OPTIMALITY ANALYSIS ON THE BASIS OF RECTANGULAR (MANHATTAN) DISTANCE MEASURE FOR MAXIMIN LHDS OBTAINED BY THE ITERATED LOCAL SEARCH HEURISTICS APPROACH

By

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Declaration

This is to certify that the thesis work entitled *"Optimality Analysis on the Basis of Rectangular (Manhattan) Distance Measure for Maximin LHDs Obtained by the Iterated Local Search Heuristics Approach"* has been carried out by *Md. Ishaque Ali* 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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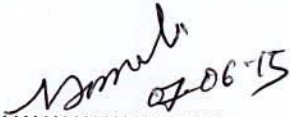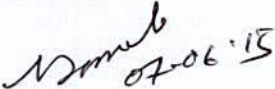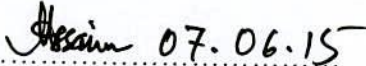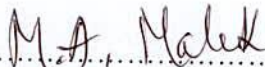Department of Mathematics, KUET.

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Dedication

To

my parents

Md. Abul Hashem & Nurjahan Begum

whose pains helped me see the light of the Earth

Acknowledgement

Abstract

Design of Experiment (DoE) is an important issue for developing mathematical model of any physical problem especially when there exist large numbers of factors. Optimal Latin Hypercube Design (LHD) is one of the well-known and used tools among the experimental designs. For obtaining optimal LHD, Iterated Local Search (ILS) is one of the best way among the heuristic approaches. Grosso et al. (2009) showed that ILS approach has the ability to obtain a large number of maximin (Optimizations by maximizing minimum pair-wise distance) LHD where distances are measured in terms of Euclidian distance measure. Several authors showed that rather than Euclidean distance measure other measures may suitable for good DoE. Manhattan distance measure is one of them [Morris and Mitchell (1995)]. In this research work, the main objective is to study the optimality of the maximin LHD obtained by ILS approach regarding Manhattan distance measure. For this purpose, ILS approach is implemented in windows environment (rather than Sun cluster, as Gross et al. (2009) done). Extensive experiments are performed to obtain maximin LHD measured in Euclidian distance measure. Then further experiments are reformed on those LHDs to find the minimum pair-wise distance of each LHD measured in Manhattan distance. Those values are compared with available one in the literature. It is noted that few values (maximin LHD measured in Manhattan distance measure) are available in the literature. It seems that the minimum pair-wise distance measured in Manhattan distance measure of the maximin LHDs obtained by ILS approach, optimized in Euclidian distance measure are comparable with those maximin LHDs obtained through other approaches but optimized in the Manhattan distance measure. Moreover some further experiments are performed to find out some new characteristics of those LHDs which may be used for further study. Some improved maximin LHDs are also obtained in this experimental arena and are presented in the thesis.

Publications

The following papers have been extracted from this thesis:

1. A.R.M. J. U. Jamali, **M. Ishaque Ali** and A. Grosso, *"Analysis the Optimality in Rectangular Distance Measure for the maximin LHDs measured in Euclidean Distance Measure Obtained by the ILS Approach"*, 18th International Mathematics Conference (IMC-2014) 20-22 March, 2014 (presented).

2. A. R. M. Jalal Uddin Jamali, **M. Ishaque Ali**, Rafiqul Islam and A. Grosso, *"Optimality Analysis of LHDs Obtained by ILS on the Basis of Manhattan Distance Measure"*, National Conference on Mathematics and Its Applications (NCMA-2015, Chittagong University of Engineering & Technology (CUET), Chittagong-4349, Bangladesh on 15th March 2015 (accepted).

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CHAPTER I

Introduction

1.1 Background

In the design of complex systems, computer experiments are the only practical approach to obtain a solution. Typically, a simulation model of system performance is constructed based on knowledge of how the system operates. Performance measures are specified to be incorporated into optimization criteria and constraints, and the design parameters which affect performance are identified. The design solution method depends on the computational demands of the simulation model. In the simplest case, the simulation model may be used directly to calculate performance measures and optimize the system. If a performance measure is not straightforward to calculate, such as one that involves an integral, then sampling via computer experiments may be employed to estimate the measure. If the simulation model is computationally expensive, then the optimization may instead rely on a metamodel, i.e., a mathematical model surrogate of system performance, to approximate the relationship between system performance and the design parameters [Chen et al. (2003)]. In computer experiments, instead of physically doing an experiment on the product, mathematical models describing the performance of the product are developed using laws of engineering/physics 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); Sacks et al. (1989)]. Many simulation models involved 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 projecting the design on to these factors, replication is not required.

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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. There is another important property for the design of experiments – the multicollinearity property. That is the factors /coordinates should be uncorrelated or they are mutually (approximately) orthogonal. The multicollinearity property is also important, because if two factors are correlated then it will not possible to distinguish between the effects of the two factors based on this experiment.

For the design of computer experiments **Latin Hypercube Design (LHD)**, first introduced by McKay and his coauthors in 1979, fulfill the non-collapsing property. LHDs are important in the design of computer-simulated experiments [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). It is assumed that there are N design points have to be placed and each point has k distinct parameters. The points are placed such a way that they are uniformly spread when projected along each single parameter axis. It is assumed 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 $0, 1, \ldots, N-1$ and such that there does not exist two points with one common coordinate value. This allows a non-collapsing design because points are evenly spreaded when projected along a single parameter axis. Note that the number of possible LHDs are huge: there are $(N!)^k$ possible LHDs (where N is number of design point and k is number of factors). A configuration

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

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

Unfortunately, randomly generated LHDs almost always show poor space-filling properties or / and the factors are highly correlated. On the other hand, maximin distance objective based designs proposed by Johnson et al. (1990), have very good space-filling properties but often no good projection properties under the Euclidean (L^2) or the Rectangular/Manhattan (L^1) distance. To overcome this shortcoming, Morris and Mitchell (1995) suggested for searching **maximin LHDs** which has both the important properties when looking for "optimal" designs. 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 LHDs are defined in several ways [Grosso et al. (2009)] but the main objective is identical i.e. searching the LHD with maximizing the minimum pair-wise distance. Note that, there exist several distance measures in literature.

As mention earlier, for the presence of combinatorial nature, the number of possible LHDs are 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} possible designs. If the number of variables are increased to 3, the number of possible designs are 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, Iterated Local Search (ILS) heuristic approach will be considered to find the optimal (maximin) LHDs [Grosso et al. (2009)]. For the optimal criterion the following maximin optimal will be considered which is similar to Johnson et al. (1990) but a quite different regarding computational effort:

$$\Phi_p(X) = \sum_{i=1}^{N} \sum_{j=i+1}^{N} \left[\frac{1}{d_{ij}^p} \right]^{\frac{1}{p}} \tag{1.1}$$

where $d_{ij} = d(x_i, x_j)$ be the 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). This optimal criterion is denoted as Opt(φ). Under this criterion, LHD Y is better than X if

$$\Phi_P(Y) < \Phi_P(X) \tag{1.2}$$

In Johnson et al. (1990) the definition of maximin optimal criterion is as follows:

$$\Phi_p(X) = \sum_{r=1}^{R} \left[\frac{J_r(X)}{D_r(X)^p} \right]^{\frac{1}{p}}, \tag{1.3}$$

where $D_1(X) < D_2(X), \cdots\cdots, < D_R(X)$ (pair-wise inter side distances), R is the number of different distances in LHD X. Whereas Grosso et al. (2008), Grosso et al. (2009) considered another maximin optimal criterion denoted as Opt (D1), which is also considered in Johnson et al. (1990), is given below.

$maxD_1(X)$ such that

$$D_1 = D_1(X) = \min d(x_i, x_j) \quad i \neq j; X \in LHD \tag{1.4}$$

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

Under this criteria, LHD Y is better than X if

$D_1(Y) > D_1(X)$ or

$D_1(Y) > D_1(X)$ and $J_1(Y) < J_1(X)$ (1.5)

and so on.

An apparent drawback of the Opt(φ) criterion, for maximin values (maximum D_1 value), is that LHDs with smaller (better) φ_p may have a worse (smaller) D_1 value, i.e. for X and Y, though $\varphi_p(X) < \varphi_p(Y)$ but $D_1(X) < D_1(Y)$. This phenomenon has been frequently observed in the computational experiments [Grosso et al. (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, as it will be demonstrated experimentally, it can be extremely effective. Such objective will be denoted as Opt(φ, D_1).

Different methods (e.g. the book of Santner et al. (2003), the article of Ye et al. (2000); Levy and Steinberg (2010) etc.) can be found in the literature to detect maximin LHDs. Grosso et al. (2009), successfully implemented Iterated Local Search (ILS) approach for finding maximin LHDs for k =3, 4, . . . ,10 and N= 3,......, 100. 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 used in practice. The rationale behind ILS is supported by the proximate optimality principle. This principle assumes that good solutions are similar. This assumption is reasonable for most real-world problems.

A lot of improved values (maximin LHDs values) obtained by the ILS approaches proposed by Grosso et al. (2009) 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; where it has been shown that the ILS approach not only able to obtain good LHD in the sense of maximin property but also the multicollinearity among the factors of the designs are negligible i.e. the average coefficient of correlations are low. Moreover Mridha (2013) performed several experiments for analyzing the time complexity of the ILS approach for finding maximin LHDs (as the number of possible LHDs are very high - $(N!)^k$). Experimentally, he showed that the time complexity of the ILS algorithm is of polynomial time with order four ($O(N^4)$) when algorithm considered Opt(φ,D_1) criterion and $O(N^3)$ when algorithm considered Opt (D_1,J_1) criterion.

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 (for examples, [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. (1989)]. 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 laws of engineering/physics. 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) model with 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.

As it is recognized by several authors, the choice of the design points for computer experiments should at least fulfill two requirements (details can be found in 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. 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.

The latter requirement is fulfilled by employing Latin Hypercube Designs (LHDs). Such designs, proposed by McKay and his coauthors (1979), are evenly distributed in each one-dimensional projection and are thus non-collapsing. Unfortunately, randomly generated

LHDs almost always show poor space-filling properties. On the other hand, maximin distance designs, proposed by Johnson, Moore and Ylvisaker (1990), have very good space-filling properties but often no good projection properties under the Euclidean or the Rectangular distance. To overcome this shortcoming, Morris and Mitchell (1995) suggested searching for maximin LHDs when looking for "optimal" designs. Although the search for maximin LHDs will be one of the problems discussed in this thesis, it will be important to point out that also other definitions of "optimality" for designs exist in the literature. These are not discussed in detail throughout the thesis (detail can be found in Santner et al. (2003)), but, for the sake of completeness, in the following literature review some of them will be mentioned, together with a short discussion of the methods employed to return "optimal" (according to the selected definition) designs.

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 being orthogonal. They considered projection uniformity over all sub dimensions. In Fang et al. (2000b) they classified 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. 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 (detail can be found in [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 (detail can be found in [McKay et al. (1979)]).

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Giunta and his coauthors (2003) gave an overview of pseudo- and quasi-Monte Carlo sampling, Latin hypercube sampling, orthogonal array sampling, and Hammersley sequence sampling.

McKay et al. (1979), Stein (1987) and Owen (1994)] had shown that LHDs perform much better than completely randomized designs. More recently, algorithms have been used to construct systematic LHDs under various optimality criteria. A LHD always has non-collapsing properties but not necessarily good space-filling property. In particular, as already remarked, randomly generated LHDs often show poor space-filling properties. Therefore, the search for "optimal" LHDs has attracted attention (detail can be found in 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. (1989)] and minimax and maximin distance designs [Johnson et al. (1990)].

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 (2002), in his dissertation, 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) made 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. Stocki (2005) and 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 by 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.

By using the Latin Hypercube sampling method, Hwan Yang (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.

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.

1.2.2. Optimal Criteria and Approaches

Some literature reviews will be presented here regarding optimal criteria as well as the solution approaches regarding experimental design. As the complexity of the problem is, to the authors' knowledge, open (but suspected to be NP-complete [Grosso et al. (2008)]. So, for detecting optimal experimental designs, several heuristics approaches (rather than exact optimization methods) have been proposed in the literature.

Fang et al. (2006) considered Simulated Annealing approach to detect maximin LHD. Li and Wu (1997) proposed a class of algorithms based on column pair-wise exchange 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). A general formulae for maximin LHDs with $k = 2$ are given by Dam and his coauthors (2007a) with the 1-norm (L^1) and infinite norm (L^∞) distances. Morover, for the Euclidean distance 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 et al. (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 and his coauthors (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 Opt(ϕ) 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. Grosso and his coauthors (2008) successfully implemented Iterated local search (ILS) approach for finding maximin LHDs for $k = 3, 4, ..10$, and $N = 3, ..., 100$. For the optimal criterion they considered maximin LHDs with Opt(D_1, J_1) and Opt(ϕ) optimal criteria with Euclidian distance measure (Eq. (1.1) to . Eq. (1.4)).

Dam and his coauthors (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 found 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), 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 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- and ℓ^2-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} will replace 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 (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 $\{0, 1, \ldots, N-1\}$. At each step, another permutation of $\{0, 1, \ldots, N-1\}$ is chosen to replace a column so that the LHD structure is retained.

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.

Using (adapted) periodic designs and simulated annealing, 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 of 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.

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In the simulated annealing algorithm, Husslage et al. (2006) considered four different neighborhoods. In all four neighborhoods the main idea is to change two points of the current LHD by exchanging one or more coordinate values. In three of the four neighborhoods, one point is required to be a critical point (a critical point is a point which is at separation distance, i.e., at a distance equal to the minimal one, from one of the other points). In the first neighborhood, one point j_1 is selected randomly from all critical points and the other point j_2 randomly from all remaining points. This implies that the second point can either be a critical or noncritical point. Once the points are selected, the number of coordinates to change are randomly selected. Due to symmetry, at most $[k/2]$ coordinates are changed. Subsequently, the coordinates to change are randomly selected. The values of the two points in these coordinates are then exchanged, which results in a new LHD. The second neighborhood is very similar to the first. The only difference is that always one coordinate is selected instead of a random number of coordinates. Note that for $k = 3$ the two neighborhoods are the same. In the third neighborhood, also one coordinate is changed, however, now the coordinate is not randomly selected. Instead, all coordinates are tried and the one which results in the neighbor with the largest separation distance is selected. If more coordinates result in the same separation distance, the one with the lowest index is selected. The fourth neighborhood is again very similar to the second neighborhood. The difference is that the first point is randomly selected from all points, instead of only the critical points. Although simulated annealing algorithms have been used before to deal with this type of problem, this adapted neighborhood structure, which is based on critical points, and the use of a different objective function, turned out to work well.

Jin [Jin et al. (2005)] proposed an enhanced stochastic evolutionary algorithm for finding maximin LHDs. They also applied their method to other space-filling criteria, namely the optimal entropy and centered L_2 discrepancy criteria.

Dam et al. (2007a) derived 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.

Stinstra and his coauthors (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.

It is remarked 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 (1994)] and a mixed criterion involving both maximin distance and correlation [Joseph and Hung (2008)]. For more details the book [Santner et al. (2003)] will be referred but for the completeness, in the following literature review, some articles will be mentioned in which criteria related to correlation are considered.

Dam van (2005) derived interesting results for two-dimensional minimax LHDs. Bates Bates and his coauthors (2004) proposed a permutation genetic algorithm to find optimal Audze-Eglais LHDs. Crary and his coauthors (2000) developed I-OPTTM to generate LHDs with minimal IMSE.

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 (1998) proposed a LHD by the extension of the concept of Iman and Conover (1982a), namely minimizing a polynomial canonical correlation criterion for pair-wise factors.

Park (1994)] and Sacks (1989) constructed optimal LHDs in which IMSE and entropy optimization criteria were considered. To construct optimal LHDs, Park 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 between factors and find the best exchange among them.

Ye (1998) constructed orthogonal LHDs in order to enhance the utility of LHDs for regression analysis. Ye defined an Orthogonal Latin Hypercube (OLHC) as a Latin

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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 (2008) proposed a multi-objective optimization approach to find good LHDs by combining correlation and distance performance measure. They 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, Morris and Mitchell (1995) chose them judiciously in order to achieve improvement in their multi-objective function.

Ye and his coauthors (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 and his coauthors (2000) considered maximin as an optimal criterion, whereas Li and Kenny (2009) considered both the maximin and the entropy optimal criterion.

Fang and his coauthors (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.

Sebastiani and Wynn (2000) 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 and his coauthors (1991) also considered an entropy-based design criterion for Bayesian prediction of deterministic functions. Crombecq and his coauthors (2011) considered space-filling and non-collapsing sequential design strategies for simulation based modeling.

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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 (2010) proposed a space-filling LHD design, where they considered a new optimal criterion called Kullback–Leibler criterion. This Kullback–Leibler criterion is relatively very new proposed by Jourdan and Franco (2009). The new designs are compared with several traditional optimal Latin hypercube designs.

Leary et al. proposed orthogonal-array-based LHDs for obtaining better space-filing property. As an optimal criterion, they considered the sum of (square of) reverse inter-site distances. Ye (1998) constructed orthogonal LHDs in order to enhance the utility of LHDs for regression analysis. Author defined 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.

Steinberg and Dennis (2006) 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 (1998). Butler (2001) proposed optimal and orthogonal LHDs which are suitable for factor screening. Fang and his coauthors (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.

On the other hand Joseph and Hung (2008) showed that maximization of inter-site distances criteria and minimizing the pair-wise correlation criteria need not necessarily agree with each other. In fact, maximization of inter-site distances can result in LHDs where the variables are highly correlated and vice versa. But it has been already discussed above that for the present of high correlation, the design has failed to analysis individual effect of the factors.

1.2.3 Distance Measure

Grosso et. al. (2009) considered only Euclidian distance measure. But in the literature several authors have considered DoE in rectangular (Manhattan) distance measure or more than one distance measure. Morris and Mitchell (1995) adopted a simulated annealing to find approximate maximin LHDs regarding both Euclidian as well as Rectangular distance. Chan et al. proposed an efficient algorithm for constructing Optimal Design of computer experiments but they considered both Euclidean distance as well as Manhattan distance. Crombecq et al. (2011) considered both Euclidean as well as rectangular distance measure for space-filling and non-collapsing sequential design strategies for simulation-based modeling. It is worthwhile to mention here that Rectangular (Manhattan) distance measure is also one of the important issues considered in several fields like in location theory. In this area of research, the problem is usually referred to as the max-min facility dispersion problem, see Erkut (1990), facilities are placed such that the minimal distance to any other facility is maximal. Manhattan distance matrix for a rectangular grid arise frequently from communications and facility locations and are known to be among the hardest discrete optimization problems. Mittelmann and Pengy (2001) estimated bounds for quadratic assignment problems associated with hamming and Manhattan distance matrices based on semi definite programming. Philip et al. (2009) showed that a new precision-weighted Manhattan distance and the Canberra distance are the most repeatable and they are most in agreement with the expected pattern rather than unweighted Manhattan or Euclidean distance measures. To analyze Time series correlation in Network Structure, Miskiewicz (2010) considered Manhattan Distance (MD). He showed that MD allows investigating a broader class of correlation and is more robust to the noise influence. Hasnat et al. (2014) described the comparative study of performance between the existing distance metrics like

Manhattan, Euclidean, Vector Cosine Angle and Modified Euclidean distance for finding the similarity of complexion by calculating the distance between the skin colors of two color facial images. From the above discussion it may be concluded that ILS approach is a state-of-art method to find out the maximin LHDs regarding Euclidian distance measure. The maximin LHDs obtained by ILS approach also comparable enough regarding muliticolinearity property. But how much those LHDs are fine (optimal) regarding Manhattan (Rectangular) distance measure is still unknown and require extensively analysis. Moreover, for any design, optimality measured in Euclidian distance may not be optimal regarding Manhattan distance. This is why several authors search optimal experimental measured in Manhattan distance measure rather than Euclidean distance measure. Moreover, for any design, optimality measured in Euclidian distance may not be optimal regarding Manhattan distance. This is why several authors search optimal experimental measured in Manhattan distance measure rather than Euclidean distance measure.

1.3 Goals of the Thesis

After the invention of hi-speed computer the design of computer experiments is likely to grow as more and more simulation models to carry out research. 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 projecting the design on to these factors, replication is not required. The experimental design should fulfill three important properties – Non-collapsing, Space-filling, and non-multicollinearity. Latin Hypercube Design (LHD) has good non-collapsing property. But randomly generated LHD often has poor space-filling. 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. But recently some researchers have shown that maximin LHD are highly correlated among the factors i.e. there exist multicollinearity. It is mentioned earlier that the multicollinearity property is also important, because if two factors are correlated then it will not possible to distinguish between the effects of the two factors based on this experiment. Several approaches existed in literature to find out the

maximin LHD such as simulated annealing, Tabu search, Iterated Local Search (ILS) etc. In the paper of Grosso et al. (2008), authors have shown that ILS approach able to find out a remarkable improved optimal experimental design (maximin LHD) regarding available one in the literature as multicollinearity can have serious effects on the estimates of the regression coefficients and on the general applicability of the model in this study, the multicollinearity among the factors of the design obtained by the ILS approach is investigated.

It is mentioned earlier that ILS approaches are able to find out very good DoE namely optimal LHDs regarding maximin optimal criterion and those LHDs are also good enough regarding multicolinearity as those have poor coefficient of muliticolinearity [Apparna (2012)]. It is also mentioned earlier that Manhattan Measure is another important approach regarding finding out optimal DoE which are frequently used in practical application. Morris and Mitchell (1995) and Bates et al. (2004) showed that though one approach may find optimal DoEs regarding on some distance measure but those DoEs may be poor enough regarding other distance measure. In this thesis, our main aim is to study the optimality of the maximin LHDs obtained by ILS approach on the basis of Manhattan distance measure. It is noted that those maximin LHDs obtained by ILS approach are optimal on the basis of Euclidean distance measure. Several experiments are performed to analyse and to compare our results with available ones in the literature.

Therefore the main objectives of this research are as follows:

(i) Implementation of the ILS approach to find out the optimal LHDs regarding maximin optimal criteria in Euclidean distance measure.

(ii) Analysis of those optimal maximin LHDs regarding Manhattan distance measure.

(iii) Comparison of those Manhattan distance measured LHDs (which are actually optimal regarding Euclidian distances measure) with available one in the literature.

(iv) Perform several experiments to find out several new characteristics of those optimal LHDs which might be used for further studies in future.

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1.4   Structure of the Thesis

After the introduction which is incorporated in the chapter I, the remaining thesis is organized as follow:

Chapter 2 presents the overview of several distance measures. In this chapter, the definitions of distances, metric and norms are presented. Moreover several distance measures are discussed briefly in this chapter. Mainly this chapter points out Manhattan distance measure as well as its application and schematic view of circle in different distance measures are given in this chapter.

In **Chapter 3**, at first the main concept of Iterated Local Search (ILS) approach is discussed briefly. Then several optimal criteria are also discussed briefly in this chapter. Moreover the maximin LHD is showed pictorially and is discussed briefly. ILS approach ·for optimizing LHD is also elaborately presented here.

In **Chapter 4,** optimality analysis of the experimental results regarding Euclidean distance is discussed briefly. In this chapter, several experiments are carried out for analysis the performance of 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 results it is shown that the algorithm is state-of-arts regarding maximin LHD in Euclidean distance measure. Moreover some more experiments have been performed to analyze the multicollinearity among the factors of each maximin design obtained by ILS approach.

In **Chapter 5,** the optimality analysis of maximin LHDs obtained by ILS approach is discussed elaborately in experimental point of views. Extensive experiments have been performed in maximin LHDs obtained by ILS approach regarding Manhattan distance measure and compare the experimental results with available one in the literature. Moreover some more experiments have been carried out to find out some more interesting characteristics of those maximin LHDs which might be important for further research.

References are included in the last of the thesis and publications are mentioned before the index of the thesis as well.

CHAPTER TWO

Overview of Distance Measure

2.1 Introduction

Distance is a numerical description of how far apart objects are. In physics or everyday discussion, distance may refer to a physical length, or estimation based on other criteria (e.g. "two counties over"). In mathematics, a distance function or metric is a generalization of the concept of physical distance. A metric is a function that behaves according to a specific set of rules, and is a concrete way of describing what it means for elements of some space to be "close to" or "far away from" each other. In most cases, "distance from A to B" is interchangeable with "distance between B and A".

2.2 Definition of Distance Function (Metric)

Mathematically, the definition of distance measure is given bellow:

Let $X \neq \emptyset$ be any given space.

Let $x, y, z \in X$ be arbitrary.

A function $d : X \times X \rightarrow \mathbb{R}$ having the properties listed below :

(i) $d(x, y) \geq 0$ (non negative)

(ii) $d(x, y) = 0$ iff $x = y$ (identical)

(iii) $d(x, y) = d(y, x)$ (reflection)

(iv) $d(x, y) + d(y, z) \geq d(x, z)$ (triangle inequality)

is called a distance function (in brief distance) or a metric for X. Instead of saying, "Let X be a non-empty set with a metric d defined on it, " we always say, "Let (X, d) be a metric space."

Evidently d is a real valued map and d denotes the distance between x and y. A set X, together with a metric defined on it, is called metric space [Gupta (2000)].

Example : Let $X = \mathbb{R}$ and $\rho(x, y) = |x - y|$ for all $x, y \in X$. Then ρ is a metric on X. This metric is defined as usual metric on $\mathbb{R}$. Before classifying distance measure, it is worthwhile to discuss about norm.

2.3 Norm

In linear algebra, functional analysis and related areas of mathematics, a norm is a function that assigns a strictly positive length or size to each vector in a vector space, other than the zero vector (which has zero length assigned to it). A semi-norm, on the other hand, is allowed to assign zero length to some non-zero vectors (in addition to the zero vector). A simple example is the 2-dimensional Euclidean space $\mathbb{R}^2$ equipped with the Euclidean norm. Elements in this vector space are usually drawn as arrows in a 2-dimensional Cartesian coordinate system starting at the origin (0, 0). The Euclidean norm assigns to each vector is the length of its arrow. Because of this, the Euclidean norm is often known as the magnitude. A vector space with a norm is called a normed vector space. Similarly, a vector space with a seminorm is called a seminormed vector space.

2.3.1 Definition of Norm

Given a vector space V over a subfield F of the complex numbers, a norm on V is a function $p: V \to \mathbb{R}$ with the following properties:

For all $a \in F$ and all $\mathbf{u}, \mathbf{v} \in V$,

(i) $p(a\mathbf{v}) = |a| \, p(\mathbf{v})$, (positive homogeneity or positive scalability).

(ii) $p(\mathbf{u} + \mathbf{v}) \leq p(\mathbf{u}) + p(\mathbf{v})$ (triangle inequality or subadditivity).

(iii)   If $p(\mathbf{v}) = 0$ then $\mathbf{v}$ is the zero vector (separates points).

There are mainly four classes norm as follows:

1-norm distance	$= \displaystyle\sum_{i=1}^{n} |x_i - y_i|$
2-norm distance	$= \left(\displaystyle\sum_{i=1}^{n} |x_i - y_i|^2 \right)^{1/2}$

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p-norm distance	$= \left(\sum_{i=1}^{n} |x_i - y_i|^p \right)^{1/p}$
Infinity norm distance	$= \lim_{p \to \infty} \left(\sum_{i=1}^{n} |x_i - y_i|^p \right)^{1/p}$ $= max(|x_1 - y_1|, |x_2 - y_2|, ..., |x_n - y_n|)$

p need not be an integer, but it cannot be less than 1, because otherwise the triangle inequality does not hold. Note that for $p = 1$ we get the taxicab (Manhattan) norm, for $p = 2$ we get the Euclidean norm, and as p approaches ∞ the p-norm approaches the infinity norm or maximum norm.

In the above brief discussion, it is observed that norm also gives the distance function. Anyway among several distance measures, here we will briefly discuss some of them.

2.4 Euclidean Distance

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. Older literature refers to the metric as Pythagorean metric.

On an n-dimensional Euclidean space $\mathbb{R}^n$, the intuitive notion of length of the vector x $=(x_1, x_2, ..., x_n)$ is captured by the formula

$$||x|| = \sqrt{x_1^2 + x_2^2 + ----- + x_n^2} \qquad (2.1)$$

This gives the ordinary distance from the origin to the point x, a consequence of the Pythagorean theorem. The Euclidean norm is so far the most commonly used norm on $\mathbb{R}^n$, but there are other norms on this vector space as will be shown below. However all these norms are equivalent in the sense that they all define the same topology. On an n-dimensional complex space $\mathbb{C}^n$ the most common norm is

$$||z|| := \sqrt{|z_1|^2 + ---- + |z_n|^2} = \sqrt{z_1 \bar{z}_1 + --- + z_n \bar{z}_n} \qquad (2.2)$$

In both cases we can also express the norm as the square root of the inner product of the vector and itself:

$$\|x\| := \sqrt{x^* x} \qquad (2.3)$$

where x is represented as a column vector $([x_1, x_2, ..., x_n])'$, and x^* denotes its conjugate transpose.

This formula is valid for any inner product space, including Euclidean and complex spaces. For Euclidean spaces, the inner product is equivalent to the dot product. Hence, in this specific case the formula can be also written with the following notation:

$$\|x\| := \sqrt{x.x} \qquad (2.4)$$

The Euclidean norm is also called the Euclidean length, L^2 distance, ℓ^2 distance, L^2 norm, or ℓ^2 norm.

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

$$d(p,q) = \sqrt{(q_1 - p_1)^2 + (q_2 - p_2)^2 + \cdots + (q_n - p_n)^2} = \sqrt{\sum_{i=1}^{n} (q_i - p_i)^2} \qquad (2.5)$$

The position of a point in a Euclidean n-space is a Euclidean vector. So, p and q are Euclidean vectors, starting from the origin of the space, and their tips indicate two points. The Euclidean norm, or Euclidean length, or magnitude of a vector measures the length of the vector:

$$\|p\| = \sqrt{p_1^2 + p_2^2 + - - - + p_n^2} = \sqrt{p.p} \qquad (2.6)$$

where the last equation involves the dot product.
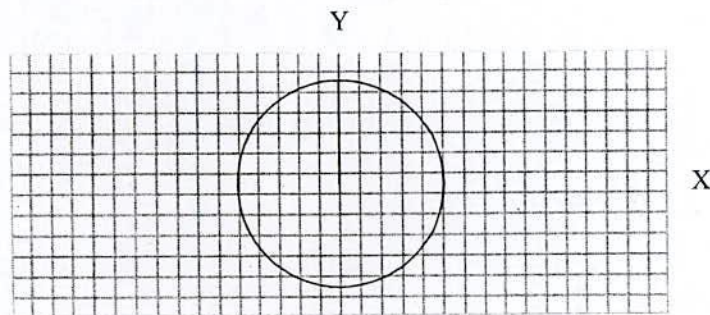
Figure 2.1: Schematic view of a circle with unit radius in Euclidean distance measure

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The schematic view of a circle with unit radius in Euclidean distance measure is given in figure 2.1. Euclidean distance is a Minkowski distance which is discussed later.

2.4.1 Squared Euclidean Distance

The standard Euclidean distance can be squared in order to place progressively greater weight on objects that are farther apart. In this case, the equation becomes

$$d^2(p,q) = (p_1 - q_1)^2 + (p_2 - q_2)^2 + \cdots + (p_i - q_i)^2 + \cdots + (p_n - q_n)^2 \qquad (2.7)$$

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.

2.5 Minkowski Distance

The Minkowski distance is a metric on Euclidean space which can be considered as a generalization of both the Euclidean distance and the Manhattan distance.

2.5.1 Definition

The Minkowski distance of order p between two points

$$P = (x_1, x_2, \ldots, x_n) \text{ and } Q = (y_1, y_2, \ldots, y_n) \in \mathbb{R}^n$$

is defined as:

$$d_p(x, y) = \left(\sum_{i=1}^{n} |x_i - y_i|^p \right)^{1/p} \qquad (2.8)$$
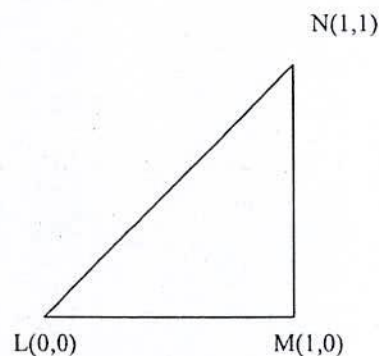
Figure 2.2: Graphical representation of the points to measure Minkowski distance for p=0.50

For $p \geq 1$, the Minkowski distance is a metric as a result of the Minkowski inequality. For $p < 1$, it is not the distance. For example, let $p = \frac{1}{2}$ and L(0,0), M(1,0) and N(1,1) are three points (see Figure 2.2). Then

$$d_p(L, N) = (|0-1|^p + |0-1|^p)^{1/p} = (1 + 1)^2 = 4$$

$$d_p(L, M) = (|0-1|^p + |0-0|^p)^{1/p} = (1 + 0)^2 = 1$$

$$d_p(M, N) = (|1-1|^p + |0-1|^p)^{1/p} = (0 + 1)^2 = 1$$

Therefore, $d_p(L, M) + d_p(M, N) = 1 + 1 = 2 < d_p(L, N)$, which violates the triangle inequality.

Minkowski distance is typically used with p being 1 or 2. The latter is the Euclidean distance, while the former is sometimes known as the Manhattan distance. In the limiting case of p reaching infinity, we obtain the Chebyshev distance which is discussed later, on the other hand, for p reaching negative infinity, we have:

$$\lim_{p \to -\infty} \left(\sum_{i=1}^n |x_i - y_i|^p \right)^{1/p} = \min_{i=1}^n |x_i - y_i| \tag{2.9}$$

The Minkowski distance can also be viewed as a multiple of the power mean of the component-wise differences between two points P and Q.

The following figure shows unit circles with various values of p:
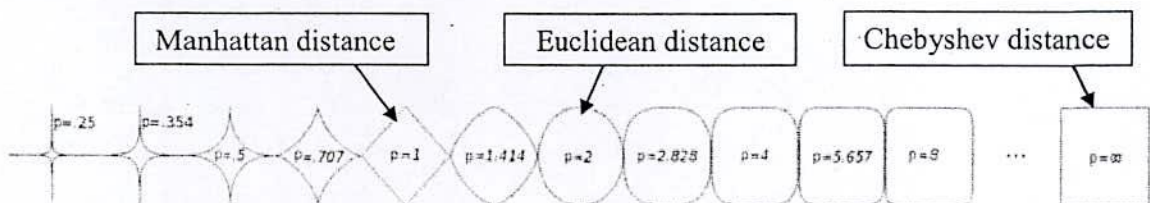
Figure 2.3: Schematic view of circles in Minkowski distance measure with several p values

Note that a circle is a set of points with a fixed distance, called the radius, from a point called the center. It is noted that Minkowski distance is refered to L_p metric. Anyway in one dimension, all L_p metrics are equal. They are just the absolute value of the difference.

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2.6 Chebyshev Distance

Minkowski distance reduces to Chebyshev distance when $p \to \infty$ i.e. The Chebyshev distance between two vectors or points P and Q, with standard coordinates x_i and y_i respectively, is

$$d_\infty(x, y) = \lim_{p \to \infty} \left(\sum_{i=1}^{n} |x_i - y_i|^p \right)^{1/p} = \max_{i=1}^{n} |x_i - y_i| \qquad (2.10)$$

Hence it is also known as the L_∞ metric.

Mathematically, the Chebyshev distance is a metric induced by the supremum norm or uniform norm. It is an example of an injective metric.

In two dimensions, i.e. plane geometry, if the points P and Q have Cartesian coordinates (x_1, y_1) and (x_2, y_2), their Chebyshev distance is

$$d_\infty(x, y) = \max(|x_2 - x_1|, |y_2 - y_1|) = \max(|1 - 2|, |1 - 3|) = \max(1, 2) = 2$$
$$[\text{say, } (x_1, y_1) = (2,3) \text{ and } (x_2, y_2) = (1,1)]$$

Under this metric, a circle of radius r, which is the set of points with Chebyshev distance r from a center point, is a square whose sides have the length $2r$ and are parallel to the coordinate axes.

On a chess board, where one is using a discrete Chebyshev distance, rather than a continuous one, the circle of radius r is a square of side lengths $2r$, measuring from the centers of squares, and thus each side contains $2r$ squares; for example, the circle of radius 1 on a chess board is a 2×2 square. The Chebyshev distance refers to L_∞ metric or norm. The Chebyshev distance is sometimes used in warehouse logistics.
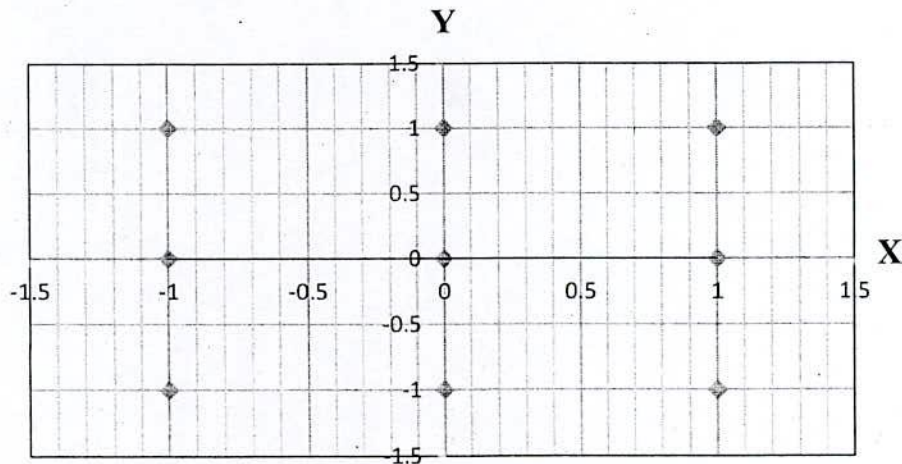
Figure 2.4: Schematic view of a circle of radius 1 in Chebyshev distance

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2.7 Rectangular / Manhattan / Taxicab Distance

Manhattan distance also a special case of Minkowski distance (Eq. (2.8)) where $p = 1$. 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. Taxicab norm or Manhattan norm of a point $\mathbf{x}$ measured from origin is given by

$$||\mathbf{x}||_1 := \sum_{i=1}^{n} |x_i| \tag{2.11}$$

The name relates to the distance a taxi has to drive in a rectangular street grid to get from the origin to the point $\mathbf{x}$.

The set of vectors, whose 1-norm is a given constant, forms the surface of a cross polytope of dimension equivalent to that of the norm minus 1. The Taxicab norm is also called the L_1 norm. The distance derived from this norm is called the Manhattan distance or L_1 distance. It is noted that $\sum_{i=1}^{n} x_i$ is not a norm because it may yield negative results.

2.7.1 Formal Definition

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,

$$d_1(\mathbf{x}, \mathbf{y}) = ||\mathbf{x} - \mathbf{y}||_1 = \sum_{i=1}^{n} |x_i - y_i| \tag{2.12}$$

Where $\mathbf{X} = (x_1, x_2, ..., x_n)$ and $\mathbf{Y} = (y_1, y_2, ..., y_n)$ are vectors.

For example, in the plane, the taxicab distance between (x_1, y_1) and (x_2, y_2) is

$$|x_1 - y_1| + |x_2 - y_2|.$$

2.7.2 Properties

Taxicab distance depends on the rotation of the coordinate system, but does not depend on its reflection about a coordinate axis or its translation. Taxicab geometry satisfies all of Hilbert's axioms (a formalization of Euclidean geometry) except for the side-angle-side axiom, as one can generate two triangles each with two sides and the angle between them the same, and have them not be congruent.

In taxicab geometry, distance is determined by a different metric than in Euclidean geometry and the shape of circles changes as well. Taxicab circles are squares with sides

oriented at a 45° angle to the coordinate axes. The image to the right shows why this is true, by showing in red the set of all points with a fixed distance from a center, shown in blue. As the size of the city blocks diminishes, the points become more numerous and become a rotated square in continuous taxicab geometry. While each side would have length $\sqrt{2}r$ using a Euclidean metric, where r is the circle's radius, its length in taxicab geometry is $2r$. Thus, a circle's circumference is $8r$. Thus, the value of a geometric analog to π is 4 in this geometry. The formula for the unit circle in taxicab geometry is $|x| + |y| = 1$ in Cartesian coordinates and $r = \dfrac{1}{|\sin\theta| + |\cos\theta|}$ in polar coordinates.

A circle of radius r for the Chebyshev distance (L_∞ metric) on a plane is also a square with side length $2r$ parallel to the coordinate axes, so planar Chebyshev distance can be viewed as equivalent by rotation and scaling to planar taxicab distance. However, this equivalence between L_1 and L_∞ metrics does not generalize to higher dimensions. A sphere formed using the Chebyshev distance as a metric is a cube with each face perpendicular to one of the coordinate axes, but a sphere formed using Manhattan distance is an octahedron: these are dual polyhedra, but among cubes, only the square (and 1-dimensional line segment) are self-dual polytopes. The Chebyshev distance refers to L_∞ metric or norm. The Chebyshev distance is sometimes used in warehouse logistics.
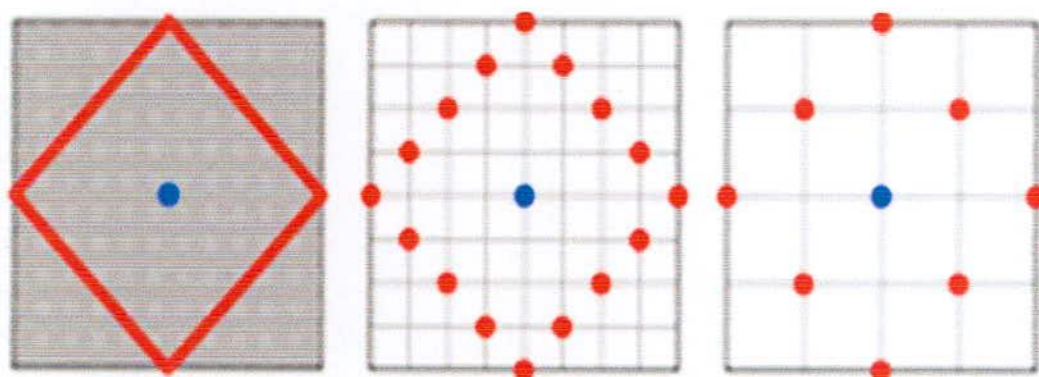
Figure 2.5: Circles in continuous and discrete taxicab geometry

Whenever each pair in a collection of these circles has a nonempty intersection, there exists an intersection point for the whole collection; therefore, the Manhattan distance forms an injective metric space. A circle of radius 1 (using this distance) is the von Neumann neighborhood of its center; see figure (2.5).

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2.7.3 Applications

It is worthwhile to mention here that Rectangular (Manhattan) distance measure is also one of the important issues considered in several fields like 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. Manhattan distance matric for a rectangular grid arise frequently from communications and facility locations and are known to be among the hardest discrete optimization problems. Mittelmann and Pengy (2001) estimated bounds for quadratic assignment problems associated with hamming and Manhattan distance matrices based on semi definite programming. They considered the issue of how to obtain lower bounds for those two classes of Quadratic Assignment Problems (QAPs) based on Semi Definite Programming (SDP). Philip et al. (2009) showed that a new precision-weighted Manhattan distance and the Canberra distance are the most repeatable and the most in agreement with the expected pattern rather than unweighted Manhattan or Euclidean distance measures. To analyse Time series correlation in Network Structure, Miskiewicz (2010) considered Manhattan Distance (MD). He showed that MD allows investigating a broader class of correlation and is more robust to the noise influence. Hasnat et al. (2014) described the comparative study of performance between the existing distance metrics like Manhattan, Euclidean, Vector Cosine Angle and Modified Euclidean distance for finding the similarity of complexion by calculating the distance between the skin colors of two color facial images. Vadivel and Majumdar (2003) described the performance comparison of distance metrics in content-based image retrieval applications. They have done a detailed study of the performance of different distance metrics for a number of color histograms on a large database of images. They use Manhattan distance, Euclidean distance, Vector Cosine Angle distance and Histogram Intersection distance for performance comparison. Five standard and well-known color histograms were considered for evaluation and the results show that the Manhattan distance performs better than the other distance metrics for all the five types of histograms. Manhattan distance is also use for measure the change of geometry of objects and clustering [Singla and Karambir (2012)].

2.7.4 Taxicab Distance Versus Euclidean Distance

In taxicab geometry all three pictured lines (red, yellow, and blue) have the same length (12) for the same route. In Euclidean geometry, the green line has length $6\sqrt{2} \approx 8.48$, and is the unique shortest path.
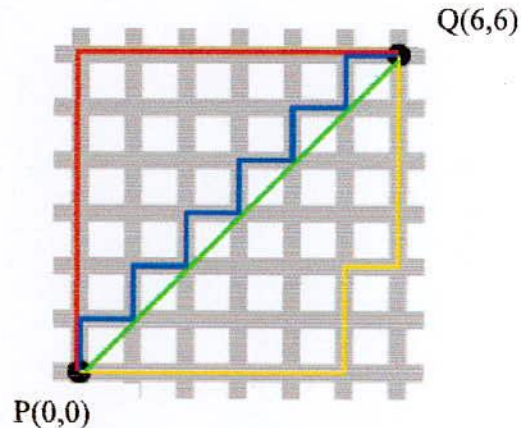
Figure 2.6: Distance measure between point P(0,0) and Q(6,6) ; in Euclidean measure $d_2(P,Q) = \sqrt{72}$ and in Manhattan measure $d_1(P,Q) = 12$.

Taxicab geometry, considered by Hermann Minkowski in the 19th century, is a form of geometry in which the usual distance function or metric of Euclidean geometry is replaced by a new metric in which the distance between two points is the sum of the absolute differences of their Cartesian coordinates. The taxicab metric is also known as rectilinear distance, L_1 distance or L_1 norm, city block distance, Manhattan distance, or Manhattan length, with corresponding variations in the name of the geometry.The latter names allude to the grid layout of most streets on the island of Manhattan, which causes the shortest path a car could take between two intersections in the borough to have length equal to the intersections' distance in taxicab geometry.

Now for completeness some other well-known distances will discuss below.

2.8 Hamming Distance

In information theory, the Hamming distance between two strings of equal length is the number of positions at which the corresponding symbols are different. In another way, it measures the minimum number of substitutions required to change one string into the other, or the minimum number of errors that could have transformed one string into the other.

2.8.1 Special Properties

For a fixed length n, the Hamming distance is a metric on the vector space of the words of length n, as it fulfills the conditions of non-negativity, identity of indiscernibles and symmetry, and it can be shown by complete induction that it satisfies the triangle inequality as well. The Hamming distance between two words a and b can also be seen as the Hamming weight of $a - b$ for an appropriate choice of the operator.

For binary strings a and b the Hamming distance is equal to the number of ones (population count) in a XOR b. The metric space of length-n binary strings, with the Hamming distance, is known as the Hamming cube; it is equivalent as a metric space to the set of distances between vertices in a hypercube graph. One can also view a binary string of length n as a vector in $\mathbb{R}^n$ by treating each symbol in the string as a real coordinate; with this embedding, the strings form the vertices of an n-dimensional hypercube, and the Hamming distance of the strings is equivalent to the Manhattan distance between the vertices.

Examples

The Hamming distance between:

- "**toned**" and "**roses**" is 3.
- **1011101** and **1001001** is 2.
- **2173896** and **2233796** is 3.

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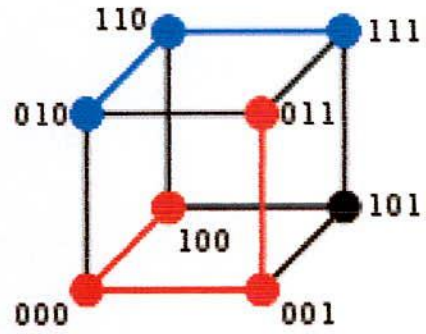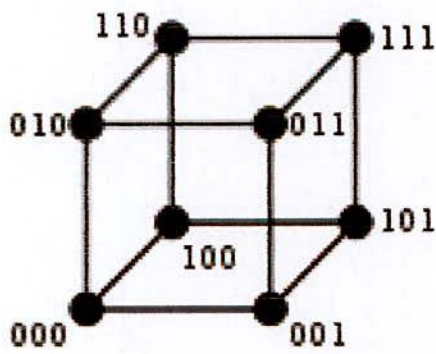
(a) 3-bit binary cube for finding Hamming distance

Hamming Distance :

From 100 to 011 has distance 3 (red path); and form 010- to 111 has distance 2 (blue path)
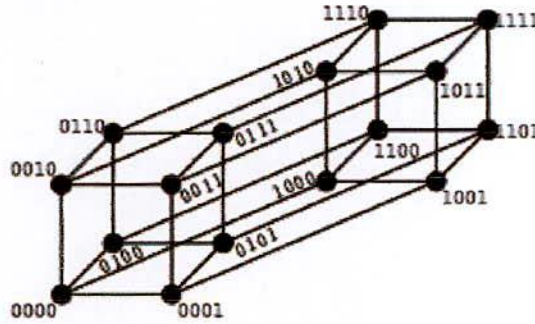
(b) 4-bit binary tesseract for finding Hamming distance
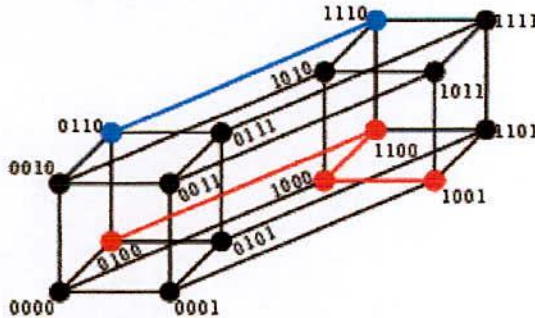
Hamming Distance :

From 0100 to 1001 has distance 3 (red path); and

From 0110-to 1110 has distance 1 (blue path)

Figure 2.7: Graphical view of measuring Hamming distance

2.8.2 Applications

The Hamming distance is named after Richard Hamming, who introduced it in his fundamental paper on Hamming codes Error detecting and error correcting codes in 1950. It is used in telecommunication to count the number of flipped bits in a fixed-length binary word as an estimate of error, and therefore is sometimes called the signal distance. Hamming weight analysis of bits is used in several disciplines including information theory, coding theory, and cryptography. However, for comparing strings of different lengths, or strings where not just substitutions but also insertions or deletions have to be expected, a more sophisticated metric like the Levenshtein distance is more appropriate. For q-ary strings over an alphabet of size $q \geq 2$ the Hamming distance is applied in case of orthogonal modulation, while the Lee distance is used for phase modulation. If $q = 2$ or $q = 3$ both distances coincide.

The Hamming distance is also used in systematics as a measure of genetic distance.

On a grid such as a chessboard, the Hamming distance is the minimum number of moves it would take a rook to move from one cell to the other.

2.9 Levenshtein Distance

In information theory and computer science, the Levenshtein distance is a string metric for measuring the difference between two sequences. Informally, the Levenshtein distance between two words is the minimum number of single-character edits (insertion, deletion, substitution) required to change one word into the other. The phrase edit distance is often used to refer specifically to Levenshtein distance. It is named after Vladimir Levenshtein, who considered this distance in 1965. It is closely related to pairwise string alignments.

2.9.1 Definition

Mathematically, the Levenshtein distance between two strings a, b is given by $lev_{a,b}(|a|,|b|)$ where

$$
lev_{a,b}(i,j) = \begin{cases} \max(i,j) \; if \; \min(i,j) = 0, \\ \min \begin{cases} lev_{a,b}(i-1,j) + 1 \\ lev_{a,b}(i,j-1) + 1 \\ lev_{a,b}(i-1,j-1) + [a_i \neq b_j] \end{cases} & \text{otherwise.} \end{cases}
$$

Note that the first element in the minimum corresponds to deletion (from a to b), the second to insertion and the third to match or mismatch, depending on whether the respective symbols are the same.

Example

For example, the Levenshtein distance between "kitten" and "sitting" is 3, since the following three edits change one into the other, and there is no way to do it with fewer than three edits:

1. kitten → sitten (substitution of "s" for "k")
2. sitten → sittin (substitution of "i" for "e")
3. sittin → sitting (insertion of "g" at the end).

Upper and Lower Bounds

The Levenshtein distance has several simple upper and lower bounds. These include:

*   It is always at least the difference of the sizes of the two strings.
*   It is at most the length of the longer string.
*   It is zero if and only if the strings are equal.
*   If the strings are the same size, the Hamming distance is an upper bound on the Levenshtein distance.
*   The Levenshtein distance between two strings is no greater than the sum of their Levenshtein distances from a third string (triangle inequality).

2.9.2 Applications

In approximate string matching, the objective is to find matches for short strings in many longer texts, in situations where a small number of differences is to be expected. The short strings could come from a dictionary, for instance. Here, one of the strings is typically short, while the other is arbitrarily long. This has a wide range of applications, for instance, spell checkers, correction systems for optical character recognition, and software to assist natural language translation based on translation memory.

The Levenshtein distance can also be computed between two longer strings, but the cost to compute it, which is roughly proportional to the product of the two string lengths, makes

this impractical. Thus, when used to aid in fuzzy string searching in applications such as record linkage, the compared strings are usually short to help improve speed of comparisons.

2.10 Lee Distance

In coding theory, the Lee distance is a distance between two strings $x_1, x_2,..., x_n$ and $y_1, y_2,...., y_n$ of equal length n over the q-ary alphabet $\{0, 1, ..., q-1\}$ of size $q \geq 2$. It is a metric, defined as

$$\sum_{i=1}^{n} \min(|x_i - y_i|, q - |x_i - y_i|).$$

If $q = 2$ the Lee distance coincides with the Hamming distance.

The metric space induced by the Lee distance is a discrete analog of the elliptic space.

Example

If $q = 6$, then the Lee distance between 3140 and 2543 is $1 + 2 + 0 + 3 = 6$.

The Lee distance is named after C. Y. Lee. It is applied for phase modulation while the Hamming distance is used in case of orthogonal modulation.

CHAPTER III

Iterated Local Search Approach for Maximin Latin Hypercube Designs

3.1 Introduction

The Latin hypercube design is a popular choice of experimental design when computer simulation is used to study a physical process. These designs guarantee uniform samples for the marginal distribution of each single input. A number of methods have been proposed [Lourenco et al. (2002), Martin and Otto(1996)] for extending the uniform sampling to higher dimensions. We show how to construct Latin hypercube designs in which all main effects are orthogonal. Our method can also be used to construct Latin hypercube designs with low correlation of first-order and second-order terms. Our method generates orthogonal Latin hypercube designs that can include much more factors than those proposed by Ye [Ye (1998)].

3.2 Iterated Local Search

The importance of high performance algorithms for tackling difficult optimization problems cannot be understated, and in many cases the only available methods are metaheuristics. The word metaheuristics contains all heuristics methods that show evidence of achieving good quality solutions for the problem of interest within an acceptable time. Metaheuristic techniques have become more and more competitive. When designing a metaheuristic, it is preferable that it be simple, both conceptually and in practice. Naturally, it also must be effective, and if possible, general purpose. The main advantage of this approach is the ease of implementation and the quickness.

As metaheuristics have become more and more sophisticated, this ideal case has been pushed aside in the quest for greater performance. As a consequence, problem-specific knowledge (in addition to that built into the heuristic being guided) must now be incorporated into metaheuristics in order to reach the state of the art level. Unfortunately,

this makes the boundary between heuristics and metaheuristics fuzzy, and we run the risk of losing both simplicity and generality.

Here a well-known metaheuristics approaches, namely general Iterated Local Search (ILS) has been discussed. Iterated Local Search is a metaheuristic designed to embed another, problem specific, local search as if it were a black box. This allows Iterated Local Search to keep a more general structure than other metaheuristics currently in practice.

The essence of metaheuristic - the iterated local search - 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. This simple idea [Baxter (1981)] has a long history, and its rediscovery by many authors has led to many different names for iterated local search like iterated descent [Baum (1986a), Baum (1986b)], large-step Markov chains [Martin et al. (1991)], iterated Lin-Kernighan [Johnson (1990)], chained local optimization [Martin and Otto (1996)], or combinations of these [Applegate et al. (1999)]. There are two main points that make an algorithm an iterated local search: (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 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^*)

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

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

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 $s^{*\prime}$ in S^*. If $s^{*\prime}$ 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 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 $s^{*\prime}$ 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

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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 [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 fixed number of cycles have finished;
- the best solution has not changed for a predefined number of cycles;

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- a solution has been found that is beyond some predefined threshold.

ILS has many of the desirable features of a metaheuristic: 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 straight-forward 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, $\forall\ i, j = 1, 2, \cdots$, N:

$$d_p = \| x_i - x_j \|_p \tag{3.1}$$

Unless otherwise mentioned, we will only consider the Euclidean distance measure ($p = 2$) and Rectangular distance ($p = 1$). In fact, we will usually consider the squared value of d_p (in brief d), i.e. d^2 (saving the computation of the square root) in case of Euclidean

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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, $x_i = (x_{i1}, x_{i2}, \cdots, x_{ik}) : i = 0, 1, \ldots, N-1$, 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 $0, 1, \cdots, N-1$ (note that each factor range is normalized to the interval $[0, N-1]$) so that for each dimension j all x_{ij}, $i = 0, 1, \cdots, N-1$ 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:

$$\mathbf{X} = \begin{pmatrix} \mathbf{x}_0 \\ \vdots \\ \mathbf{x}_{N-1} \end{pmatrix} = \begin{pmatrix} x_{01} & \cdots & x_{0k} \\ \vdots & \cdots & \vdots \\ x_{(N-1)1} & \cdots & x_{(N-1)k} \end{pmatrix} \tag{3.2}$$

such that for each $j \in \{1, 2, \cdots, k\}$ and for all $p, q \in \{0, 1, \cdots, N-1\}$ 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 $\mathbf{X}$.

Figure 3.1 show the randomly generated LHD (Fig(a)) and maximin LHD (Fig(c)) regarding Euclidean distance measure obtained by ILS approach. Fig(b) shows the intermediate semi optimal LHD during ILS algorithm run.
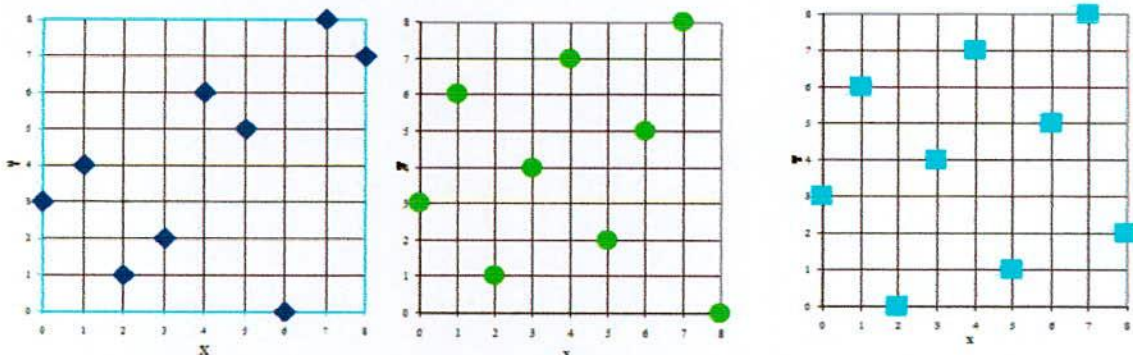
Fig: (a) $D_1^{(2)}(X_r)=2$, $J_1^{(2)}(X_r)=4$
and $D_1^{(1)}(X_r)=2$, $J_1^{(1)}(X_r)=4$

Fig: (b) $D_1^{(2)}(X_{sm})=8$, $J_1^{(2)}(X_{sm})=4$
and $D_1^{(1)}(X_{sm})=4$, $J_1^{(1)}(X_{sm})=13$

Fig: (c) $D_1^{(2)}(X_M)=8$, $J_1^{(2)}(X_M)=2$
and $D_1^{(1)}(X_M)=4$, $J_1^{(1)}(X_M)=9$

Figure 3.1: Some LHDs and their corresponding (D_1, J_1) values in L^2 and L^1 distance measures

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.

3.5 Optimality Criteria

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(D_1, J_1) Optimality Criterion : Under this criterion a LHD Y can be considered better than another one X if a lexicographic ordering holds:

$$D_1(\mathbf{Y}) > D_1(\mathbf{X}) \quad \text{or}$$
$$D_1(\mathbf{Y}) = D_1(\mathbf{X}) \quad \text{and} \quad J_1(\mathbf{Y}) < J_1(\mathbf{X}). \tag{3.3}$$

We illustrate this optimality criterion as follows. Note that we consider here only Euclidean distance measure. In Figure 3.1(a) $\mathbf{X_r}$ is a randomly generated LHD with $(N, k,) = (9,2)$ where $D_1(\mathbf{X_r}) = 2$ and $J(\mathbf{X_r}) = 4$; Figure 3.1 (b) presents an improved configuration $\mathbf{X_{sm}}$ where $D_1(\mathbf{X_{sm}}) = 8$ with $J(\mathbf{X_{sm}}) = 4$. A third LHD X_M is given in Figure 3.1 (c) where $D_1(\mathbf{X_M}) = 8$ and $J_1(\mathbf{X_M}) = 2$; by the Opt(D_1,J_1) criterion this is the best configuration among the three.

By generalizing this approach, we can consider the problem like a multi-objective problem with priorities: maximize the objective with highest priority D_1; within the set of optimal solutions with respect to D_1, minimize the objective with second highest priority J_1. Note that Johnson et al. [Johnson et al. (1990)] first proposed this optimality criterion.

Opt(φ) Optimality Criterion : As previously remarked, if there exist different LHDs with equal D_1 and J_1 values, i.e. in case there exist at least two LHDs $\mathbf{X}$, $\mathbf{Y}$ such that $D_1(\mathbf{X}) = D_1(\mathbf{Y}) = D_1$ and $J_1(\mathbf{X}) = J_1(\mathbf{Y}) = J_1$, we could further consider the objective D_2 and maximize $D_2(\mathbf{X})$, the second smallest distance in $\mathbf{X}$, and, if equality still holds, minimize

$J_2(\mathbf{X})$, the number of occurrence of $D_2(\mathbf{X})$, and so on. Then an optimal design $\mathbf{X}$ sequentially maximizes D_{is} and minimizes J_{is} in the following order: $D_1, J_1; D_2, J_2, \cdots, D_m, J_m$. Morris and Mitchell [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

$$\phi_p(x) = \sum_{r=1}^{m} \left[\frac{J_r(X)}{(D_r(X))^p} \right]^{\frac{1}{p}} \tag{3.4}$$

where p is a positive integer parameter. Under this criterion, LHD $\mathbf{Y}$ is better than $\mathbf{X}$ if

$$\phi_P(\mathbf{Y}) < \phi_R(\mathbf{X}).$$

Note that for large enough p, each term in the sum in (3.4) dominates all subsequent terms. Through p we can control the impact of the different D_r distances: as p increases, the impact of distance D_1 becomes more and more relevant. In the form (3.4), the evaluation of ϕ_p would be computationally costly. However, it has a computationally cheaper form (see [Jin et al. (2005)]). Indeed, (3.4) can be simplified as

$$\phi_P(X) = \left[\sum_{i=1}^{N} \sum_{j=i+1}^{N} \frac{1}{d_{ij}^P} \right]^{\frac{1}{P}} \tag{3.5}$$

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

An apparent drawback of the Opt(ϕ) criterion, if we are interested in maximin 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 $\mathbf{X}$ and $\mathbf{Y}$ such that $\emptyset_p(\mathbf{X}) < \emptyset_p(\mathbf{Y})$ and $D_1(\mathbf{X}) < D_1(\mathbf{Y})$. This phenomenon has been frequently observed in our computational experiments. 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 mixed approach might appear strange but, as we will demonstrate experimentally, it can be extremely effective.

While the two criteria above are strictly related to maximin values and they will be widely employed in the definition of approaches for detecting maximin solutions, for the sake of completeness, we also mention that also other optimality criteria, not necessarily related

with maximin values, are available in the literature. We present a couple of them as well as the approaches for constructing the optimal Latin hypercube design in Table 3.1.

Table 3.1: Some well know approaches as well as optimal criterion for optimal experimental designs

Researchers	Year	Algorithm	Objective functions
Audze and Eglajs	1977	Coordinates Exchange Algorithm	Potential Energy
Park	1994	A 2-stage(exchange-and Newton-type) algorithm	Integrated mean squared error and entropy criteria
Morris and Mitchell	1995	Simulated annealing	ϕ_p criterion
Ye et al.	2000	Columnwise-pairwise	ϕ_p and entropy criteria
Fang et al.	2000(a)	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	Minimum distance and Audze-Eglajs function
Dam et al.	2007(b)	Branch-and-bound algorithm	1-norm and infinite norm distances
Grosso et al.	2008	Iterated local search and simulated annealing algorithms	ϕ_p criterion

3.6 ILS Heuristic 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), Local Search (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 bellow:

Step 1. **Initialization** : $X = I_S(\{0, 1, \ldots, N-1\})$

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

Each component of the algorithm is briefly discussed below.

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 $h \in \{1, 2, \ldots, k\}$ a random permutation $v_0, v_1, \ldots, v_{N-1}$ of the integers $0, 1, \ldots, N-1$ is generated and we set

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

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 $\mathbf{X} = (x_1, x_2, \ldots, x_N)$, its neighborhood is made of

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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 **X**, if

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

i.e., the minimum distance from $\mathbf{x}_i$ to all other points is also the minimum one among all the distances in **X**. We denote by $I(X)$ $\{1, 2, \ldots, N\}$ 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 **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:

$$x_{i1,p} \leftrightarrow x_{i2,q} \, \forall \, p, q = 1, 2, \ldots, k : p \neq q,$$

and finds the best exchange among them. The CP algorithm proposed by Morris and Mithchell [Morris and Mitchell (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 Opt(ϕ) optimal criteria.

The definition of Rowwise-Pairwise Critical Local Moves (we call it LM_{RpD1}) 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 $i \in I(X)$, $r, j \in \{1, 2, \ldots, N\}$, $h, \ell \in \{1, 2, \ldots, k\}$, swapping the ℓ-th component gives the neighbor Y defined by

$$y_{rh} = \begin{cases} x_{rh} & \text{if } r \neq i \text{ or } h \neq \ell \\ x_{ih} & \text{if } r = j \text{ and } h = \ell \\ x_{jh} & \text{if } r = i \text{ and } h = \ell \end{cases} \tag{3.6}$$

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.

| Initial solution – LHD A | After single Local Move, nbh sol. LHD B | After complete LS – LHD C |

Fig: (a) $D_1^{(2)}(X_A)=2$, $J_1^{(2)}(X_A)=3$ Fig: (b) $D_1^{(2)}(X_B)=2$, $J_1^{(2)}(X_B)=1$ Fig: (c) $D_1^{(2)}(X_C)=8$, $J_1^{(2)}(X_C)=4$
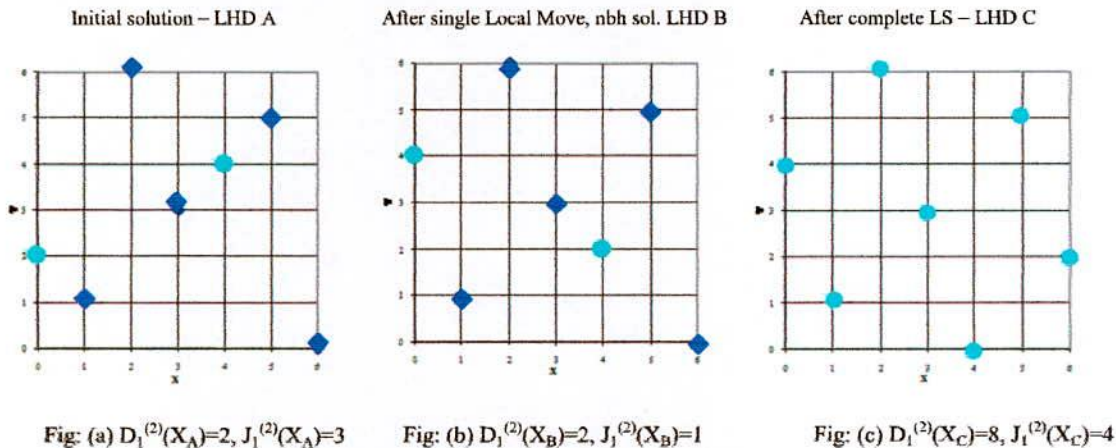
Figure 3.2: Illustration of Neighborhood solutions for LM_{RpD1} based local search (LS) procedure

We now illustrate the RP based local moves by considering a randomly generated initial design A: $(N, k) = (7, 2)$ (see 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 $(4, 4)$ (See Figure 3.2 (b)).

Also note that LHD **B** is an improving neighbor of LHD **A**, since $(D_1, J_1)(\mathbf{B}) = (2, 1)$ whereas $(D_1, J_1)(\mathbf{A}) = (2, 3)$. Finally Figure 3.2 (c) shows the maximin LHD produced by the Local search procedure. Though the algorithm optimized the LHD regarding Euclidean distance measure but the LHD is improved regarding Manhattan distance measure too (see 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 (see [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(ϕ) optimality criterion. So for the Opt(D_1, J_1) optimality criterion: "**Y** is better than **X**" if

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

On the other hand for Opt(ϕ) optimality criterion : "**Y** is better than **X**" if

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

where ϕ_p is defined by (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 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.
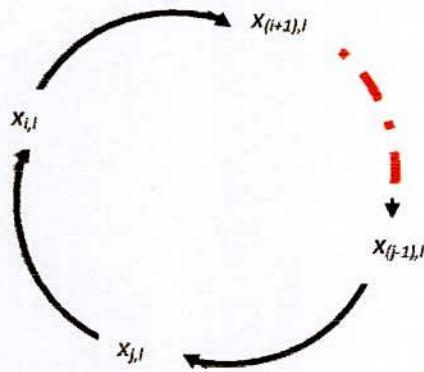
Figure 3.3: Illustration of Cyclic Order Exchange perturbation technique

(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 m. Finally, we swap in cyclic order the value of component m from point x_i to point x_j. The pseudo-code structure for SCOE is the following.

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 m

Step 3a: set temporarily $x'_{jm} = x_{jm}$

for $t = j, j - 1, \ldots, i - 1$ **do**

Step 3b: Replace the component $x_{(t)m}$ by $x_{(t-1)m}$

end for

Step 3c: and replace x_{im} by x'_{jm}

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 $N = 6$ and $k = 8$(see Eq. (3.7)).

$$\mathbf{X^*} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{pmatrix} = \begin{pmatrix} 0 & 2 & 1 & 3 & 5 & 5 & 4 & 2 \\ 1 & 3 & 2 & 2 & 0 & 3 & 3 & 4 \\ 2 & 1 & 4 & 5 & 2 & 2 & 1 & 3 \\ 3 & 4 & 5 & 0 & 3 & 1 & 0 & 1 \\ 4 & 5 & 0 & 4 & 1 & 4 & 2 & 0 \\ 5 & 0 & 3 & 1 & 4 & 0 & 5 & 5 \end{pmatrix} \tag{3.7}$$

Now we randomly choose two rows (points), say x_2 and x_5 and we randomly choose the column (component) $m = 4$. Then, after the SCOE perturbation we get the following LHD $\mathbf{X'}$ (Eq. (3.8), note that bold faces indicate the values modified with respect to $\mathbf{X^*}$).

$$\mathbf{X'} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{pmatrix} = \begin{pmatrix} 0 & 2 & 1 & 3 & 5 & 5 & 4 & 2 \\ 1 & 3 & 2 & \mathbf{4} & 0 & 3 & 3 & 4 \\ 2 & 1 & 4 & \mathbf{2} & 2 & 2 & 1 & 3 \\ 3 & 4 & 5 & \mathbf{5} & 3 & 1 & 0 & 1 \\ 4 & 5 & 0 & \mathbf{0} & 1 & 4 & 2 & 0 \\ 5 & 0 & 3 & 1 & 4 & 0 & 5 & 5 \end{pmatrix} \tag{3.8}$$

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.

2. 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).

$$X* = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{pmatrix} = \begin{pmatrix} 5 & 2 & 1 & 3 & 5 & 5 & 4 & 2 \\ 0 & 3 & 2 & 4 & 0 & 3 & 3 & 4 \\ 1 & 1 & 4 & 2 & 2 & 2 & 1 & 3 \\ 2 & 4 & 5 & 5 & 3 & 1 & 0 & 1 \\ 3 & 5 & 0 & 0 & 1 & 4 & 2 & 0 \\ 4 & 0 & 3 & 1 & 4 & 0 & 5 & 5 \end{pmatrix} \tag{3.9}$$

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(2a) 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 $1, 2, \ldots, l$ 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 $k = 1, 2, \ldots, l$ do

   Step 3: swap(x_{ik}, x_{jk})

  end for

Before Crossover

$$x_i = \boxed{\begin{array}{cc} 0 & 3 \end{array}} \begin{array}{cccccc} 2 & 4 & 0 & 3 & 3 & 4 \end{array}$$

$$x_j = \boxed{\begin{array}{cc} 4 & 0 \end{array}} \begin{array}{cccccc} 3 & 1 & 4 & 0 & 5 & 5 \end{array}$$

After Crossover

$$x_i' = \boxed{\begin{array}{cc} 4 & 0 \end{array}} \begin{array}{cccccc} 2 & 4 & 0 & 3 & 3 & 4 \end{array}$$

$$x_j' = \boxed{\begin{array}{cc} 0 & 3 \end{array}} \begin{array}{cccccc} 3 & 1 & 4 & 0 & 5 & 5 \end{array}$$
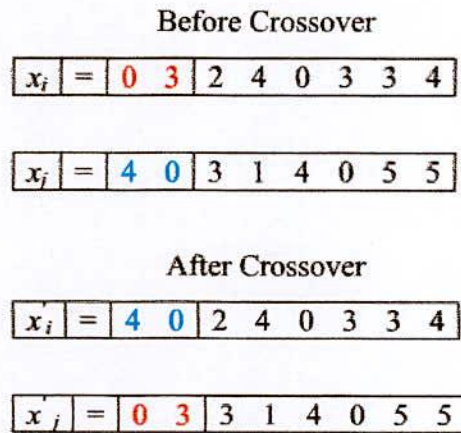
Figure 3.4: Illustration of Single Pair Crossover perturbation technique

$$X^* = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{pmatrix} = \begin{pmatrix} 0 & 2 & 1 & 3 & 5 & 5 & 4 & 2 \\ 4 & 5 & 0 & 4 & 0 & 3 & 3 & 4 \\ 2 & 1 & 4 & 5 & 2 & 2 & 1 & 3 \\ 3 & 4 & 5 & 0 & 3 & 1 & 0 & 1 \\ 1 & 3 & 2 & 2 & 1 & 4 & 2 & 0 \\ 5 & 0 & 3 & 1 & 4 & 0 & 5 & 5 \end{pmatrix} \tag{3.10}$$

Now we illustrate the SPC perturbation by an example; we again consider the LHD X^* (Eq. (3.10)). We randomly choose a pair of rows (points), say x_2 and x_6, and randomly fix a column, say $l_2 = 2$. Then after SPC perturbation on X^* we get the following final LHD X ' (Eq. (3.11) note that the bold faces denote the values modified with respect to X^*).

$$X' = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{pmatrix} = \begin{pmatrix} 0 & 2 & 1 & 3 & 5 & 5 & 4 & 2 \\ \mathbf{5} & \mathbf{0} & 0 & 4 & 0 & 3 & 3 & 4 \\ 2 & 1 & 4 & 5 & 2 & 2 & 1 & 3 \\ 3 & 4 & 5 & 0 & 3 & 1 & 0 & 1 \\ 1 & 3 & 2 & 2 & 1 & 4 & 2 & 0 \\ \mathbf{4} & \mathbf{5} & 3 & 1 & 4 & 0 & 5 & 5 \end{pmatrix} \tag{3.11}$$

3.6.6 Stopping Rule (S_R)

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

CHAPTER IV

Optimality Analysis of the Experimental Results Regarding
Euclidean Distance

4.1 Introduction

In this chapter we will discuss about the optimality of the experimental results obtained by ILS approach. At first we will display the optimal LHDs to show the performance of ILS approach regarding Euclidean distance measure. Then we will also briefly discuss about the multicollinearity of the optimal LHDs obtained by ILS approach.

4.2 Experimental Results and Discussion for Euclidean Measure

The parameter setting for the experiments, as Jamali (2009) considered, is given in Table 4.1 and 4.2. For the comparison of ILS approach with the existing literatures, we will refer to [Jamali (2009)]. In that dissertation the approach in [Morris and Mitchell (1995)] denoted as SA_M (simulated Annealing (modified), and the approaches proposed in [Husslage et al. (2006)] denoted as PD (periodic Design), SA (simulated Annealing) and MS denoted multi-start random generated approaches. We have also denoted the updated website values as Web (or Best known) values. The improvements obtained through the PD and SA approaches are discussed in Husslage et al. (2006).

Table 4.1: Parameter setting for the experiments of ILS approach

Experimental design	LHD	Perturbation Technique	SCOE
Method	ILS	Stopping Rule	MaxNonImp parameter value
Optimal Criteria	Opt(ϕ)	MaxNonImp setting	100
Local Move	RP	Parameter, p	20
Acceptance Rule	BI		

Table 4.2: The setting of number of runs (R) for the ILS approach

k	N	R
3-10	2-25	500
3-10	26-50	100
3,4,5	51-100	50
6-10	51-100	10

The experimental results of ILS approach regarding Euclidean measure [Jamali, 2009] are given in the Table 4.3 and Table 4.4. We observe that ILS is able to detect a very large amount of improved solutions with respect to the best known ones. It is worthwhile to remark that for large (k, N) values the improvement of each LHD obtained by ILS approach is very significance. For the better visualization of the above results, Table 4.5 displays the summary of the performance of the several approaches. In the first row of Table 4.5 identical means, ILS approach able to identical solution compare to the best known results available in the literature whereas Worse means the solution obtained by ILS approach are worse compare to best known results. The performance of ILS approach regarding maximin LHDs in L^2 measure is remarkable compare to other approaches available in the literature. This is, especially, true at large k values. For $k \geq 6$, with the exception of few numbers of low N values, all the solutions returned by ILS are better compare to the best known results. 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 4.6. 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. 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.

Table 4.3: Comparison among PD, SA, Web 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	Web	ILS	PD	SA	Web	ILS	PD	SA	Web	ILS	PD	SA	Web	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	50	50	55	82	82	82	62	91	91	92
11	24	30	30	30	39	55	55	55	55	80	80	81	62	108	108	110
12	30	36	36	36	46	63	63	63	62	91	91	93	91	136	139	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	54	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	121	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	243	266	269	258	343	374	378
25	91	81	91	86	156	162	178	181	205	255	285	286	286	368	400	408
26	91	86	91	89	156	171	188	189	226	269	302	306	296	387	426	439
27	91	90	91	91	157	178	198	198	238	287	310	326	310	410	447	474
28	94	94	94	98	174	188	210	212	258	302	331	349	339	427	479	494
29	94	98	101	102	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	114	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	133	126	230	244	273	274	358	403	445	460	470	586	648	668
35	133	122	133	129	234	255	286	289	366	418	467	482	495	601	683	697
36	133	129	133	136	250	261	297	298	400	427	486	502	518	631	719	739
37	152	131	152	140	266	275	309	308	408	454	520	530	528	648	744	775
38	152	134	152	142	283	279	321	322	415	464	541	557	561	681	788	813
39	152	139	152	149	283	290	330	330	439	486	566	575	561	706	816	846
40	155	146	155	152	291	301	342	345	492	505	575	590	632	739	876	886
41	162	147	162	155	293	309	355	354	492	525	596	618	632	776	882	938
42	168	152	168	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	186	178	331	349	396	393	548	582	680	688	696	862	992	1041
45	186	166	186	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	774	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	213	206	415	414	478	473	663	699	830	830	893	1042	1203	1218
51	213	189	213	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	233	227	477	454	534	526	760	783	932	935	1019	1171	1359	1392
55	243	214	243	233	483	471	546	541	760	805	956	966	1082	1198	1421	1432
56	243	216	243	235	515	479	558	565	784	830	982	992	1104	1236	1431	1484
57	261	221	261	241	515	490	574	570	846	854	1007	1018	1136	1265	1488	1523
58	261	227	261	246	539	500	594	591	846	878	1035	1046	1166	1303	1554	1559
59	266	229	266	254	544	519	609	607	849	903	1063	1064	1223	1328	1564	1615
60	273	237	273	258	568	530	618	622	904	928	1094	1101	1242	1381	1631	1647
61	274	244	274	262	620	538	630	641	904	939	1128	1134	1258	1413	1667	1703
62	283	245	283	269	620	554	657	645	934	991	1150	1156	1306	1450	1715	1756
63	297	249	297	276	620	575	670	666	967	989	1178	1187	1380	1497	1781	1781
64	297	258	297	281	625	579	684	678	985	1009	1206	1223	1430	1526	1804	1834
65	314	260	314	286	630	583	694	701	997	1035	1216	1239	1430	1565	1868	1884
66	314	269	314	294	666	603	718	706	1050	1051	1261	1272	1476	1590	1874	1926
67	314	270	314	297	666	614	735	726	1072	1085	1299	1283	1482	1646	1954	1977
68	314	278	314	306	685	623	746	738	1087	1119	1330	1360	1538	1664	1983	2014
69	324	280	324	310	698	650	765	754	1112	1114	1351	1399	1588	1704	2028	2070
70	325	285	325	313	716	658	779	773	1150	1135	1378	1439	1633	1759	2094	2116
71	325	289	325	325	716	665	793	795	1150	1187	1413	1416	1644	1783	2141	2168
72	341	296	341	326	750	678	810	810	1203	1197	1430	1454	1768	1863	2136	2215
73	350	299	350	329	759	688	834	818	1229	1243	1462	1549	1768	1872	2197	2252
74	350	306	350	341	767	703	842	845	1229	1269	1512	1562	1774	1910	2291	2299
75	350	310	350	345	771	714	867	854	1274	1283	1530	1571	1862	1963	2303	2365
76	363	324	363	349	813	750	882	877	1300	1318	1569	1597	1935	2024	2387	2415
77	363	325	363	355	823	762	894	890	1308	1331	1591	1631	1947	2051	2433	2456
78	387	337	387	362	844	761	910	906	1382	1360	1621	1654	2014	2079	2479	2502
79	387	333	387	376	848	788	927	921	1382	1399	1639	1668	2037	2120	2498	2550
80	403	344	403	371	873	786	949	943	1395	1430	1691	1690	2037	2154	2554	2597
81	406	338	406	381	916	783	963	972	1406	1431	1730	1731	2064	2217	2648	2665
82	406	353	406	389	938	825	989	979	1475	1483	1742	1773	2141	2239	2680	2715
83	417	369	417	401	940	825	1002	1006	1501	1509	1762	1804	2141	2290	2696	2752
84	426	363	426	401	967	838	1021	1015	1534	1510	1818	1825	2229	2325	2790	2803
85	426	369	426	406	967	877	1043	1032	1552	1566	1866	1871	2232	2399	2819	2877
86	428	376	428	422	967	867	1053	1047	1573	1578	1882	1890	2375	2437	2875	2929
87	428	374	428	419	976	877	1073	1062	1598	1589	1934	1922	2375	2476	2913	2988
88	437	374	437	426	1050	890	1086	1079	1685	1629	1954	1963	2398	2513	2975	3075
89	443	378	443	432	1050	907	1102	1102	1690	1654	1990	2009	2400	2562	3067	3104
90	481	384	481	437	1060	940	1134	1116	1710	1696	2027	2032	2516	2633	3104	3134
91	481	393	481	450	1089	951	1134	1146	1748	1724	2031	2054	2516	2674	3143	3192
92	481	394	481	457	1089	966	1149	1154	1805	1756	2100	2117	2599	2729	3216	3243
93	481	402	481	456	1098	963	1171	1169	1813	1795	2130	2122	2604	2726	3283	3305
94	481	405	481	461	1124	986	1199	1198	1881	1811	2169	2165	2747	2788	3348	3360
95	481	413	482	474	1135	1010	1219	1223	1901	1846	2206	2202	2747	2817	3335	3455
96	509	414	509	475	1261	1023	1261	1228	1965	1863	2227	2261	2769	2911	3451	3497
97	515	419	515	489	1261	1027	1261	1245	1965	1899	2299	2269	2817	2960	3514	3546
98	531	429	531	486	1261	1055	1283	1266	1965	1929	2299	2309	2850	3001	3560	3606
99	531	449	531	497	1261	1040	1298	1290	2009	1950	2338	2356	2878	3041	3628	3652
100	554	451	554	502	1261	1074	1305	1313	2053	1975	2401	2388	3000	3117	3648	3710

Table 4.4: Comparison among PD, SA, Web 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	Web	ILS	SA	Web	ILS	SA	Web	ILS	SA	Web	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	54	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	110	111	130	131	133	154	154	157	172	172	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	219	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	4809	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	6227	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	8258	8344	9617	9998
	3903	4335	5040	5184	5597	6617	6692	6983	8228	8464	8450	9835	10233

Table 4.5: Summary of the comparison among several approaches of finding maximin LHDs for *N*=2 to 100

k	Number of best solutions (maximin LHD)						Identical	Worse
	PD	SA	SA_M	Web	MS	ILS	ILS	ILS
3	61	0	0	65	0	14	20	65
4	02	0	0	47	0	34	18	47
5	00	0	0	11	0	78	10	11
6	00	0	0	00	0	90	09	00
7	00	0	0	00	0	92	07	00
8		0	0	00	0	93	06	00
9		0	0	00	0	93	06	00
10		0	0	00	0	92	07	00

Table 4.6: 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
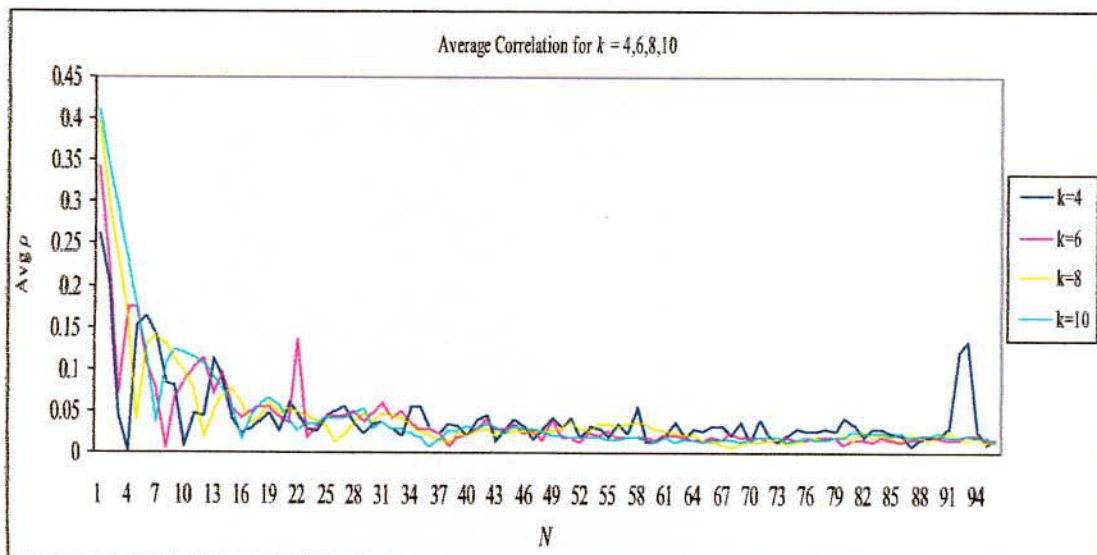
Figure 4.1: Muliticollinearity analysis of the LHDs obtained by ILS approach

From the above discussion it is clear that ILS approach is state-of arts for optimality analysis regarding Euclidian distance measure as well as computational cost. Aparna (2012) also analyzed the performance of ILS approach regarding multicollinearity of the optimal LHD measured in Euclidean distance. The experimental results regarding average correlation are given in the Figure 4.1. It is noted that the average coefficient of correlation are calculated as define in [Aparna 2012]. We observe that, except few LHDs, the average coefficients of correlations among factors are less than 0.2. It may conclude that the optimal LHDs optioned by ILS approach regarding Euclidean measure have poor multicollinearity i.e. among the factors of each LHD exists good orthogonality property. It is also remarkable that the avarage coeffient of correlations are decreses with the increases of number of factors. It is whorthwhile to mention here that the performance of ILS approach is increase with the increase of factors as well as incerasing of number of design points (see Table 4.5).

CHAPTER 5

Optimality Analysis and Discussion of the Experimental Results
Regarding Manhattan Distance

5.1 Introduction

In the previous section we have performed several experiments in ILS approach for LHDs regarding Euclidean distance measure. In this chapter at first we will perform several experiments on the LHDs obtained by ILS approach regarding Manhattan distance measure. Then we will compare the experimental results with available ones in the literature. Moreover we also perform some more experiments on the maximin LHDs obtained by ILS approach to find out some more interesting characteristics.

5.2 Experimental Results and Comparison for Manhattan Measure

It is noted that finding optimal LHD in Manhattan (Rectangular) distance measure is more complicated [Toth (1971)]. Anyway the purpose is not to perform experiments to optimize LHD by ILS in Manhattan distance measure; rather the maximin LHD in Rectangular distance measure will be studied where the designs are optimized by ILS approach regarding Euclidian distance measure.

Actually in this study, the optimal LHD namely maximin LHD obtained by the ILS approach (MLH-ILS) will be considered in which distance is measured in Euclidian distance measure (L^2). Then the minimum inter-site distance will be measured among the design points of the MLH-ILS design by Rectangular distance measure (L^1). In what follow the notation – $D_1^{(L1)}$ or $D_1(J_1)^{(L1)}$ and $D_1^{(L2)}$ or $D_1(J_1)^{(L2)}$ denote the minimum inter-site distance of an LHD measured by the Manhattan distance measure and Euclidean distance measure respectively. Note that in the above notation J_1 means number of duplications of D_1 value in the LHD. In these experiments we considered ρ, ρ_{max}, $D_1(J_1)^{(L1)}$,

$\Phi^{(L1)}$, $D_1(J_1)^{(L2)}$ and $\Phi^{(L2)}$ properties. Here the notation ρ and ρ_{max} denote average pairwise correlation maximum pair-wise correlation among the factors of the LHD measured as follows(Aparna 2012):

$$\rho^2 = \frac{\sum_{i=2}^{k}\sum_{j=1}^{i-1}\rho_{ij}^2}{k(k-1)/2} \quad \text{and} \quad \rho_{max} = \max_{1 \le i,j \le k} \rho_{ij},$$

where ρ_{ij} be the pairwise linear product-moment coeffient of corelation between factors i and j.

The notation $\Phi_p^{(L1)}$ and $\Phi_p^{(L2)}$ indicate the value of Φ_p (see Eq. (1.1)) measured by Manhattan distance measure and Euclidean distance measure respectively. The optimal criterion (Φ_p, ρ^2) denotes the multi-objective function where the algorithm optimized $\omega_1\rho^2 + \omega_2\Phi_p$ criterion [Joseph and Hung (2008)] where ω_1, ω_2 are weight factors (optimized both minimum distance criterion as well as correlation criterion). On the other hand the optimal criterion (Φ, D1) indicates optimized Φ_p value but tracking the best $D_1(J_1)$ during algorithm searches feasible space. That is though ILS algorithm optimize Φ_p criterion but it does not consider LHD which corresponding to best Φ_p rather it considers LHD which has best $D_1(J_1)$ value in the track of search. The optimal criterion $\rho = 0$ means the optimal LHD must has zero correlation among the factors.

For the first experiment, we first consider optimal LHD (with (N, k) = (5, 3)) denoted as MLH-ILS. Now we have performed experiments on that LHD to find out $D_1(J_1)^{(L1)}$ and characteristics as indicated with first column of the Table 5.1. The experimental result is given in the Table 5.1.

It is observed in the Table 5.1 which is also eventually true that MLH-SA is better in $D_1(J_1)^{(1)}$ value as it is optimized regarding L^1 measure; similarly **OMLH –MSA** is better than others LHDs regarding correlation. Similar case is occurred in the Table 5.2 also. It is worthwhile to mention here that **OLH-Y** is better compare to OMLH – MSA, off course, as well as to other LHDs regarding multicollinearity because the LHDs, considered in **OLH- Y,** has inherently zero multicollinearity. It is also no doubt that **MLH -ILS** is the best compare to all other LHDs regarding $D_1(J_1)^{(L2)}$ and $\Phi_p^{(L2)}$ as ILS approach considered L^2 distance measure. But it is remarkable that $D_1(J_1)^{(2)}$ value is significantly better in **MLH -ILS** obtained by ILS approach. It is also noted that though, in **MLH-SA,** SA approach

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considered L^1 measure whereas, in **MLH –ILS,** ILS approach considered L^2 measure for obtaining maximin LHD, the $D_1(J_1)^{(L1)}$ value of **MLH -ILS** is comparable with **MLH-SA.** Moreover the $D_1(J_1)^{(L1)}$ value of **ILS** approach is almost identical with other approach in both the design considered here. It is observed in the table that though in MLH-ILS, considered L^2 distance measure, the $\Phi^{(L1)}$ values of MLH-ILS design is comparable of the other two designs. On the other hand the $\Phi^{(L2)}$ values of MLH-ILS design is significantly better than those of the other two designs. It is also observed that the design OMLH-MSA is best than the other two regarding multicollinearity, since the designs are optimized regarding average correlation ρ value. But MLH-ILS design is better than the design MLH-SA regarding both ρ and ρ_{max} values.

Table 5.1: The comparison of MLH-ILS vs MLH-SA and OMLH – MSA for $(N, k) = (5, 3)$

Method →	MLH-SA	OMLH-MSA	MLH-ILS
Optimal Latin Hypercube Design Matrix →	1 1 2 2 5 3 3 2 5 4 3 1 5 4 4	1 2 3 2 4 5 3 5 1 4 1 2 5 3 4	1 3 5 2 2 2 3 5 1 4 4 4 5 1 3
Optimal Criteria →	Φ_p	(Φ_p, ρ^2)	(Φ, D_1)
Distance measure →	L^1	L^1	L^2
PROPERTIES ↓			
ρ →	0.265	**0.0816**	0.200
ρ_{max} →	0.4	**0.1**	0.200
$D_1(J_1)^{(L1)}$ →	**5(3)**	5(4)	5(6)
$\Phi_p^{(L1)}$ →	**0.2170**	.2201	0.21879
$D_1(J_1)^{(L2)}$ →	9(1)	9(2)	**11(6)**
$\Phi_p^{(L2)}$ →	0.1113	0.1151	**0.09956**

Similarly we have again performed experiment on optimal LHD (with $(N, k) = (9, 4)$) denoted as MLH-ILS. The experimental results are given in the Table 5.2.

Table 5.2: The comparison of MLH-ILS vs MLH-SA, OMLH – MSA and OLH-Y for $(N, k) = (9, 4)$

Method →	MLH-SA	OMLH - MSA	OLH- Y	MLH- ILS
Optimal Latin Hypercube Design Matrix →	1 3 3 4	1 5 3 3	1 2 6 3	1 5 8 4
	2 5 8 8	2 2 5 8	2 9 7 6	2 7 4 9
	3 8 6 2	3 9 7 5	3 4 2 9	3 2 1 6
	4 7 1 6	4 3 8 1	4 7 1 2	4 8 3 3
	5 2 9 3	5 7 1 7	5 5 5 5	5 1 5 1
	6 9 5 9	6 6 9 9	6 3 9 8	6 3 7 8
	7 1 4 7	7 1 2 4	7 6 8 1	7 6 9 2
	8 4 2 1	8 8 4 2	8 1 3 4	8 9 6 7
	9 6 7 5	9 4 6 6	9 8 4 7	9 4 2 5
Optimal Criteria →	Φ_p	(Φ_p, ρ^2)	$\rho = 0$	Φ_p, D_1
Distance measure →	L^1	L^1	L^1	L^2
PROPERTIES ↓				
ρ →	0.108	0.063	0.000	0.151
ρ_{max} →	0.217	0.117	0.000	0.233
$D_1(J_1)^{(L1)}$ →	**11(3)**	11(4)	10(8)	10(4)
$\Phi_p^{(L1)}$ →	**0.105**	**0.105**	0.115	0.108
$D_1(J_1)^{(L2)}$ →	33(2)	31(1)	30(8)	**42(6)**
$\Phi_p^{(L2)}$ →	0.031	0.033	0.037	**0.026**

Again in the Table 5.2, it is observed that the designs MLH-SA, OMLH-MSA and OLH-Y are optimized regarding Rectangular distance measure (L^1) whereas the proposed design – MLH-ILS is optimized regarding Euclidian distance measure (L^2). It is observed in the table that though L^2 distance measure is considered in MLH-ILS design, the $D_1(J_1)^{(L1)}$ and $\Phi^{(L1)}$ values of MLH-ILS design are comparable with respect to the other three designs. On the other hand $D_1(J_1)^{(L2)}$ and $\Phi^{(L2)}$ values of MLH-ILS design are significantly better than the other three designs considered. It is also noticed that regarding correlation parameters ρ and ρ_{max}, OLH-Y design is better comparing with the other three designs but regarding $D_1(J_1)^{(L2)}$, OLH-Y design is worst one. It is noted that in the design OMLH-MSA, correlation criterion ρ is partially minimized and in the OLH-Y design, designs are chosen so that ρ be zero. On the other hand MLH-ILS design is comparable with both the designs MLH-SA and

OMLH-MSA with respective to correlation parameter ρ and ρ_{max}. That is except OLH-Y the multicolinearity of MLH- ILS is comparable with other approaches.

Now some experiments will be performed for comparison of $D_1(J_1)^{(L1)}$ values (minimum inter-site distance measured in Manhattan distance measure) of the designs available in the web www.spacefillingdesigns.nl. The Manhattan distance measure (L^1) based maximin LHDs, available in the web, are denoted by MLH-Web. Note that the maximin designs, considered here from the web, are optimized regarding Manhattan distance measure. On the other hand it is mentioned here again that the proposed designs MLH- ILS is optimized regarding Euclidian distance measure (L^2).

Table 5.3: The comparison of MLH-ILS vs MLH-Web regarding Manhattan distance measure (L^1) for $k = 3, 4, 5, 6$

N	k=3		k=4		k=5		k=6	
	MLH-ILS $(D_1^{(L1)})$	MLH-Web $(D_1^{(L1)})$	MLH-ILS $(D_1^{(L1)})$	MLH-Web $(D_1^{(L1)})$	MLH-ILS $(D_1^{(L1)})$	MLH-Web $(D_1^{(L1)})$	MLH-ILS $(D_1^{(L1)})$	MLH-Web $(D_1^{(L1)})$
4	4	4	6	6	8	8	10	10
5	5	5	7	7	10	10	11	12
6	6	6	8	8	10	11	14	14
7	6	6	8	10	12	12	14	16
8	7	7	10		13		16	
9	8	8	10		13		17	
1	7	8	12		15		19	
1	8	8	11		15		19	
1	8	9	13		17		23	
1	9	10	12		17		21	
1	9	10	14		19		24	
1	10	11	14		17		22	
1	9	11	14		19		24	
1	10		14		19		26	
1	10		16		19		27	
1	10		16		21		26	
2	10		18		21		29	
2	11		20		25		29	
2	11		17		23		31	
2	11		18		26		32	
2	11		19		26		33	
2	13		19		27		34	

So in this experiments the $D_1^{(L1)}$ values are just calculated from the MLH-ILS designs which is optimized regarding Euclidean distance measure. For this experiments, we consider factors : $k = 3, 4, \ldots, 6$ and number of points : $N = 4, 5, \ldots, 25$ are considered. Now we have performed experiment on those optimal (MLH-ILS) LHDs to find out $D_1^{(L1)}$) values. The experimental results are shown in the Table 5.3. Note that in the Table 5.3 the symbol $D_1^{(L1)}$ denotes minimum inter-site distance among the points of a design in which distance is measured in Rectangular distance measure. It is noted that there are few values are available in the literature regarding Manhattan distance measure.

Table 5.4: The comparison of MLH-ILS vs MLH-Web regarding Euclidian distance measure (L^2) for $k = 3, 4, 5, 6$

N	k =3		k =4		k=5		k=6	
	MLH-ILS $(D_1^{(L2)})$	MLH-Web $(D_1^{(L2)})$	MLH-ILS $(D_1^{(L2)})$	MLH-Web $(D_1^{(L2)})$	MLH-ILS $(D_1^{(L2)})$	MLH-Web $(D_1^{(L2)})$	MLH-ILS $(D_1^{(L2)})$	MLH-Web $(D_1^{(L2)})$
3	6	6	7	7	8	8	12	8
4	6	6	12	12	14	14	20	18
5	11	9	15	13	24	22	27	24
6	14	14	22	18	32	27	40	36
7	17	12	28	26	40	32	52	52
8	21	21						
9	22	22						
10	27	22						
11	30	22						
12	36	27						
13	41	36						
14	42	34						
15	48	41						
16	50	41						

Again some experiments will be performed to find out the $D_1^{(L2)}$ values of the MLH-Web designs considered in the previous experiment. Note that, the designs MLH-Web are optimized regarding Rectangular (L^1) distance measure rather than Euclidean (L^2) distance measure whereas MLH-ILS designs are optimized regarding Euclidian distance measure (L^2) measure. Now regarding $D_1^{(L2)}$ values of MLH-ILS, which is optimized in L^2 measure, are compared with MLH-Web, which is optimized in L^1 measure. The experimental results are reputed in the Table 5.4. As mentioned earlier that there are few designs are available in the web regarding Manhattan distance based optimized. It is observed that the designs MLH- ILS's outperform the designs MLH-web regarding Euclidean distance measure

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significantly. It is remarked that when number of N and/ or k of LHD are large, the performance of ILS approach is much better.   It is worthwhile to mention here that in the research paper Morris and Mitchell (1995), few points were considered with Euclidian distance measure, and results of the column **Web** are taken from the "Archived results for 3-10 dimensional L^2 -maximin Latin hypercube designs $-14/3/2006$" of the web www.spacefillingdesigns.nl. Note that this web portal is updated by Grosso et al. (2009) for maximin LHDs, where updated values are obtained by the proposed ILS approach.

5.3 Experimental Results of Optimal LHDs Regarding Manhattan Measure

Now we will perform several experiments on optimal LHDs obtained by ILS approach regarding Manhattan distance measure. In these experiments we have considered those optimal LHDs obtained by ILS approach which are better than available ones obtained by other approaches. The experimental results are reputed in the Tables 5.5 and 5.6. In the tables k denotes number of dimension, N denotes number of design points, $D_1^{(L1)}$ denotes D_1 (minimum inter-site distance) value of the maximin LHD measure in Manhattan distance and $\emptyset_p$ denotes optimal $\emptyset_p$ value of the maximin LHD measured in Euclidean distance measure. As there is no more available data regarding $D_1^{(L1)}$ and $\emptyset_p$ values except displayed in above section, so we cannot able to compare the computational results. But these results may be used for further experimental studies regarding Manhattan distance measure. Anyway though we could not comment about the $D_1^{(L1)}$ and $\emptyset_p$ displayed in the tables, but we may expect that these values might be comparable with other values of LHDs which will be optimized in Rectangular distance measure.

Table 5.5: The $\mathbf{D_1}^{(L1)}$ and $\emptyset_p$ values of maximin LHD obtaining by ILS approach for $k = 3, 4, 5$ and 6

	$k=3$			$k=4$			$k=5$			$k=6$	
N	$\emptyset_p$	$D_1^{(L1)}$	N	$\emptyset_p$	$D_1^{(L1)}$	N	$\emptyset_p$	$D_1^{(L1)}$	N	$\emptyset_p$	$D_1^{(L1)}$
17	0.051031	10	14	0.06428	14	11	0.068843	15	9	0.077615	17
18	0.048795	10	15	0.05607	14	12	0.066372	17	10	0.070186	17
19	0.044324	10	16	0.05109	14	13	0.060302	17	11	0.0635	19
20	0.041345	10	17	0.04569	14	14	0.055385	19	12	0.059131	23
21	0.041523	11	18	0.04467	16	15	0.053376	17	13	0.05547	21
22	0.040456	11	19	0.04449	16	16	0.050833	19	14	0.052632	24
23	0.037063	11	20	0.04068	18	17	0.047782	19	15	0.048168	22
24	0.035136	11	21	0.03904	20	18	0.045549	19	16	0.045268	24
27	0.030571	13	22	0.03719	17	19	0.040723	21	17	0.041849	26
28	0.029722	13	23	0.03526	18	20	0.040291	21	18	0.041849	27
29	0.02794	13	25	0.03272	19	21	0.037716	25	19	0.039841	26
30	0.026603	13	26	0.03028	19	22	0.032325	23	20	0.036911	29
31	0.025846	13	27	0.02972	20	23	0.031466	26	21	0.035669	29
32	0.0254	13	28	0.02863	20	24	0.030151	26	22	0.034606	31
33	0.024261	14	29	0.02666	19	25	0.02921	27	23	0.033205	32
35	0.023669	14	30	0.02602	20	26	0.028548	29	24	0.031342	33

Continuing

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N	Øₙ	D₁^(L1)	N	Øₙ	D₁^(L1)	N	Øₙ	D₁^(L1)	N	Øₙ	D₁^(L1)
36	0.023076	15	31	0.02489	21	27	0.027503	29	25	0.030964	34
39	0.020806	16	32	0.02461	21	28	0.026594	28	26	0.02954	35
40	0.019838	15	33	0.02393	22	29	0.025624	30	27	0.02815	34
51	0.015833	17	34	0.02238	22	30	0.024419	33	28	0.024522	36
52	0.01532	18	35	0.02172	23	31	0.024398	31	29	0.022233	37
53	0.014543	17	36	0.02121	22	32	0.023505	31	30	0.022559	40
54	0.014677	19	37	0.02019	20	33	0.02257	31	31	0.02176	37
56	0.014004	19	38	0.01918	25	34	0.022394	28	32	0.021186	35
70	0.011102	21	39	0.01911	22	35	0.021724	30	33	0.020628	42
71	0.010706	21	40	0.01898	25	36	0.020833	30	34	0.020129	44
75	0.010239	22	41	0.01738	25	37	0.020633	31	35	0.019153	46
77	0.010107	22	42	0.01848	25	38	0.019988	34	36	0.019136	45
			43	0.01765	24	39	0.019548	35	37	0.018474	45
			44	0.01733	25	40	0.018888	35	38	0.017929	49
			45	0.01584	26	41	0.018679	34	39	0.017803	47
			46	0.01533	26	42	0.017963	34	40	0.017265	48
			47	0.01494	25	43	0.017683	37	41	0.016857	54
			48	0.0161	27	44	0.017387	39	42	0.016582	56
			49	0.01476	29	45	0.016935	36	43	0.01599	46
			50	0.01457	29	46	0.016167	36	44	0.014822	49
			51	0.01519	30	47	0.015766	36	45	0.014799	48
			52	0.01458	29	48	0.014306	38	46	0.01378	50
			53	0.01437	29	49	0.014979	37	47	0.014362	50
			54	0.01388	29	50	0.014178	41	48	0.01457	49
			55	0.01384	29	51	0.014258	40	49	0.014236	55
			56	0.01361	31	53	0.013691	41	50	0.014066	53
			60	0.01211	32	54	0.012908	42	51	0.013388	52
			61	0.01226	30	55	0.013169	42	52	0.013563	56
			64	0.01167	35	56	0.012613	44	53	0.013061	54
			65	0.01127	36	57	0.012019	42	54	0.013009	57
			68	0.01055	37	58	0.012092	42	55	0.012788	59
			71	0.01003	36	59	0.01213	42	56	0.012595	56
			72	0.01009	38	60	0.011536	44	57	0.012413	57
			74	0.00965	37	61	0.011664	43	58	0.012051	58
			77	0.00929	38	62	0.011011	46	59	0.011886	62
			78	0.00893	36	63	0.010711	45	60	0.011795	55
			79	0.00944	38	64	0.010744	49	61	0.011451	60
			81	0.00880	37	65	0.010822	45	62	0.011391	59
			83	0.00877	38	66	0.010615	49	63	0.011224	61
			86	0.00788	39	68	0.009962	57	64	0.010866	61
			89	0.00808	39	69	0.010026	52	65	0.01081	65
			91	0.00775	42	70	0.009914	53	66	0.010441	58
			92	0.00771	41	71	0.00957	51	67	0.010272	66
			93	0.00771	40	72	0.009662	49	68	0.010439	66
			94	0.00770	42	73	0.009345	62	69	0.010105	65
			95	0.00737	43	74	0.009019	52	70	0.009885	70
			100	0.00692	43	75	0.009219	56	71	0.00967	64
						76	0.008919	51	72	0.009625	69
						77	0.00897	57	73	0.00937	64
						78	0.008537	51	74	0.009135	70
						79	0.00878	55	75	0.009259	74
						81	0.008384	59	76	0.008735	72
						82	0.008597	56	77	0.008791	71
						83	0.00833	53	78	0.008937	68
						84	0.008281	56	79	0.008872	71
						85	0.008301	56	80	0.008582	75
						86	0.008095	61	81	0.008294	79
						88	0.007715	62	82	0.008008	83
						89	0.007977	60	83	0.008213	80
						90	0.007684	62	84	0.008172	77
						91	0.00765	63	85	0.007885	78
						92	0.007322	60	86	0.007632	70
						93	0.007409	62	87	0.007518	71
						94	0.007223	64	88	0.007438	85
						96	0.007207	68	89	0.007413	81
						97	0.006933	67	90	0.007407	79
						98	0.006973	64	91	0.007353	77
						99	0.007136	65	92	0.00701	79
									93	0.007152	84
									94	0.006767	81
									95	0.006602	88
									96	0.006794	81
									97	0.006547	75
									98	0.006562	80
									99	0.006411	83
									100	0.006638	83

Table 5.6: The $D_1^{(L1)}$ and $\emptyset_p$ values of maximin LHD obtaining by ILS approach for $k = $ 7, 8, 9 and 10

	k=7			k=8			k=9			k=10	
N	$\emptyset_p$	$D_1^{(L1)}$	N	$\emptyset_p$	$D_1^{(L1)}$	N	$\emptyset_p$	$D_1^{(L1)}$	N	$\emptyset_p$	$D_1^{(L1)}$
7	0.12126	18	7	0.0845	14	8	0.064018	23	9	0.053683	29
8	0.10206	18	8	0.0944	22	9	0.080064	27	10	0.07036	33
9	0.06757	19	9	0.0857	23	10	0.074125	29	11	0.06455	32
10	0.06166	22	10	0.0581	24	11	0.049447	31	12	0.042993	37
11	0.05822	23	11	0.0529	27	12	0.045883	33	13	0.039968	38
12	0.05407	26	12	0.0497	28	13	0.043234	35	14	0.037716	44
13	0.04975	26	13	0.0462	30	14	0.040825	37	15	0.035944	43
14	0.04647	29	14	0.0429	30	15	0.038152	39	16	0.033748	47
15	0.04335	28	15	0.0401	35	16	0.035852	42	17	0.031814	46
16	0.04252	30	16	0.0379	39	17	0.033768	43	18	0.030179	52
17	0.04022	30	17	0.0358	38	18	0.031863	47	19	0.028607	57
18	0.03843	34	18	0.0346	38	19	0.030248	49	20	0.027096	59
19	0.03625	31	19	0.0326	40	20	0.029828	48	21	0.026189	59
20	0.03483	35	20	0.0328	39	21	0.028502	51	22	0.025616	59
21	0.03369	34	21	0.0310	42	22	0.027514	53	23	0.024671	63
22	0.03186	38	22	0.0299	44	23	0.026803	54	24	0.024105	61
23	0.03020	36	23	0.0285	49	24	0.025854	56	25	0.023383	64
24	0.02909	38	24	0.0277	49	25	0.024822	60	26	0.022911	68
25	0.02794	40	25	0.0262	50	26	0.023662	58	27	0.021552	69
26	0.02706	42	26	0.0253	52	27	0.023076	59	28	0.021124	70
27	0.02616	43	27	0.0242	51	28	0.022086	61	29	0.020563	69
28	0.02475	45	28	0.0235	54	29	0.021219	64	30	0.019699	72
29	0.02418	46	29	0.0229	58	30	0.020952	67	31	0.019245	81
30	0.02401	48	30	0.0221	57	32	0.019869	67	32	0.01844	78
31	0.02218	40	31	0.0213	58	33	0.01916	70	33	0.017739	76
32	0.02191	51	32	0.0209	58	34	0.018634	69	34	0.017541	75
33	0.02153	53	33	0.0201	61	35	0.017969	72	35	0.01685	81
34	0.02059	55	34	0.0195	56	36	0.017555	77	36	0.016602	88
35	0.02031	54	35	0.0187	57	37	0.016966	77	37	0.016195	87
36	0.01886	48	36	0.0188	64	38	0.016611	81	38	0.0158	94
37	0.01808	59	37	0.0182	63	39	0.016254	78	39	0.015719	98
38	0.01637	52	38	0.0177	65	40	0.015875	75	40	0.015361	94
39	0.01662	56	39	0.0170	68	41	0.015597	80	41	0.014781	90
40	0.01574	55	40	0.0168	75	42	0.014952	88	42	0.014183	101
41	0.01551	57	41	0.0163	75	43	0.014987	91	43	0.013928	97
42	0.01498	59	42	0.0161	76	44	0.014608	82	44	0.013626	101
43	0.01464	66	43	0.0153	73	45	0.01439	90	45	0.013447	105
44	0.01428	59	44	0.0148	73	46	0.013861	94	46	0.013058	99
45	0.01419	62	45	0.0132	69	47	0.013727	94	47	0.012876	108
46	0.01395	62	46	0.0129	72	48	0.013314	93	48	0.012634	110
47	0.01358	67	47	0.0131	84	49	0.012929	91	49	0.012359	114
48	0.01331	69	48	0.0123	77	50	0.012578	96	50	0.012271	106
49	0.01316	70	49	0.0122	84	51	0.012339	93	51	0.012019	112
50	0.01286	69	50	0.0118	80	52	0.011894	107	52	0.011703	121
51	0.01257	67	51	0.0116	80	53	0.010515	108	53	0.011464	122
52	0.01228	75	52	0.0114	84	54	0.011299	106	54	0.011334	127
53	0.01214	81	53	0.0113	85	55	0.011392	95	55	0.011022	130
54	0.01193	80	54	0.0110	88	56	0.010885	107	56	0.010744	123
55	0.01163	82	55	0.0109	86	57	0.010233	111	57	0.010747	130
56	0.01146	88	56	0.0106	80	58	0.01015	116	58	0.010344	131
57	0.01114	89	57	0.0105	89	59	0.009988	110	59	0.010219	132
58	0.01054	81	58	0.0103	92	60	0.009572	106	60	0.01019	124
59	0.01067	64	59	0.0102	99	61	0.009546	110	61	0.009884	131
60	0.01028	82	60	0.0100	102	62	0.009083	122	62	0.009609	142
61	0.01023	68	61	0.0098	97	63	0.009193	113	63	0.009476	137
62	0.01034	73	62	0.0096	90	64	0.008898	124	64	0.009186	138
63	0.01001	74	63	0.0094	107	65	0.00865	127	65	0.008483	132
64	0.01001	73	64	0.0093	104	66	0.008565	112	66	0.008871	144
65	0.00981	77	65	0.0091	106	67	0.008428	120	67	0.008658	147
66	0.00966	82	66	0.0090	112	68	0.008355	116	68	0.008615	152
67	0.00958	74	67	0.009	105	69	0.008166	115	69	0.008463	150
68	0.00951	77	68	0.0088	106	70	0.008086	125	70	0.008233	150
69	0.00934	76	69	0.0086	109	71	0.007978	123	71	0.007847	152
70	0.00907	87	70	0.0085	124	72	0.007898	138	72	0.007614	152

Continuing

N	$\emptyset_n$	$D_1^{(L1)}$	N	$\emptyset_n$	$D_1^{(L1)}$	N	$\emptyset_n$	$D_1^{(L1)}$	N	$\emptyset_n$	$D_1^{(L1)}$
71	0.00919	89	71	0.0084	121	73	0.007772	129	73	0.007951	159
72	0.00895	82	72	0.0083	129	74	0.007714	130	74	0.007341	160
73	0.00895	85	73	0.0082	124	75	0.007559	142	75	0.00718	145
74	0.00882	84	74	0.0078	116	76	0.007457	134	76	0.007081	156
75	0.00855	85	75	0.0079	110	77	0.007389	140	77	0.007038	156
76	0.00864	94	76	0.0077	116	78	0.007322	141	78	0.00693	163
77	0.00843	88	77	0.0077	112	79	0.007153	142	79	0.0069	156
78	0.00837	94	78	0.0076	111	80	0.007117	151	80	0.006748	168
79	0.00821	87	79	0.0074	117	81	0.007051	149	81	0.006693	160
80	0.00795	91	80	0.0073	127	82	0.006954	156	82	0.006638	155
81	0.00813	100	81	0.0070	115	83	0.006912	150	83	0.006505	171
82	0.00785	97	82	0.0070	126	84	0.006745	158	84	0.006396	171
83	0.00798	103	83	0.0072	116	85	0.006671	144	85	0.006379	174
84	0.00786	89	84	0.0070	123	86	0.006579	154	86	0.006256	176
85	0.00774	90	85	0.0071	124	87	0.006484	165	87	0.006182	176
86	0.00771	102	86	0.0070	125	88	0.00633	167	88	0.006138	174
87	0.00763	96	87	0.0070	130	89	0.006388	166	89	0.006065	182
88	0.00746	104	88	0.0069	132	90	0.006301	173	90	0.006024	163
89	0.00740	102	89	0.0068	121	91	0.006223	168	91	0.00595	189
90	0.00726	103	90	0.0068	132	92	0.006063	175	92	0.005876	181
91	0.00732	103	91	0.0067	128	93	0.005961	169	93	0.005823	192
92	0.00708	110	92	0.0066	128	94	0.006024	167	94	0.005771	195
93	0.00716	109	93	0.0065	128	95	0.0059	167	95	0.005708	193
94	0.00692	101	94	0.0065	123	96	0.005852	161	96	0.005648	195
95	0.00672	105	95	0.0064	131	97	0.005838	181	97	0.005594	194
96	0.00679	107	96	0.0064	130	98	0.005726	166	98	0.005505	212
97	0.00676	99	97	0.0064	122	99	0.005672	181	99	0.005493	204
98	0.00671	113	98	0.0063	128	100	0.005594	182	100	0.005436	205
99	0.00662	105	99	0.0062	135						
100	0.00654	99	100	0.0061	130						

5.4 Experimental Study for Impact of Trials

Now we have performed further experiments to study the effect of trials in the ILS algorithm for finding maximin LHDs. In the same time, we would like to find some new characteristics of the maximin LHDs obtained by ILS approach. At first we would like to observe about the effect of trials on $D_1^{(L2)}$ values of maximin LHD. For this experiments we have considered dimension $k = 3$ to 9. The experimental results are displayed in Figures 5.1(a) – 5.1(g). The N values for each experiment are shown in the right side of the figures. It is noted that the abscissa of each figure indicates number of trials on the other hand ordinate indicates $D_1^{(L2)}$ values. Now it is observed in the Figure 5.1(a), in which we have considered dimension of LHD is $k = 3$, for $N = 5$ to 25, that the $D_1^{(L2)}$ values are almost identical for all trials. Moreover for $N = 30$ to 50 though the $D_1^{(L2)}$ values are not almost identical but not significantly different. We also observed that the increase of trials do not increase the $D_1^{(L2)}$ values monotonically. It is noted that for $N = 50$ few trial corresponds good $D_1^{(L2)}$ values rather than large trial value namely $trial = 40$. It means a good initial solution has significant effect on good optimal solution for ILS heuristic approach.
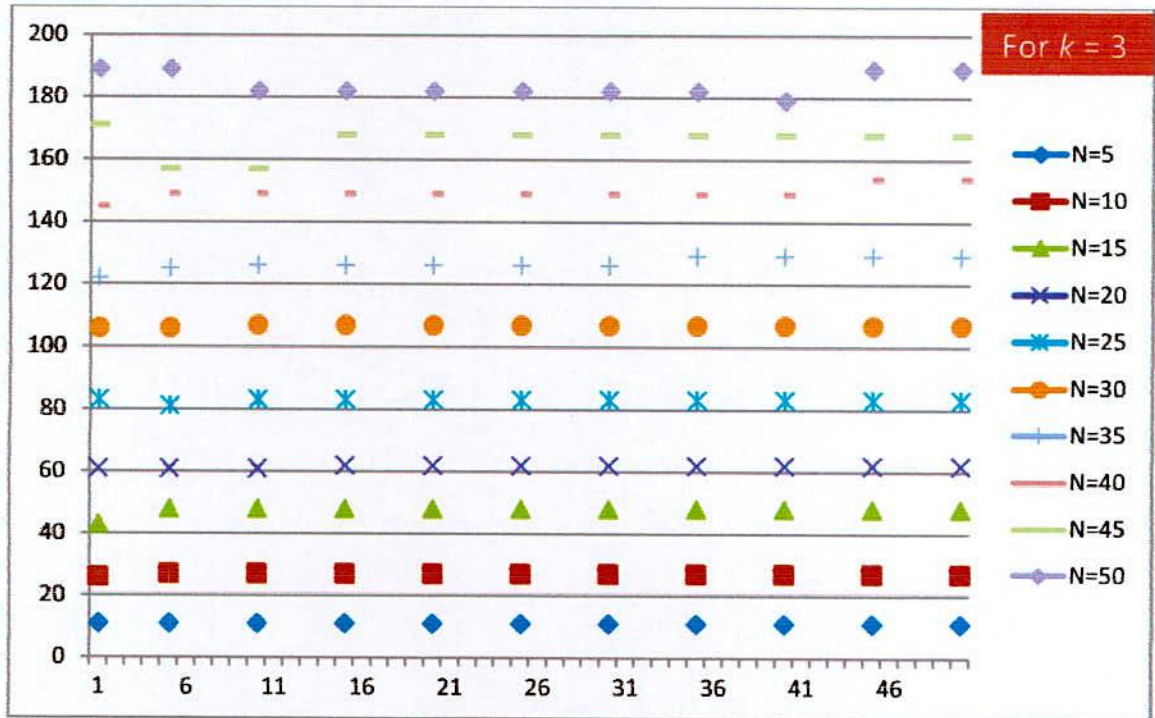
Figure 5.1(a): Impact of trials in ILS approach regarding $D_1^{(L2)}$ values for $k = 3$

Now in the Figure 5.1(b) we have considered dimension of LHD is $k = 4$, for $N = 5$ to 15, in the Figure 5.1(c) we have considered dimension of LHD is $k = 5$, for $N = 5$ to 25, in the Figure 5.1(d) we have considered dimension of LHD is $k = 6$, for $N = 5$ to 15, in the Figure 5.1(e) we have considered dimension of LHD is $k = 7$, for $N = 5$ to 25, in the Figure 5.1(f) we have considered dimension of LHD is $k = 8$, for $N = 5$ to 15. It is observed that the $D_1^{(L2)}$ values are almost identical for all trials.
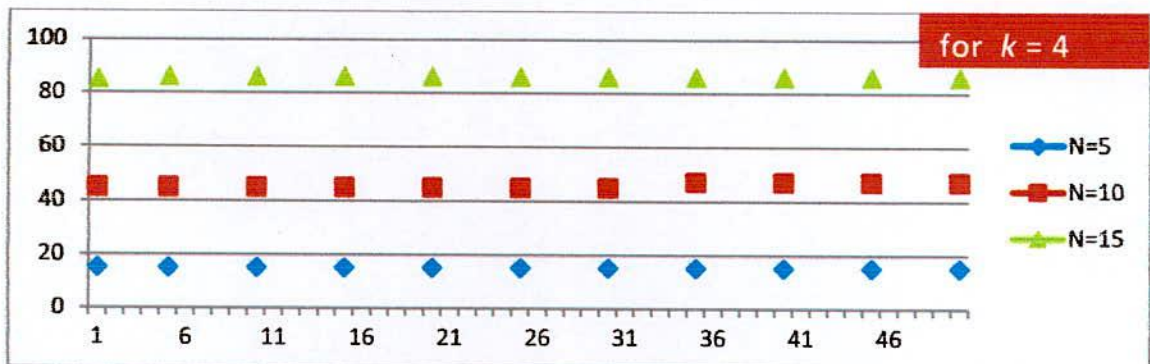

Figure 5.1(b): Impact of trials in ILS approach regarding $D_1^{(L2)}$ values for $k = 4$
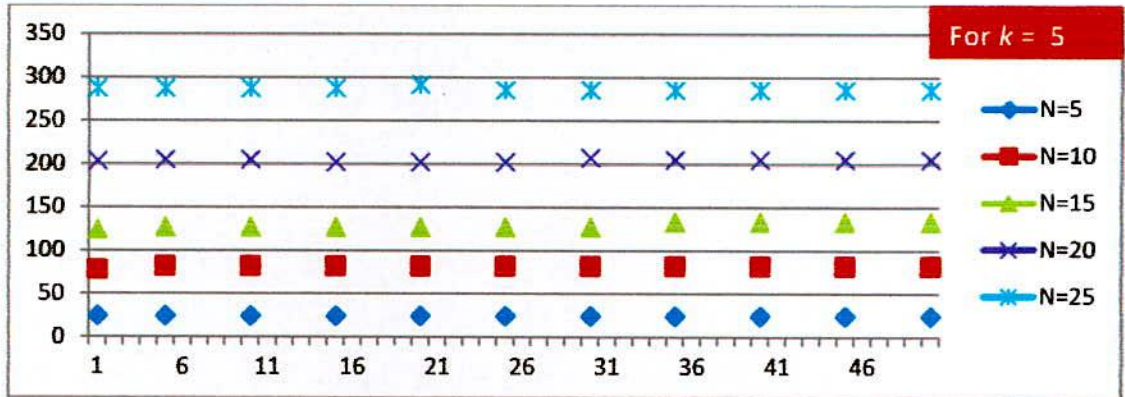
Figure 5.1(c): Impact of trials in ILS approach regarding $D_1^{(L2)}$ values for $k=5$

Figure 5.1(d): Impact of trials in ILS approach regarding $D_1^{(L2)}$ values for $k = 6$

Figure 5.1(e): Impact of trials in ILS approach regarding $D_1^{(L2)}$ values for $k = 7$
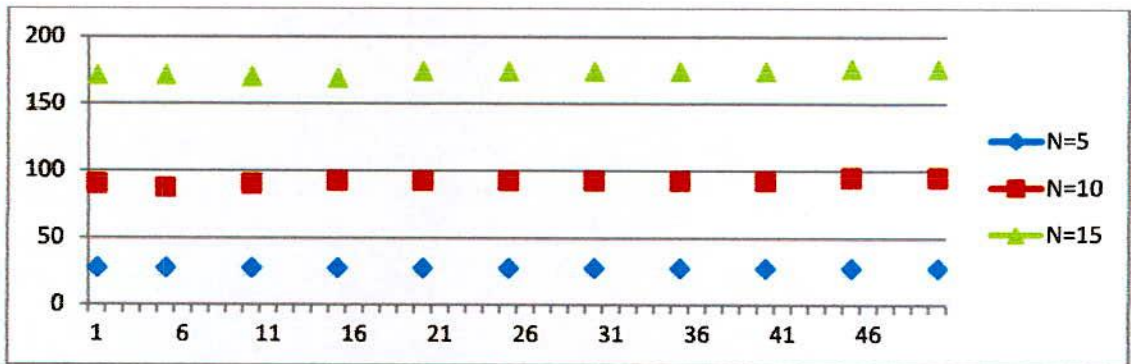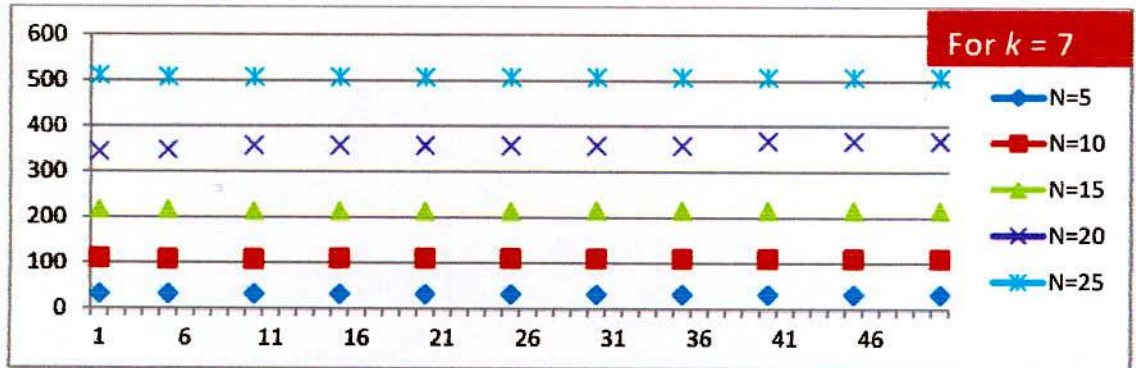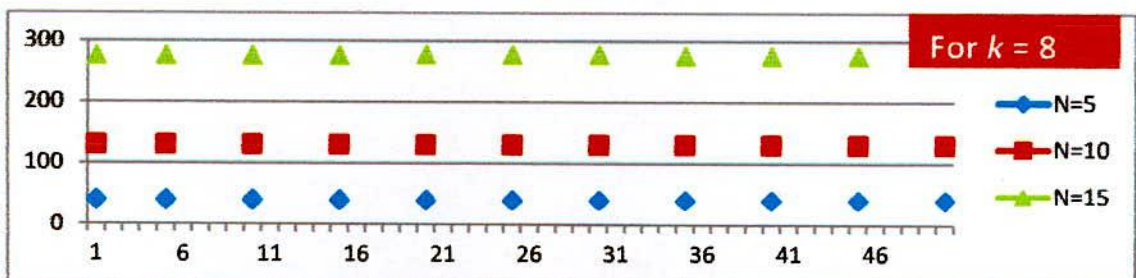

Figure 5.1(f): Impact of trials in ILS approach regarding $D_1^{(L2)}$ values for $k = 8$
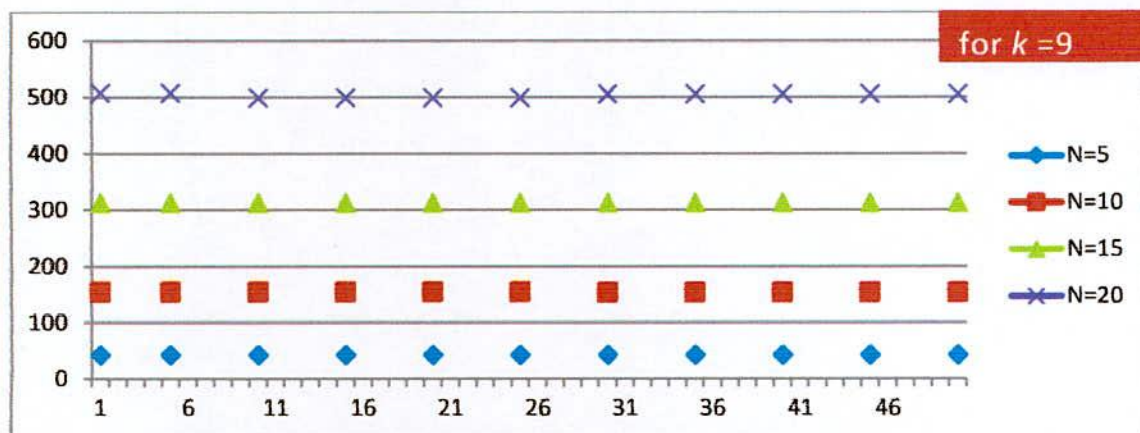
Figure 5.1(g): Impact of trials in ILS approach regarding $D_1^{(L2)}$ values for $k = 9$

Similarly in the Figure 5.1(g) we have considered dimension of LHD is $k = 9$, for $N = 5$ to 20. Here we also observed that the impact of trial regarding the $D_1^{(L2)}$ values is not significant.

Now we would like to observe about the effect of trials on corresponding $D_1^{(L1)}$ values. For this experiments we have considered dimension $k = 3$ to 9. The N values for each experiment are shown in the right side of the figures. The experimental results are displayed in figures 5.2(a) – 5.2(g). It is noted that the abscissa of each figure indicates number of trials on the other hand ordinate indicates $D_1^{(L1)}$ values. Now it is observed in all the Figure 5.2(a) – 5.2(g) except few N values, the impact of trial on LHD regarding $D_1^{(L1)}$ values are not significant.

Figure 5.2(a): Impact of trials in ILS approach regarding $D_1^{(L1)}$ values for $k = 3$

Figure 5.2 (b): Impact of trials in ILS approach regarding $D_1^{(L1)}$ values for $k = 4$

Figure 5.2 (c): Impact of trials in ILS approach regarding $D_1^{(L1)}$ values for $k = 5$
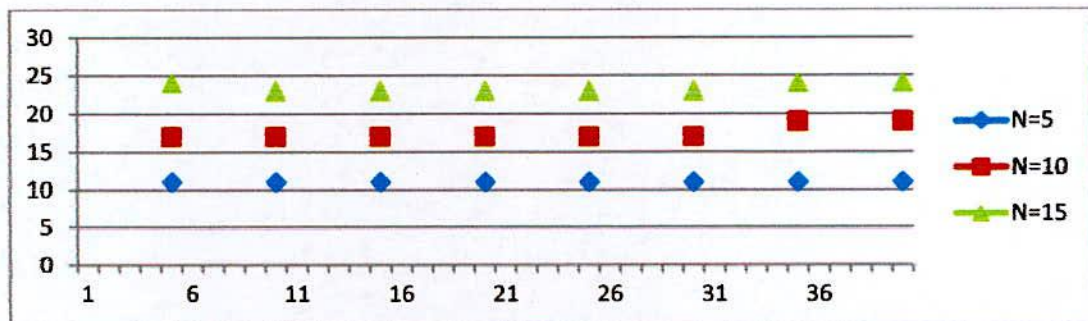
Figure 5.2 (d): Impact of trials in ILS approach regarding $D_1^{(L1)}$ values for $k = 6$
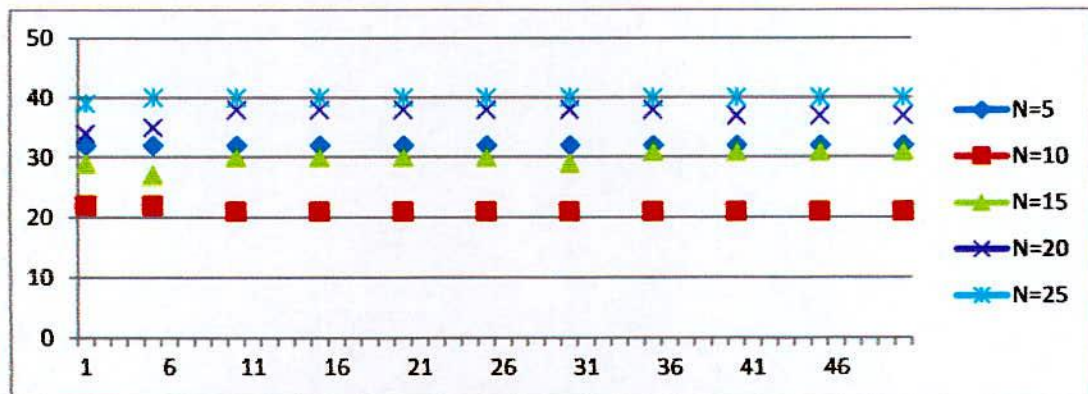
Figure 5.2 (e): Impact of trials in ILS approach regarding $D_1^{(L1)}$ values for $k = 7$
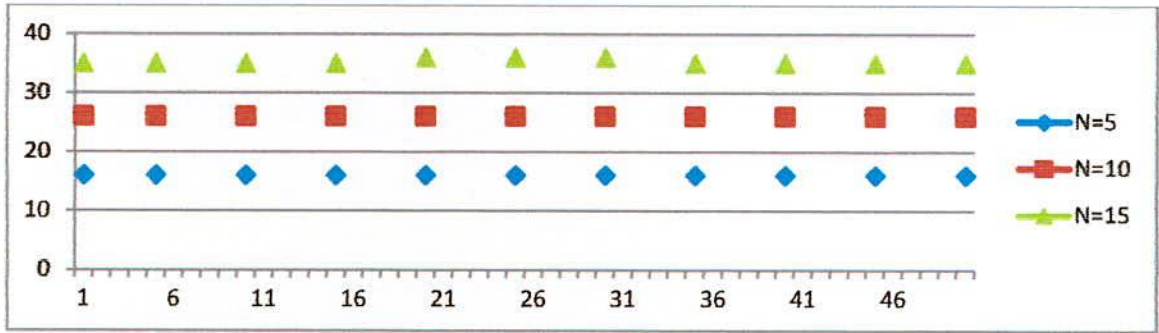
Figure 5.2 (f): Impact of trials in ILS approach regarding $D_1^{(L1)}$ values for $k = 8$
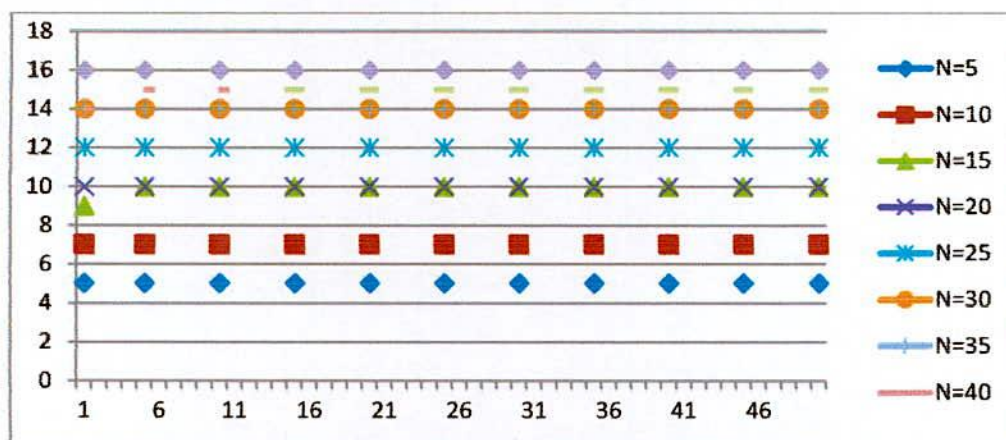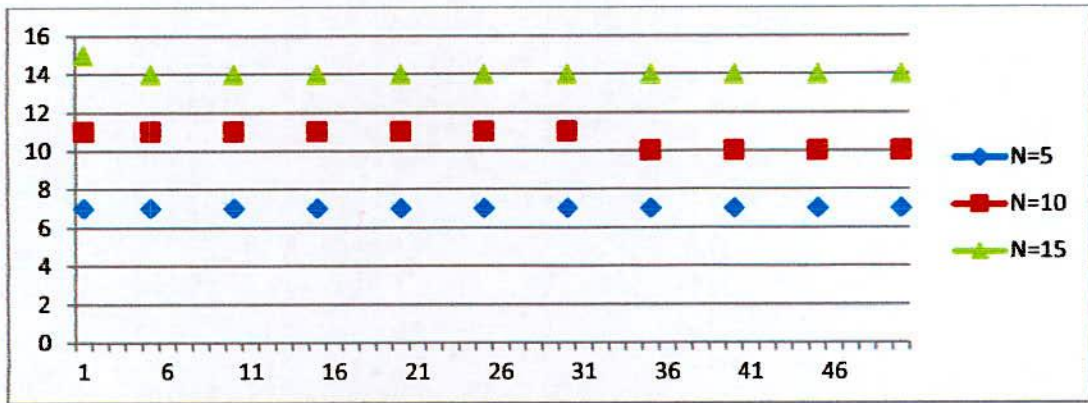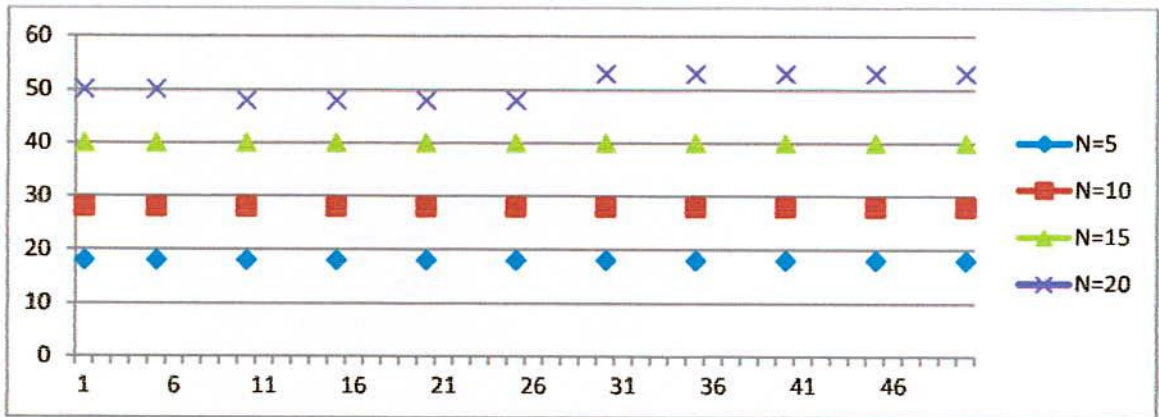

Figure 5.2 (g): Impact of trials in ILS approach regarding $D_1^{(L1)}$ values for $k = 9$
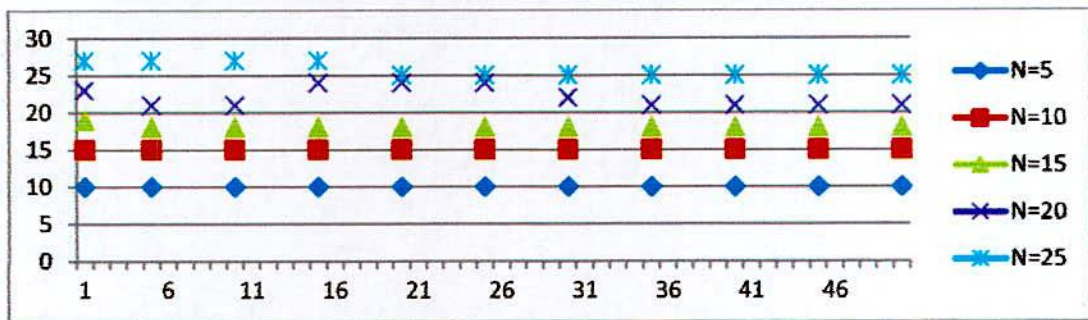
Table 5.7 (a): Impact of trials in ILS approach regarding $D_M^{(L2)}$ and $D_M^{(L1)}$ values for $k = 3$

	$k=3$									
	$N=5$		$N=10$		$N=15$		$N=20$		$N=25$	
Trials	$D_M^{(L2)}$	$D_M^{(L1)}$	$D_M^{(L2)}$	$D_M^{(L1)}$	$D_M^{(L2)}$	$D_M^{(L1)}$	$D_M^{(L2)}$	$D_M^{(L1)}$	$D_M^{(L2)}$	$D_M^{(L1)}$
1	24	8	114	16	266	28	561	39	977	53
5	24	8	104	16	278	28	561	39	827	49
10	24	8	104	16	278	28	554	40	929	51
15	24	8	104	16	278	28	507	38	929	51
20	24	8	104	16	278	28	507	38	929	51
25	24	8	104	16	278	28	507	38	929	51
30	24	8	104	16	278	28	507	38	929	51
35	24	8	104	16	278	28	507	38	929	51
40	24	8	104	16	278	28	507	38	929	51
45	24	8	104	16	278	28	507	38	929	51
50	24	8	104	16	278	28	507	38	929	51

Now we have performed further experiments to find out some new characteristics of those maximin LHDs. The experimental results are given in the Tables 5.3(a) – 5.3(h). In the tables $D_M^{(L1)}$ and $D_M^{(L2)}$ denote D_M value (maximum inter-site pair-wise distance value of LHD) of the maximin LHD regarding Manhattan and Euclidean distance measure respectively. It is remarked that the $D_M^{(L1)}$ and $D_M^{(L2)}$ values, shown in the tables are new characteristics of the maximin LHDs which are not available in the literature. So we could not compare the results. It is observed in the tables that the impact of trials is not significance regarding the $D_M^{(L1)}$ and $D_M^{(L2)}$ values too. But there is one important observation is that when $D_1^{(L2)}$ value is unchanged then corresponding $D_M^{(L2)}$, $D_1^{(L1)}$, $D_M^{(L1)}$ and $D_M^{(L2)}$ values are also almost unchanged regarding number of trials.

Table 5.7 (b): Impact of trials in ILS approach regarding $D_M^{(L2)}$ and $D_M^{(L1)}$ values for $k = 3$

Trials	N=30 $D_M^{(L2)}$	$D_M^{(L1)}$	N=35 $D_M^{(L2)}$	$D_M^{(L1)}$	N=40 $D_M^{(L2)}$	$D_M^{(L1)}$	N=45 $D_M^{(L2)}$	$D_M^{(L1)}$	N=50 $D_M^{(L2)}$	$D_M^{(L1)}$
1	1341	63	1785	71	2561	87	3140	94	4371	113
5	1341	63	2025	77	2718	90	3158	96	4371	113
10	1358	61	1883	75	2718	90	3158	96	4083	108
15	1358	61	1883	75	2718	90	3181	97	4083	108
20	1358	61	1883	75	2718	90	3181	97	4083	108
25	1358	61	1883	75	2718	90	3181	97	4083	108
30	1358	61	1883	75	2718	90	3181	97	4083	108
35	1358	61	1770	72	2718	90	3181	97	4083	108
40	1358	61	1770	72	2718	90	3181	97	4580	114
45	1358	61	·1770	72	2406	84	3181	97	4371	113
50	1358	61	1770	72	2406	84	3181	97	4371	113

Table 5.7 (c): Impact of trials in ILS approach regarding $D_M^{(L2)}$ and $D_M^{(L1)}$ values for $k = 4$

Trials	N=5 $D_M^{(L2)}$	$D_M^{(L1)}$	N=10 $D_M^{(L2)}$	$D_M^{(L1)}$	N=15 $D_M^{(L2)}$	$D_M^{(L1)}$
1	25	9	138	21	305	33
5	25	9	138	21	290	32
10	25	9	138	21	290	32
15	25	9	138	21	290	32
20	25	9	138	21	290	32
25	25	9	138	21	290	32
30	25	9	138	21	290	32
35	25	9	138	22	290	32
40	25	9	138	22	290	32
45	25	9	138	22	290	32
50	25	9	138	22	290	32

Table 5.7 (d): Impact of trials in ILS approach regarding $D_M^{(L2)}$ and $D_M^{(L1)}$ values for $k = 5$

Trials	$N=5$ $D_M^{(L2)}$	$D_M^{(L1)}$	$N=10$ $D_M^{(L2)}$	$D_M^{(L1)}$	$N=15$ $D_M^{(L2)}$	$D_M^{(L1)}$	$N=20$ $D_M^{(L2)}$	$D_M^{(L1)}$	$N=25$ $D_M^{(L2)}$	$D_M^{(L1)}$
1	26	10	173	27	376	42	640	54	1165	73
5	26	10	165	25	333	38	622	53	1165	73
10	26	10	165	25	333	38	622	53	1165	73
15	26	10	165	25	333	38	615	53	1165	73
20	26	10	165	25	333	38	615	53	1148	67
25	26	10	165	25	333	38	615	53	1119	69
30	26	10	165	25	333	38	618	54	1119	69
35	26	10	165	25	336	38	754	60	1119	69
40	26	10	165	25	336	38	754	60	1119	69
45	26	10	165	25	336	38	754	60	1119	69
50	26	10	165	25	336	38	754	60	1119	69

Table 5.7 (e): Impact of trials in ILS approach regarding $D_M^{(L2)}$ and $D_M^{(L1)}$ values for $k = 6$

Trials	$N=5$ $D_M^{(L2)}$	$D_M^{(L1)}$	$N=10$ $D_M^{(L2)}$	$D_M^{(L1)}$	$N=15$ $D_M^{(L2)}$	$D_M^{(L1)}$
1	36	14	217	31	420	48
5	36	14	214	34	420	48
10	36	14	215	34	418	45
15	36	14	206	32	406	48
20	36	14	206	32	422	48
25	36	14	206	32	422	48
30	36	14	206	32	422	48
35	36	14	206	32	422	48
40	36	14	206	32	422	48
45	36	14	214	30	413	48
50	36	14	214	30	413	48

Table 5.7 (f): Impact of trials in ILS approach regarding $D_M^{(L2)}$ and $D_M^{(L1)}$ values for $k = 7$

Trials	$N=5$ $D_M^{(L2)}$	$D_M^{(L1)}$	$N=10$ $D_M^{(L2)}$	$D_M^{(L1)}$	$N=15$ $D_M^{(L2)}$	$D_M^{(L1)}$	$N=20$ $D_M^{(L2)}$	$D_M^{(L1)}$	$N=25$ $D_M^{(L2)}$	$D_M^{(L1)}$
1	39	15	253	39	535	56	845	72	1305	90
5	39	15	253	39	529	55	840	70	1304	90
10	39	15	262	39	534	56	811	73	1304	90
15	39	15	255	39	534	56	811	73	1304	90
20	39	15	255	39	534	56	811	73	1304	90
25	39	15	255	39	534	56	811	73	1304	90
30	39	15	255	39	535	55	811	73	1304	90
35	39	15	255	39	546	58	811	73	1304	90
40	39	15	255	39	546	58	821	71	1304	90
45	39	15	255	39	546	58	821	71	1304	90
50	39	15	255	39	546	58	821	71	1304	90

Table 5.7 (g): Impact of trials in ILS approach regarding $D_M^{(L2)}$ and $D_M^{(L1)}$ values for $k = 8$

Trials	N=5		N=10		N=15	
	$D_M^{(L2)}$	$D_M^{(L1)}$	$D_M^{(L2)}$	$D_M^{(L1)}$	$D_M^{(L2)}$	$D_M^{(L1)}$
1	40	16	295	45	616	66
5	40	16	314	48	616	66
10	40	16	314	48	616	66
15	40	16	314	48	616	66
20	40	16	314	48	615	63
25	40	16	314	48	615	63
30	40	16	314	48	615	63
35	40	16	314	48	612	64
40	40	16	314	48	612	64
45	40	16	314	48	612	64
50	40	16	314	48	612	64

Table 5.7 (h): Impact of trials in ILS approach regarding $D_M^{(L2)}$ and $D_M^{(L1)}$ values for $k = 9$

Trials	N=5		N=10		N=15		N=20	
	$D_M^{(L2)}$	$D_M^{(L1)}$	$D_M^{(L2)}$	$D_M^{(L1)}$	$D_M^{(L2)}$	$D_M^{(L1)}$	$D_M^{(L2)}$	$D_M^{(L1)}$
1	46	18	179	36	692	72	1145	90
5	46	18	179	36	692	72	1145	90
10	46	18	177	37	692	72	1138	93
15	46	18	177	37	692	72	1138	93
20	46	18	177	37	692	72	1138	93
25	46	18	177	37	692	72	1138	93
30	46	18	174	38	692	72	1138	94
35	46	18	174	38	692	72	1138	94
40	46	18	174	38	692	72	1138	94
45	46	18	174	38	692	72	1138	94
50	46	18	174	38	692	72	1138	94

5.5 Some New Best Optimal LHDs Regarding ILS Approach

In the experimental study we have obtained some best maximin LHDs compare to available one in the literature namely web portal http://www.spacefillingdesigns.nl. The experimental results are displayed in the Table 5.8. In the table 5.8 Pre_$D_1^{(L2)}$ denotes maximin LHDs given in (Grosso et al. 2009) measured in Euclidean distance measure and New_$D_1^{(L2)}$ denotes the maximin LHDs obtained by our experiments measured in Euclidean distance measure too. It is noted that the initial solution of Grosso et al. (2009) and that of our experiments for the ILS algorithm are might be different. From this observation it may again conclude that the initial solution may effect on finding the optimal solution.

Table 5.8: Some improved LHDs values compared to previous ones by ILS approach

k	N	Pre_$D_1^{(L2)}$	New_$D_1, J_1^{(L2)}$
3	30	105	**[109,2]**
3	40	152	**[161,1]**
5	15	131	**[133,1]**
5	25	286	**[291,1]**
7	20	360	**[368,2]**
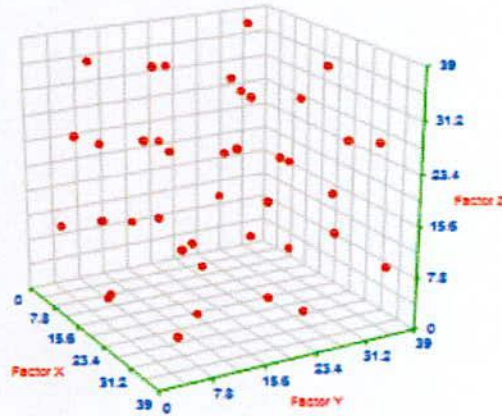
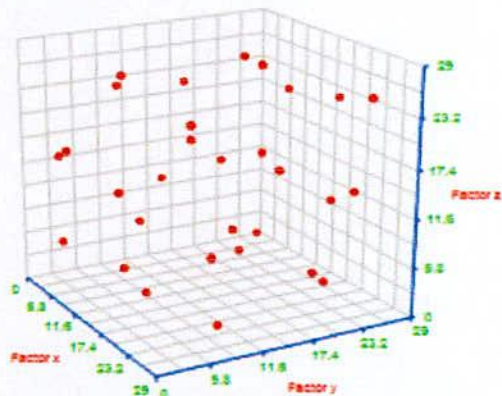Figure 5.3: Improved maximin LHD for $(N, k) = (40, 3)$ where $D_1^{(L2)} = 161$

Figure 5.4 : Improved maximin LHD for $(N, k) = (30, 3)$ where $D_1^{(L2)} = 109$

Now we have displayed graphically two three-dimensional improved maximin LHDs in Figure 5.3 and 5.4 for $(N, k) = (40, 3)$ and $(30, 3)$ respectively. Since for more than three factors it is impossible to display the LHD graphically, so we have displayed other improved maximin LHDs in tabular form. Table 5.9, 5.10 and 5.11 display remaining improved maximin LHDs namely $(N, k) = (16, 5)$, $(25, 5)$ and $(20, 7)$.

Table 5.9: Improved (Best) maximin LHD for $(N, k) = (16, 5)$ obtained by ILS approach

Points	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5
x_0	0	16	9	20	15
x_1	1	8	5	4	9
x_2	2	5	22	9	7
x_3	3	20	15	8	2
x_4	4	17	17	3	19
x_5	5	0	8	19	10
x_6	6	7	4	11	24
x_7	7	21	24	17	13
x_8	8	23	2	7	12
x_9	9	6	20	18	20
x_{10}	10	9	19	24	3
x_{11}	11	1	16	2	18
x_{12}	12	11	3	15	0
x_{13}	13	24	10	22	6
x_{14}	14	22	12	16	23
x_{15}	15	10	13	0	4

Table 5.10: Improved (Best) maximin LHD for $(N, k) = (25, 5)$ obtained by ILS approach

N	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5
x_0	0	16	9	20	15
x_1	1	8	5	4	9
x_2	2	5	22	9	7
x_3	3	20	15	8	2
x_4	4	17	17	3	19
x_5	5	0	8	19	10
x_6	6	7	4	11	24
x_7	7	21	24	17	13
x_8	8	23	2	7	12
x_9	9	6	20	18	20
x_{10}	10	9	19	24	3
x_{11}	11	1	16	2	18
x_{12}	12	11	3	15	0
x_{13}	13	24	10	22	6
x_{14}	14	22	12	16	23
x_{15}	15	10	13	0	4
x_{16}	16	12	1	21	16
x_{17}	17	3	0	5	11
x_{18}	18	15	7	1	21
x_{19}	19	18	21	12	1
x_{20}	20	13	23	6	17
x_{21}	21	2	14	14	5
x_{22}	22	14	18	23	14
x_{23}	23	4	11	13	22
x_{24}	24	19	6	10	8

Table 5.11: Improved (Best) maximin LHD for $(N, k) = (20, 7)$ obtained by ILS approach

N	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5	Factor 6	Factor 7
x_0	0	18	8	8	2	12	6
x_1	1	7	12	12	14	4	0
x_2	2	13	2	16	12	3	15
x_3	3	4	14	4	6	6	16
x_4	4	2	4	18	4	14	7
x_5	5	16	6	0	18	8	8
x_6	6	10	16	14	17	16	14
x_7	7	5	9	2	9	19	1
x_8	8	11	0	6	8	18	17
x_9	9	19	18	11	10	0	10
x_{10}	10	0	1	9	19	9	9
x_{11}	11	8	19	13	1	11	2
x_{12}	12	14	10	17	0	10	18
x_{13}	13	9	3	5	3	2	5
x_{14}	14	3	13	19	11	1	11
x_{15}	15	17	15	1	5	15	12
x_{16}	16	15	5	15	13	13	3
x_{17}	17	6	17	3	16	7	4
x_{18}	18	12	7	7	15	5	19
x_{19}	19	1	11	10	7	17	13

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