results available in the literature whereas worse means the maximin LHDs obtained by ILS approach are worse compare to best known results. Notice that the maximin LHDs obtained by SA_M approach are not reported in the Table 4.1 and Table 4.2 as there are few values available in the literature [Morris and Mitchel (1995)] and all of which are worse with respect to MLH_ILS [Jamali (2009)] as shown in the Table 4.3. Moreover in the Table 4.2 the maximin LHDs obtained by ESE approach are not reported in Table 4.2. As ESE approach performs relatively better compare to PD or SA, so we will compare ILS with ESE separately. It is observed that except dimension $k = 3$, in which PD performs better, ILS outperforms compared to other approaches considered. We observe that ILS is able to detect a very large amount of improved solutions with respect to the best known ones. This is, especially, true at large k values. For $k \geq 6$, with the exception of few numbers of N values, all the solutions returned by ILS are better compare to the best known results. It is worthwhile to remark that for large (k, N) values the improvement of each LHD obtained by ILS approach is very significance.

Table 4.3: the comparison among several approaches for finding maximin LHDs for $N=2$ to 100 in each dimension k

k	Number of best			<i>Web</i>	<i>ILS</i>	Identical	Worse
	<i>PD</i>	<i>SA</i>	<i>SA_M</i>			<i>ILS</i>	<i>ILS</i>
3	61	0	0	65	14	20	65
4	02	0	0	47	34	18	47
5	00	0	0	11	78	10	11
6	00	0		00	90	09	00
7	00	0		00	92	07	00
8		0		00	93	06	00
9		0		00	93	06	00
10		0		00	92	07	00

Though the performance of ILS approach is significantly better compare to other approaches consider here, but the approach will be effective if it is efficient i.e. the algorithm performs the job within acceptable time. So it is needed to comment about the computation times. It is worthwhile to mention here that there is no information regarding

times to obtain the Web's results. Anyway for this demand, the computational cost of the approaches is reported in the Table 4.4. It is noted that the elapsed time of ESE approach is not available. It is, however, quite clear that ILS is more computationally demanding with respect to PD and SA. Such higher costs are clearly rewarded in terms of quality of the results but the quality of the results might be wondered if the time restrictions are imposed on ILS. According to some further experiments that were performed, it would be realized that, especially at large k values, equivalent or better results with respect to the PD and SA ones, could quickly be reached by ILS [Jamali (2009)]. Therefore, it seems that at large k values even few and short runs of ILS are able to deliver results better than those reached by PD and SA. That is ILS approach outperforms compare to other approaches considered regarding L^2 distance measure.

Table 4.4: Comparison of computational cost

Total Elapsed Time (hrs)			
k	PD	SA	ILS
3	145	500	164
4	61	181	507
5	267	152	767
6	108	520	1235
7	232	246	698
8	--	460	846
9	--	470	1087
10	--	470	1166

Now we will compare the performance of ILS with respect to ESE regarding maximin LHDs by summing the above maximin LHDs values for ILS and ESE approach. Table 4.5 displays the intimate comparison between ILS and ESE approach regarding maximin LHD's values. It is observed that except dimension 4, in which performance of both approaches are comparable, ILS always outperforms significantly. Moreover we notice that for $k > 5$, the almost all maximin LHDs obtained by ILS approach are the better.

Table 4.5: Comparison between ESE and ILS regarding Maximin LHDS

$N=2,\dots,100$	No. of Best LHDS in	
	ESE	ILS
3	24	43
4	45	35
5	11	77
6	0	92
7	1	91
8	0	92
9	0	93
10	0	92

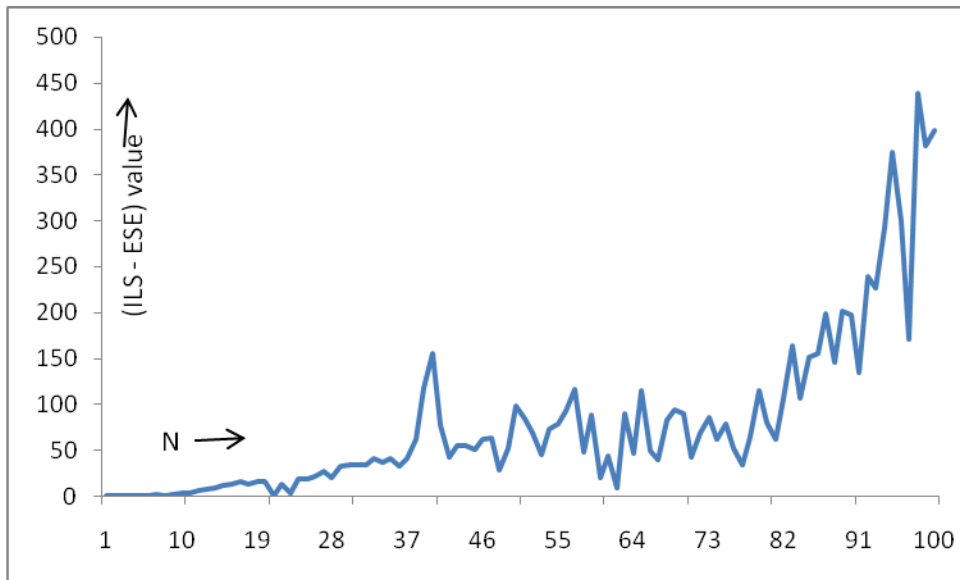


Figure 4.1 Effect of N on the performance of ILS approach upon ESE approach for $k = 10$

Now what are the effects of increasing of N on the performance of ILS approach upon ESE approach is depicted in the Figure 4.1. For this contest we consider $k = 10$ and $N = 2, \dots, 100$. In the Figure 4.1 the horizontal line indicates N (number of design point) and vertical line indicates the difference between the D_1 value of MLH_{ILS} and MLH_{ESE} ($MLH_{ILS} - MLH_{ESE}$). It is observed in the figure that there is a significant effect on

N. For the increasing of N , ILS approach find out much better LHDs compare to ESE approach. From the above discussion it is clear that ILS approach is state-of arts regarding maximin optimality in Euclidian distance measure as well as computational cost.

CHAPTER V

EXPERIMENTS ON OPTIMAL LHDS REGARDING AUDZE-EGLAIS DISTANCE MEASURE

5.1 Introduction

In chapter IV, we have performed experiments to analyse the effectiveness and robustness of ILS approach on the basis of maximin LHDS on (ϕ_p, D_1) optimal criterion in which pair-wise distances of points are measured by square of L^2 distance measure. On the basis of those experimental study we may conclude that ILS outperforms to find maximin LHDS measured L^2 distance measure by taking (ϕ_p, D_1) optimal criterion. Anyway in the literature there exist several types of optimal LHDS according to different kind of optimal criteria as well as distance measure considered. Here we will perform several experiments in this contest.

5.2 Experiments on individual optimal LHD for details characteristics

0	4	8	5	2	10
1	3	4	9	5	0
2	6	1	4	11	8
3	10	6	0	4	2
4	11	9	10	8	6
5	2	11	3	10	4
6	9	0	8	1	7
7	0	2	1	3	5
8	1	5	11	7	9
9	5	10	7	0	3
10	8	7	2	6	11
11	7	3	6	9	1

0	7	1	4	9	3
1	0	8	5	7	9
2	10	11	8	5	5
3	5	2	10	0	7
4	3	7	2	1	0
5	9	5	0	3	10
6	2	6	11	8	1
7	8	4	9	10	11
8	6	9	1	11	4
9	1	0	3	6	6
10	11	3	6	4	2
11	4	10	7	2	8

To view the details characteristics of optimal LHD regarding both the maximin (ϕ_p, D^1) criterion and Audze-Eglais criterion, we have first considered LHD $(k, N) = (6, 12)$. Table

5.1 displays the optimal LHD regarding the maximin ϕ_p criterion obtained by ILS approach [Grosso et al. (2009)] and denoted as maximin LHD **A**. On the other hand Table 5.2 presents the optimal LHD regarding the Audze-eglais criterion obtained by Enhanced Stochastic Evolutionary (ESE) algorithm [Jin et al. (2005) and Husslage et al. (2011)] and denoted as Audze-eglais LHD **B**. In both the cases, Euclidian distance measure is used.

0	143	143	144	144	142	286	143	143	143	143	142
143	0	142	143	143	143	143	142	144	144	286	143
143	142	0	143	143	143	143	142	286	144	144	143
144	143	143	0	142	286	142	143	143	143	143	144
144	143	143	142	0	144	142	143	143	143	143	286
142	143	143	286	144	0	144	143	143	143	143	142
286	143	143	142	142	144	0	143	143	143	143	144
143	142	142	143	143	143	143	0	144	286	144	143
143	144	286	143	143	143	143	144	0	142	142	143
143	144	144	143	143	143	143	286	142	0	142	143
143	286	144	143	143	143	143	144	142	142	0	143
142	143	143	144	286	142	144	143	143	143	143	0

0	25	23	24	24	26	36	27	23	27	25	26
25	0	26	27	23	27	25	26	24	24	36	23
23	26	0	25	27	25	23	26	36	24	24	27
24	27	25	0	26	36	26	23	25	23	27	24
24	23	27	26	0	24	26	25	27	25	23	36
26	27	25	36	24	0	24	23	25	23	27	26
36	25	23	26	26	24	0	27	23	27	25	24
27	26	26	23	25	23	27	0	24	36	24	25
23	24	36	25	27	25	23	24	0	26	26	27
27	24	24	23	25	23	27	36	26	0	26	25
25	36	24	27	23	27	25	24	26	26	0	23
26	23	27	24	36	26	24	25	27	25	23	0

Now we have performed further experiments on both LHDs to find out the pair-wise distances of the design points in each distance measure namely L^1 and L^2 . The experimental results regarding LHD **A** are displayed in the Table 5.3 and 5.4. In Table 5.3 we have distance matrix **P** measured in Euclidean distance measure whereas in Table 5.4 we have distance matrix **Q** measured in Manhattan distance measure respectively.

Similarly performing experiments on LHD **B**, we have obtained the distance matrices **R** and **S** given in Table 5.5 and Table 5.6 regarding Euclidean and Manhattan distance measure respectively.

0	140	149	147	145	146	140	149	143	137	150	294
140	0	139	143	145	148	134	145	143	143	286	150
149	139	0	140	146	139	139	140	142	278	143	137
147	143	140	0	144	147	135	146	286	142	143	143
145	145	146	144	0	149	137	294	146	140	145	149
146	148	139	147	149	0	278	137	135	139	134	140
140	134	139	135	137	278	0	149	147	139	148	146
149	145	140	146	294	137	149	0	144	146	145	145
143	143	142	286	146	135	147	144	0	140	143	147
137	143	278	142	140	139	139	146	140	0	139	149
150	286	143	143	145	134	148	145	143	139	0	140
294	150	137	143	149	140	146	145	147	149	140	0

0	24	25	25	27	28	26	25	23	23	24	38
24	0	23	27	25	26	24	27	27	23	36	24
25	23	0	24	28	25	27	26	26	34	23	23
25	27	24	0	24	25	25	24	36	26	27	23
27	25	28	24	0	23	21	38	24	26	27	25
28	26	25	25	23	0	34	21	25	27	24	26
26	24	27	25	21	34	0	23	25	25	26	28
25	27	26	24	38	21	23	0	24	28	25	27
23	27	26	36	24	25	25	24	0	24	27	25
23	23	34	26	26	27	25	28	24	0	23	25
24	36	23	27	27	24	26	25	27	23	0	24
38	24	23	23	25	26	28	27	25	25	24	0

Now we have performed experiments on those distance matrices **P**, **Q**, **R** and **S** to find out some interesting characteristics of the LHD **A** and **B** respectively. The experimental results are shown in the Table 5.7. In the table “ D_{Max} ” means maximum pair-wise distance of design points in any LHD, “ J_{Max} ” means number of D_{Max} values in that LHD and “AE value” means Audze- Eglais distance value. As mentioned earlier that Euclidean distance measure is considered for the both optimal LHDs **A** and **B**. At first we will compare D_1J_1 value measured in L^2 distance measure of the two optimal LHDs. It is observed (in column

4) that Maximin LHD **A** is much better than Audze-Eglais LHD **B** regarding maximin value D_1J_1 in Euclidean measure (L^2) where LHD **A** is optimized regarding (ϕ_p, D_1) [Grosso et al. (2009)] optimal criterion by ILS approach and Audze-Eglais LHD **B** is optimized regarding Audze-Eglais criterion by ESE approach. Though Maximin LHD **A** is optimized regarding L^2 measure but in this experiment we notice that Maximin LHD **A** is better than Audze-Eglais LHD **B** regarding D_1J_1 value measured in Manhattan measure (L^1) too.

Table 5.7: Comparison of Maximin LHD **A** and Audze-Eglais LHD **B** in various aspects regarding ILS and ESE approaches respectively

LHD	k	N	In Euclidean measure (L^2)			In Manhattan measure (L^1)		
			D_1J_1	D_{Max}, J_{Max}	AE value	D_1J_1	D_{Max}, J_{Max}	AE value
A	6	12	142, 12	286, 6	0.440568	23, 12	36, 6	2.57439
B	6	12	134, 2	294, 2	0.440954	21, 2	38, 2	2.57795

It is remarkable that though Audze-Eglais LHD **B** is optimized by the Audze-eglais criterion but in the table we observe , in column 6 (L^2) and in column 9 (L^1), that Maximin LHD **A** is also better than Audze-Eglais LHD **B** regarding Audze-Eglais (AE) value. Moreover It is notice that Maximin LHD **A** is better than Audze-Eglais LHD **B** regarding D_{Max}, J_{Max} values measured both L^1 and L^2 respectively. In this experimental study it may be said that Maximin LHD **A** obtained by ILS approach with (ϕ_p, D_1) optimal criterion is better than Audze-Eglais LHD **B** with Audze-Eglais optimal criterion in all aspects.

Again, to view the details characteristics of optimal LHD regarding both the maximin ϕ_p criterion and Audze-Eglais criterion, we have considered LHD $(k, N) = (6, 9)$. Table 5.8 displays the optimal LHD regarding the maximin ϕ_p criterion obtained by ILS approach on the other hand Table 5.9 presents the optimal LHD regarding the Audze-Eglais criterion obtained by Enhanced Stochastic Evolutionary algorithm (ESE) [Husslage et al. (2011)]. In both the cases we used Euclidian distance measure and the optimal LHDs are denoted as maximin LHD **C** and Audze-Eglais LHD **D** respectively.

Table 5.8 Optimal maximin
LHD C

0	8	5	5	4	4
1	1	2	3	2	0
2	0	6	7	7	5
3	2	8	1	1	6
4	3	0	4	3	8
5	4	4	0	8	3
6	5	1	8	6	1
7	7	3	2	0	2
8	6	7	6	5	7

Table 5.9 Optimal Audze-Eglais
LHD D

0	4	2	8	5	2
1	3	8	4	2	7
2	1	1	1	1	3
3	8	5	2	3	0
4	6	0	3	6	8
5	2	6	0	8	4
6	7	7	7	7	5
7	0	4	6	4	1
8	5	3	5	0	6

Table 5.10 Distance matrix **L** in L^2 measure
for maximin LHD C

0	82	84	166	83	83	84	82	83
82	0	82	84	83	83	166	84	83
84	82	0	82	83	83	84	166	83
166	84	82	0	83	83	82	84	83
83	83	83	83	0	84	83	83	84
83	83	83	83	84	0	83	83	84
84	166	84	82	83	83	0	82	83
82	84	166	84	83	83	82	0	83
83	83	83	83	84	84	83	83	0

Table 5.11 Distance matrix **M** in L^1
measure for maximin LHD C

0	18	20	30	17	21	20	18	19
18	0	18	20	17	19	30	20	21
20	18	0	18	21	19	20	30	17
30	20	18	0	19	21	18	20	17
17	17	21	19	0	20	19	21	20
21	19	19	21	20	0	17	17	20
20	30	20	18	19	17	0	18	21
18	20	30	20	21	17	18	0	19
19	21	17	17	20	20	21	19	0

Now we have performed further experiments on both LHDs C and D to find out the pair-wise distances of the design points in each distance measure namely L^1 and L^2 . The experimental results regarding LHD C are displayed in the Table 5.10 and 5.11. In Table 5.10 we have distance matrix **L** measured in Euclidean distance measure whereas in Table 5.11 we have distance matrix **M** measured in Manhattan distance measure respectively. Similarly performing experiments on LHD D, we have obtained the distance matrices **U** and **V** given in Table 5.12 and Table 5.13 regarding Euclidean and Manhattan distance measure respectively.

Table 5.12 Distance matrix **U** in L^2 measure for
Audze- Eglais LHD D

0	88	80	78	86	122	84	75	116
88	0	80	92	100	82	80	105	84
80	80	0	80	84	86	164	73	82
78	92	80	0	104	86	80	99	92
86	100	84	104	0	82	80	123	70
122	82	86	86	82	0	78	73	120
84	80	164	80	80	78	0	85	78
75	105	73	99	123	73	85	0	68
116	84	82	92	70	120	78	68	0

Table 5.13 Distance matrix **V** in L^1
measure for Audze- Eglais LHD D

0	20	18	20	20	24	20	17	22
20	0	18	20	20	20	20	23	18
18	18	0	18	20	18	30	19	20
20	20	18	0	20	20	20	19	22
20	20	20	20	0	20	18	25	18
24	20	18	20	20	0	16	19	24
20	20	30	20	18	16	0	19	18
17	23	19	19	25	19	19	0	17
22	18	20	22	18	24	18	17	0

Table 5.14: Comparison of Maximin LHD **C** and Audze-eglais LHD **D** in various aspects regarding ILS and ESE approaches respectively

LHD	k	N	In Euclidean measure (L^2)			In Manhattan measure (L^1)		
			D_1J_1	D_{Max}, J_{Max}	AE value	D_1J_1	D_{Max}, J_{Max}	AE value
C	6	9	82, 6	166, 3	0.415	17, 6	30, 3	1.834
D	6	9	69, 1	164, 1	0.414	16, 1	30, 1	1.826

Again we have performed experiments on those distance matrices **L**, **M**, **U** and **V** to find out the characteristics of the LHD **C** and **D** respectively. The experimental results are displayed in the Table 5.14. Again it is notice (in column 4) that Maximin LHD **C** is much better than Audze-eglais LHD **D** regarding maximin value D_1J_1 in Euclidean measure (L^2) where LHD **C** is optimized regarding (ϕ_p, D_1) [Grosso et al. (2009)] optimal criterion by ILS approach and Audze-eglais LHD **B** is optimized regarding Audze-eglais criterion by ESE approach. Though Maximin LHD **C** is optimized regarding L^2 measure but in this experiment we again notice that Maximin LHD **C** is better than Audze-eglais LHD **D** regarding D_1J_1 value according to Manhattan measure (L^1) too. On the other hand, it is notice that Maximin LHD **C** and Audze-Eglais LHD **D** are comparable regarding D_{Max}, J_{Max} values measured both L^1 and L^2 respectively. Note that LHD **C** is a bit worse compare to Audze-Eglais LHD **D** regarding Audze-Eglais (A-E) value.

Now we will perform another experiment to analysis the Maximin LHD and Audze-Eglais LHD according to the ILS [Grosso et al (2009)] and Genetic Algorithm (GA) [Bates et al. (2003)] approaches respectively. In this context we consider $(k, N) = (3, 10)$ and the optimal LHDs are experimental results are **Maximin LHD F** and **Audze-Eglais LHD G**.

Maximin LHD F			Audze-eglais LHD G		
1	7	5	1	3	5
2	2	6	2	7	3
3	4	1	3	9	8
4	5	10	4	2	2
5	9	2	5	5	10
6	10	7	6	1	7
7	1	8	7	10	4
8	3	3	8	6	1
9	6	9	9	8	9
10	8	4	10	4	6

The experimental results are shown in Table 5.15. It is observe that Maximin LHD **F** is significantly better compare to Audze-Eglais LHD **G** as well regarding D_1J_1 and D_{Max} , J_{Max} value in Euclidean distance measure. But there is a remarkable observation is that Maximin LHD **F** is better that Audze-Eglais LHD **G** regarding Audze-Eglais (A-E) value, though Audze-eglais LHD **G** is optimized regarding Audze-Eglais optimal criterion.

Table 5.15: Comparison of Maximin LHD and Audze-Eglais LHD in various aspects regarding ILS and GA approaches respectively

LHD	k	N	In Euclidean measure (L^2)			In Manhattan measure (L^1)		
			D_1J_1	D_{Max}, J_{Max}	A-E value	D_1J_1	D_{Max}, J_{Max}	A-E value
Maximin LHD F	3	10	27, 3	104, 3	1.0258	7, 3	16, 3	4.3706
Audze-eglais LHD G	3	10	19, 1	110, 1	1.0401	7, 2	18, 1	4.3504

From the above experiments, we observe that maximin LHDs obtained by ILS approach are always significantly better regarding D_1 and D_{Max} values measured L^2 distance measure. On the other hand according to A-E value maximin LHDs obtained by ILS approach are at least comparable with that of Audze-Eglais LHDs obtained by ESE algorithm. Similarly according to D_1 and D_{Max} values measured L^1 distance measure maximin LHD is better or at least comparable with Audze-Eglais LHDs.

5.3 Comparison on ILS VS Other Approach Regarding Audze-Eglais distance measure

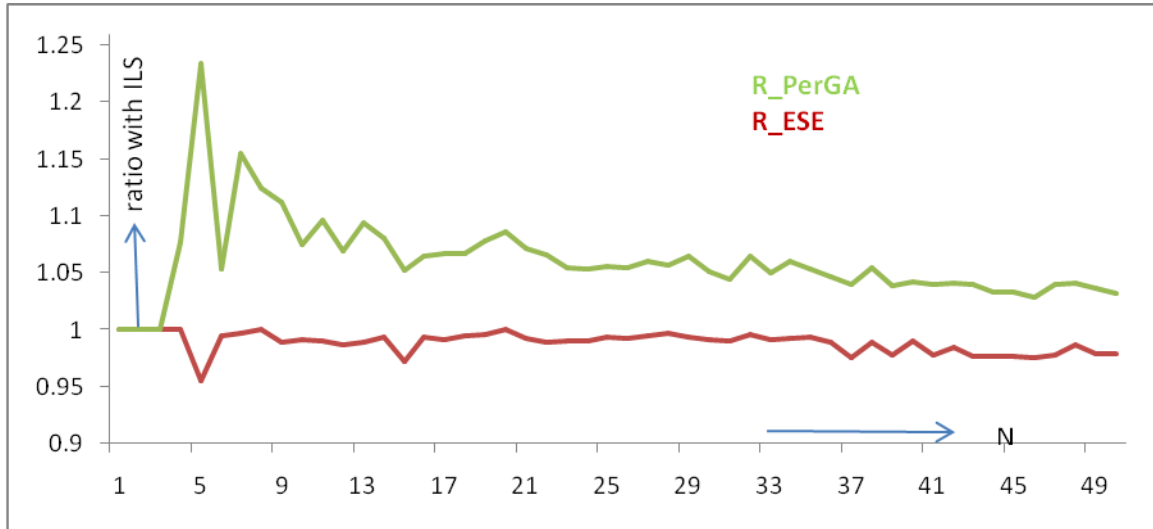


Figure 5.1 Comparison of ILS vs PerGA and ESE approaches regarding **Audze-Eglais** values of LHDs for $k=4$ and $N=3, \dots, 50$

Now we consider several optimal LHDs optimized by different approaches as well as different optimal criteria to analyze the **Audze-Eglais** values. In this experiment we will compare **maximin** LHDs (optimized by (ϕ_p, D^1) criterion) obtained by ILS approach regarding **Audze-Eglais** values with **Audze-Eglais** LHDs (optimized by **Audze-Eglais** criterion) obtained by Permutation Genetic Algorithm (PerGA) and Enhanced Stochastic Evolutionary (ESE) algorithm regarding **Audze-Eglais** values. It is noted that maximin LHDs is optimized on the basis of (ϕ_p, D^1) criterion not **Audze-Eglais** criterion. For this comparison we will calculate the **Audze-Eglais** value of each maximin LHDs.

At first we consider $k = 4$ and $N = 3, \dots, 50$. The experimental results are displayed in the Figure 5.1. In the figure **R_PerGA** indicates the ratio **PerGA/ILS** regarding **Audze-Eglais** values of the LHDs, **R_ESE** indicates the ratio **ESE/ILS** regarding **Audze-Eglais** values of the LHDs. In the Figure 5.1 it is observed that the ratio **ESE/ILS** is almost equal to unity. On the other hand the ratio **PerGA /ILS** is always greater than one. It is also remark that **the ratio PerGA /ILS** decrease with the increasing of N . From the Figure 5.1 it may conclude that the **Audze-Eglais** values of **maximin** LHDs obtained by ILS approach are comparable with other **Audze-Eglais** LHDs obtained by ESE algorithm

in dimension $k=4$. Moreover the **Audze-Eglais** values of **maximin** LHDs obtained by ILS approach are better than that of **Audze-Eglais** LHDs obtained by **PerGA** approach.

Again we have performed further similar experiments for $k=4$, $k=6$ and $k=8$ for all $N=4, \dots, 50$. In this experiments we have compared **Audze-eglais** values of **maximin** LHDs (optimized by (ϕ_p, D^1) criterion) obtained by ILS approach regarding with **Audze-Eglais** values of **Audze-Eglais** LHDs (optimized by **Audze-Eglais** criterion) obtained by Enhanced Stochastic Evolutionary (ESE) algorithm and **Audze-Eglais** LHDs (optimized by **Audze-Eglais** criterion) obtained in Web [www.spacefillingdesigns.nl (2015)]. The experimental results are reported in the Table 5.16. It is notice that though **maximin** LHDs are optimized regarding (ϕ_p, D^1) criterion but till **Audze-Eglais** values of **maximin** LHDs are comparable with **Audze-Eglais** LHDs obtained by ESE algorithm mentioned in [Husslage et al. (2011)] as well as and ESE algorithm mentioned in Web [www.spacefillingdesigns.nl (2016)]. It is also

Table 5.16 Comparison of **maximin** LHDs vs **Audze-Eglais** LHDs in Euclidean measure regarding **Audze-Eglais** values

N	Audze-eglais values of optimal LHDs								
	(k=4)			(k=6)			(k=8)		
	ILS	ESE	AE_Web	ILS	ESE	AE_Web	ILS	ESE	AE_Web
4	0.454	.454	0.454	0.300	0.300	0.300	0.225	0.225	0.225
5	0.533	0.509	0.509	0.484	0.336	0.518	0.250	0.250	0.250
6	0.564	0.561	0.561	0.359	0.358	0.358	0.268	0.268	0.268
7	0.601	0.599	0.600	0.377	0.376	0.376	0.359	0.282	0.359
8	0.619	0.619	0.620	0.399	0.398	0.398	0.292	0.292	0.292
9	0.667	0.660	0.660	0.415	0.414	0.414	0.301	0.301	0.300
10	0.692	0.686	0.687	0.427	0.425	0.425	0.311	0.311	0.311
11	0.716	0.709	0.709	0.435	0.434	0.434	0.320	0.319	0.319
12	0.734	0.724	0.724	0.440	0.441	0.441	0.326	0.326	0.326
13	0.754	0.746	0.746	0.454	0.453	0.453	0.331	0.331	0.331
14	0.767	0.762	0.762	0.464	0.462	0.461	0.335	0.335	0.335
15	0.777	0.755	0.774	0.473	0.470	0.470	0.339	0.339	0.338
16	0.796	0.791	0.790	0.480	0.477	0.476	0.341	0.341	0.341
17	0.812	0.805	0.805	0.484	0.483	0.483	0.348	0.347	0.346
18	0.820	0.816	0.816	0.489	0.488	0.488	0.289	0.350	0.350
19	0.830	0.827	0.827	0.493	0.492	0.492	0.356	0.354	0.354
20	0.835	0.835	0.835	0.497	0.496	0.496	0.359	0.358	0.357
21	0.853	0.847	0.848	0.456	0.501	0.501	0.361	0.361	0.360
22	0.865	0.856	0.856	0.507	0.505	0.505	0.364	0.363	0.363
23	0.877	0.868	0.867	0.511	0.510	0.509	0.367	0.366	0.365
24	0.884	0.875	0.875	0.514	0.513	0.513	0.368	0.368	0.368
25	0.890	0.884	0.884	0.517	0.516	0.516	0.370	0.370	0.370

26	0.898	0.891	0.890	0.519	0.518	0.518	0.372	0.372	0.371
27	0.903	0.898	0.896	0.521	0.521	0.520	0.374	0.373	0.373
28	0.909	0.906	0.906	0.525	0.524	0.524	0.375	0.375	0.375
29	0.918	0.912	0.912	0.529	0.527	0.527	0.377	0.376	0.376
30	0.927	0.919	0.919	0.532	0.530	0.530	0.378	0.378	0.378
31	0.934	0.925	0.925	0.534	0.533	0.532	0.380	0.380	0.379
32	0.935	0.931	0.930	0.537	0.535	0.535	0.382	0.381	0.381
33	0.943	0.935	0.935	0.539	0.537	0.537	0.383	0.383	0.382
34	0.948	0.941	0.941	0.541	0.540	0.539	0.384	0.384	0.384
35	0.952	0.946	0.946	0.544	0.542	0.541	0.385	0.385	0.385
36	0.960	0.950	0.950	0.544	0.543	0.543	0.386	0.386	0.386
37	0.980	0.956	0.956	0.547	0.545	0.545	0.387	0.387	0.387
38	0.970	0.959	0.959	0.548	0.547	0.547	0.388	0.388	0.388
39	0.987	0.965	0.965	0.549	0.548	0.549	0.389	0.389	0.389
40	0.978	0.968	0.968	0.550	0.550	0.549	0.390	0.390	0.390
41	0.993	0.971	0.971	0.551	0.551	0.551	0.391	0.391	0.390
42	0.990	0.975	0.974	0.552	0.552	0.552	0.392	0.392	0.391
43	1.002	0.979	0.978	0.555	0.554	0.554	0.393	0.393	0.392
44	1.007	0.983	0.982	0.556	0.555	0.555	0.394	0.394	0.393
45	1.010	0.986	0.986	0.559	0.557	0.557	0.395	0.394	0.394
46	1.015	0.990	0.990	0.560	0.559	0.558	0.396	0.395	0.395
47	1.015	0.993	0.993	0.561	0.560	0.560	0.397	0.396	0.396
48	1.010	0.997	0.997	0.563	0.561	0.561	0.397	0.397	0.397
49	1.022	1.001	1.001	0.565	0.563	0.563	0.398	0.398	0.397
50	1.025	1.004	1.003	0.566	0.564	0.564	0.399	0.398	0.398

worthwhile to mention here that the **Audze-Eglais** values of **maximin** LHDs are become better (more closed to **Audze-Eglais** LHDs's values) with the increasing of the dimension k . To view it clearly the difference between **maximin** LHDs and **Audze-Eglais** LHDs regarding **Audze-Eglais** values are reported in the Table 5.17. Note that negative value implies **maximin** LHDs is better than **Audze-Eglais** LHDs regarding **Audze-Eglais** values.

Table 5.17 difference between **maximin** LHDs and **Audze-Eglais** LHDs regarding **Audze-Eglais** values

N	$k = 4$	$k = 6$	$k = 8$	N	$k = 4$	$k = 6$	$k = 8$
4	0.000			28	0.003	0.001	0.000
5	0.024	-		29	0.006	0.002	0.000
6	0.003	0.001		30	0.008	0.002	0.000
7	0.002	0.001	-0.001	31	0.009	0.002	0.000
8	0.000	0.001	0.000	32	0.004	0.002	0.001
9	0.007	0.002	0.000	33	0.008	0.002	0.001
10	0.006	0.001	0.001	34	0.007	0.001	0.000
11	0.008	0.000	0.001	35	0.007	0.002	0.001
12	0.009	0.000	0.001	36	0.010	0.001	0.000
13	0.008	0.001	0.001	37	0.024	0.002	0.000
14	0.006	0.002	0.000	38	0.011	0.001	0.000
15	0.002	0.004	0.000	39	0.022	0.001	0.000
16	0.005	0.004	0.000	40	0.010	0.001	0.000

17	0.007	0.002	0.001	41	0.022	0.000	0.000
18	0.004	0.002	-0.062	42	0.016	0.000	0.000
19	0.003	0.001	0.002	43	0.024	0.001	0.001
20	0.001	0.002	0.001	44	0.024	0.001	0.001
21	0.006	-	0.001	45	0.024	0.002	0.001
22	0.009	0.001	0.001	46	0.025	0.002	0.001
23	0.009	0.001	0.001	47	0.022	0.002	0.001
24	0.009	0.002	0.001	48	0.013	0.002	0.001
25	0.007	0.001	0.001	49	0.021	0.002	0.001
26	0.007	0.001	0.001	50	0.021	0.001	0.001
27	0.005	0.000	0.001				

5.4 Comparison among several Optimal LHDs in different aspect

In order to perform experiments on several Optimal LHDs obtained by different approaches, we consider optimal LHDs with $(k, N) = (4, 9)$. In this experiment we consider five optimal LHDs namely MLH-SA, OMLH-MSA, OLH-Y, MLH-ESE, MLH-ILS. Here MLH-SA denotes Maximin LHD obtained by simulated annealing (SA) [Husslage et al. (2006)], OMLH-MSA means orthogonal maximin LHD obtained by Modified Simulated Annealing (MSA) [Husslage et al. (2006)], in which multi-objective (Φ_p, ρ^2) criteria is considered, OLH-Y indicates Orthogonal LHD mentioned in [Ye (1998)], MLH-ESE denotes Maximin LHD obtained by ESE algorithm mentioned in [Husslage et al. (2011)], MLH-ILS indicated Maximin LHD obtained by ILS approach mentioned in [Grosso et al. (2009)]. It will worthwhile to mention here that we will compare MLH-ILS optimal design with other designs considered here in various aspects. The experimental results are reputed in the Table 5. 18.

In the Table 5.19 1st row the name of the optimal LHDs, row 2nd indicated the objective function of the algorithms considered, 3rd row displays the optimal designs and 4th row indicated the type of distance measure considered to calculate the pair-wise distance of each pair of design points. The characteristic of each LHD considered is indicated in first column below the head line – “**PROPERTIES**”. The meaning of the notation of each property concise is displayed in the Table 5.18.

Table 5.18 Meaning of the symbols

Symbols	Meaning	Symbols	Meaning
ρ	Average correlation	$D_1(J_1)^{(L1)}$	$D_1(J_1)$ value in L^1
ρ_{\max}	Maximum correlation	$D_1(J_1)^{(L2)}$	$D_1(J_1)$ value in L^2
D_1	Minimum pair-wise distance in a LHD	$\Phi_p^{(L1)}$	Φ_p value in L^1
(J_1)	Number of time D_1 occur in a LHD	$\Phi_p^{(L2)}$	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
Φ_p	Φ_p optimal criterion	ω_1 and ω_2	(Weight average) constant
A-E	Audze-Eglais optimal criterion		

It is observed in the Table 5.19 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 $\rho = 0.151$.

It is also observed in the Table 5.19 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.

Table 5.19: 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

5.5 Comparison between Maximin LHD and Audze-Eglais LHD regarding Manhattan distance measure.

Now we will perform experiments extensively on Maximin LHD and Audze-Eglais LHD regarding Manhattan distance measure. For this experiments we again consider all optimal LHDs with $N = 5, \dots, 50$ for $k = 4$; $N = 5, \dots, 50$ for $k = 6$ and $N = 7, \dots, 50$ for $k = 8$ for maximin LHDs optimized by ILS approach in Euclidean distance measure and Audze-Eglais LHDs available in web [www.spacefillings.nl] optimized by ESE approach. Note that both kind of LHDs are optimized in which Euclidean distance measure were considered. In this experimental study, we calculate D_1 values as well as A-E values in

Manhattan distance measure of those optimal (maximin LHDs as well as Audze-Eglais LHDs) LHDs. The experimental results regarding D_1 values as well as A-E values are reported in Table 5.20 and Table 5.21 respectively.

Table 5.20: Comparison between Maximin LHD and Audze-Eglais LHD regarding $D_1 J_1$ value in Manhattan (L^1) distance measure

N	$k=4$		$k=6$		$k=8$	
	Maximin LHD	A-E LHD	Maximin LHD	A-E LHD	Maximin	A-E LHD
5	7, 4	7, 2	9, 1	6, 1		
6	8, 2	8, 4	14, 15	14, 15		
7	8, 2	9, 6	14, 2	15, 8	14, 1	14, 1
8	10, 8	10, 8	16, 3	14, 1	22, 4	21, 1
9	10, 4	10, 4	17, 6	16, 1	23, 1	23, 1
10	12, 16	11, 5	17, 1	19, 4	24, 1	25, 3
11	11, 3	10, 1	19, 2	20, 3	27, 1	26, 1
12	13, 9	12, 2	23, 12	21, 2	28, 2	27, 1
13	12, 3	12, 1	21, 1	22, 1	30, 1	31, 3
14	14, 4	13, 1	24, 4	21, 1	30, 1	31, 2
15	14, 3	14, 4	22, 1	23, 1	35, 1	36, 3
16	14, 1	14, 4	24, 1	20, 1	39, 4	38, 2
17	14, 2	15, 3	26, 2	24, 1	38, 1	35, 1
18	16, 2	16, 2	27, 5	26, 1	41, 3	38, 1
19	16, 2	17, 4	26, 1	24, 1	40, 1	42, 5
20	18, 4	18, 2	29, 1	24, 1	39, 1	43, 1
21	20, 10	17, 1	29, 3	29, 2	42, 2	43, 1
22	17, 1	17, 4	31, 2	30, 1	44, 1	45, 1
23	18, 5	16, 1	32, 1	29, 1	49, 3	46, 1
24	19, 2	20, 8	33, 1	31, 1	49, 2	48, 1
25	19, 4	17, 1	34, 1	33, 1	50, 1	48, 1
26	19, 2	19, 2	35, 1	35, 2	52, 1	49, 1
27	20, 3	18, 1	34, 1	35, 1	51, 2	49, 1
28	20, 1	19, 1	36, 1	33, 1	54, 1	53, 2
29	19, 1	19, 1	37, 1	34, 1	58, 1	55, 1
30	20, 1	20, 1	40, 3	34, 1	57, 1	58, 1
31	21, 2	22, 2	37, 1	36, 1	58, 1	54, 1
32	21, 1	21, 2	35, 1	38, 2	58, 1	58, 1
33	22, 1	22, 2	42, 2	38, 1	61, 1	58, 1
34	22, 1	25, 5	44, 2	39, 1	56, 1	59, 1
35	23, 1	22, 1	46, 3	45, 1	57, 1	64, 1
36	22, 2	23, 1	45, 2	44, 1	64, 1	66, 1
37	20, 2	24, 2	45, 1	44, 2	63, 1	61, 1
38	25, 2	25, 1	49, 1	45, 1	65, 1	66, 1
39	22, 1	23, 1	47, 2	50, 1	68, 1	70, 1
40	25, 1	22, 1	48, 1	49, 1	75, 3	68, 1
41	25, 2	27, 1	54, 2	51, 1	75, 1	76, 1
42	25, 1	25, 1	56, 5	55, 2	76, 1	75, 1
43	24, 2	28, 4	46, 1	46, 1	73, 1	77, 1
44	25, 1	26, 1	49, 2	43, 1	73, 1	70, 1
45	26, 2	27, 4	48, 1	45, 1	69, 1	77, 1
46	26, 1	28, 3	50, 1	46, 1	72, 1	73, 1
47	25, 1	25, 1	50, 2	52, 2	84, 1	83, 1
48	27, 1	28, 1	49, 1	52, 1	77, 1	81, 1
49	29, 1	28, 1	55, 1	49, 1	84, 1	82, 2
50	29, 1	28, 1	53, 1	52, 1	80, 1	81, 1
No of better LHDs	19	17	31	12	22	17

Table 5.21: Comparison between Maxmin LHD and Audze-Eglais LHD regarding A-E value in Manhattan (L^1) distance measure

N L^1 (Manhattan)	k=4		k=6		k=8	
	Maxmin LHD	A-E	Maxmin LHD	A-E LHD	Maxmin	A-E LHD
5	1.26865	1.25794	1.26772	1.30526		
6	1.62222	1.63182	1.07143	1.07143		
7	2.02217	2.01423	1.31967	1.31724	1.29588	1.30108
8	2.38333	2.38333	1.5625	1.57467	1.1706	1.17106
9	2.79127	2.78487	1.83778	1.82617	1.35495	1.3536
10	3.17341	3.17835	2.08095	2.06892	1.54774	1.54526
11	3.59234	3.59575	2.33314	2.32879	1.73758	1.74051
12	3.97428	3.9822	2.57439	2.57795	1.92952	1.92504
13	4.4114	4.3767	2.84969	2.83796	2.1164	2.11534
14	4.7803	4.76221	3.10912	3.10882	2.31095	2.30598
15	5.18558	5.18086	3.37413	3.36393	2.493	2.49409
16	5.58613	5.5992	3.63879	3.62587	2.67851	2.67971
17	6.03849	6.01619	3.8945	3.88882	2.8789	2.88279
18	6.40529	6.39889	4.16132	4.15049	2.79732	3.07163
19	6.82229	6.81297	4.42651	4.42582	3.27474	3.26809
20	7.20005	7.20137	4.6727	4.69583	3.4743	3.45912
21	7.62586	7.63534	4.49122	4.94098	3.66628	3.65129
22	8.0877	8.07256	5.22094	5.20809	3.85696	3.84847
23	8.52793	8.48166	5.47487	5.48996	4.05547	4.0516
24	8.92831	8.90783	5.73882	5.74939	4.24429	4.23957
25	9.36588	9.33333	5.99717	6.00637	4.44097	4.43573
26	9.78678	9.73911	6.26768	6.26077	4.63988	4.6293
27	10.2176	10.1705	6.51708	6.50478	4.83505	4.83303
28	10.5954	10.5685	6.79843	6.79677	5.02729	5.0277
29	11.0493	11.0062	7.06333	7.05678	5.21657	5.22773
30	11.4711	11.4149	7.33794	7.31486	5.4122	5.41098
31	11.9101	11.8487	7.60426	7.59101	5.61431	5.61504
32	12.3103	12.275	7.85979	7.86038	5.81396	5.80731
33	12.7262	12.6664	8.1274	8.13117	6.0043	6.00694
34	13.1139	13.0766	8.3954	8.38632	6.20803	6.19874
35	13.5561	13.5234	8.66729	8.66107	6.39657	6.39749
36	14	13.9461	8.93063	8.91809	6.59186	6.58731
37	14.5121	14.3777	9.213	9.19794	6.79099	6.79224
38	14.8598	14.8088	9.47071	9.45458	6.9779	6.98622
39	15.3224	15.2284	9.73111	9.71368	7.16866	7.17499
40	15.7008	15.6768	9.99521	9.99117	7.36554	7.37179
41	16.1839	16.0198	10.2447	10.2592	7.56359	7.56043
42	16.569	16.4718	10.5069	10.5073	7.7626	7.76136
43	17.0255	16.9111	10.7884	10.7923	7.96064	7.95536
44	17.448	17.3551	11.0672	11.0619	8.162	8.15639
45	17.8731	17.7323	11.3405	11.3206	8.3582	8.3477
46	18.3038	18.1696	11.6017	11.6082	8.55317	8.54496
47	18.7424	18.6594	11.8855	11.8693	8.74668	8.7433
48	19.1525	19.0551	12.163	12.1365	8.95038	8.93634
49	19.6131	19.4654	12.4359	12.4168	9.15127	9.13384
50	19.9985	19.8942	12.6981	12.685	9.34633	9.33574

It is observed in Table 5.20 and Table 5.21 that both maximin LHDs as well as Audze-Eglais LHDs are comparable regarding Manhattan distance measure. Especially maximin LHDs are a bit better compare to Audze-Eglais LHDs regarding D_1 values in Manhattan distance measure.

CHAPTER VI

DISCUSSION AND CONCLUSION

The optimal DoE are extremely useful in the area of computer simulation. One important area where computer simulation is used a lot is engineering. Engineers are confronted with the task of designing products and processes. Since physical experimentation is often expensive and difficult, computer models are frequently used for simulating physical characteristics. The engineer often needs to optimize the product or process design, i.e. to find the best settings for a number of design parameters that influence the critical quality characteristics of the product or process. A computer simulation run is usually time-consuming and there is a great variety of possible input combinations. For these reasons, meta-models that model the quality characteristics as explicit functions of the design parameters are constructed. Such a meta-model, also called a (global) approximation model or surrogate model, is obtained by simulating a number of design points. Well-known meta-model types are polynomials and Kriging models. Since a meta-model evaluation is much faster than a simulation run, in practice such a meta-model is used, instead of the simulation model, to gain insight into the characteristics of the product or process and to optimize it. A review of meta-modeling applications in structural optimization can be found in Barthelemy and Haftka (1993), and in multidisciplinary design optimization in Sobieszczanski-Sobieski and Haftka (1997). As observed by many researchers, there is an important distinction between designs for computer experiments and designs for the more traditional response surface methods. Physical experiments exhibit random errors and computer experiments are often deterministic (cf. Simpson et al. (2004)). This distinction is crucial and much research is therefore aimed at obtaining efficient designs for computer experiments. As is recognized by several authors, such a design for computer experiments should at least satisfy the following two criteria [Johnson et al. (1990) and Morris and Mitchell (1995)]. First of all, the design should be space-filling in some sense. When no details on the functional behavior of the response parameters are available, it is important to be able to obtain information from the entire design space. Therefore, design points should be evenly spread" over the entire region. One of the measures often used to obtain space-filling

designs is the maximin measure. The Audze-Eglais measure is another measure used for this purpose. Secondly, the design should be non-collapsing. When one of the design parameters has (almost) no influence on the function value, two design points that differ only in this parameter will collapse", i.e. they can be considered as the same point that is evaluated twice. For deterministic simulation models this is not a desirable situation. Therefore, two design points should not share any coordinate values when it is not known a priori which dimensions are important. Note that in other fields of research such designs are referred to as low discrepancy designs. To obtain non-collapsing designs the Latin hypercube structure is often enforced. It can be shown that if the function of interest is independent of one or more of the k parameters then, after removal of the irrelevant parameters, the projection of the LHD onto the reduced design space retains good spatial properties; [Koehler and Owen (1996)]. Audze-Eglais LHDs are also constructed by only a few authors. In Bates et al. (2004), the problem of finding Audze-Eglais LHDs is formulated and a permutation genetic algorithm is used to generate them. Liefvendahl and Stocki (2006) compare maximin and Audze-Eglais LHDs and recommend the Audze-Eglais criterion over the maximin criterion. Examples of practical applications of Audze-Eglais LHDs can be found in Rikards et al. (2001), Bulik et al. (2004), Stocki (2005), and Hino et al. (2006). There are several other measures proposed in the literature besides maximin and Audze Eglais, e.g. maximum entropy, minimax, IMSE, and discrepancy. For a good overview, we refer to Koehler and Owen (1996). Several type of optimal DoE are available in the frequently updated web portal www.spacefillingdesigns.nl.

ILS outperforms regarding maximin LHDs compare to several well known approaches existing in the literature. In chapter IV Maximin LHDs obtained by ILS approach are compared with maximin LHDs obtained by other well-known approaches. Most of those approaches considered ϕ_p optimal criterion with L^2 distance measure. The optimal criterion of ILS approach is also ϕ_p but the algorithm tackle the better D_1 value during the search. In consequence ILS outperforms regarding maximin LHDs compare to several well known approaches existing in the literature. From the comparison study, given in Chapter IV, it may be concluded that ILS approach is a state-of-the-arts approach for finding maximin LHDs measured in L_2 with Opt (ϕ_p, D_1) criterion.

Though ILS approach may be a state of the arts regarding D_1 (maximized minimum pairwise inter site distance), we could not conclude the MLH_ILS be best regarding space-filling property. There exist some other objective functions which are also used for optimized LHD for satisfying space-filling property. Some well-known such objective functions are briefly presented in Chapter II. Among them correlation criterion is used to make the DoE's parameters uncorrelated and Audze-Eglais optimal criterion is used for providing good space-filling DoE. Moreover in the literature it is shown that distance measures are also crucial for measurement good space-filling property of the DoEs. In this perspective extensive experiments have been performed in Chapter V. Firstly several experiments have been carried out to compare the maximin LHDs obtained by ILS approach and Audze-Eglais LHD obtained by ESE approach regarding both D_1 values as well as Audze-Eglais values. From the experimental study it is observed that maximin LHDs are significantly better compared to Audze-Eglais LHD regarding D_1 values (minimum inter-site distance value) where inter-site distance are measured in Euclidean distance measure. But it should be imposed attention that the Audze-Eglais values of maximin LHDs are comparable with that of Audze-Eglais LHD (1977).

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.

From these experimental studies It may be conclude that maximin LHDs obtained by ILS approach is state-of the-arts regarding D_1 values are comparable with other Audze-Eglais values.

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