

A STUDY ON MAXIMIN LHDS CALCULATED IN EUCLIDEAN DISTANCE MEASURE AND OPTIMIZED BY ILS APPROACH IN PERSPECTIVE OF MD MEASURE

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ABSTRACT

Maximin LHD (Latin Hypercube Design) is one of the optimal designs of experiment in which minimum inter-site distances of the design points are maximized. It is noted that several distance measures are used to calculate the inter-site pair-wise distances among the design points. Moreover several methods are also available in the literature to optimize the experiential designs such as maximin LHD. Grosso et al. (2008) proposed ILS (Iterated Local Search) for the optimization of LHD namely maximin LHD in which the inter-site distance among the design points are calculated by the Euclidean distance measure during the process of optimization. In the literature, some other approaches are available to find out maximin LHD where inter-site distances among the design points are calculated by the Manhattan distance (MD) measured and other measures during the process of optimization too. This research works is mainly a comparison study between maximin LHDS obtained by ILS approach where inter-site distance is calculated in Euclidean distance measure during the procedure of optimization and maximin LHDS obtained by other approaches where inter-site distances is calculated in Manhattan distance measure during the procedure of optimization in the platform of experiments. For the comparison of the maximin LHDS obtained by the different approaches, the optimality of the LHDS are investigated in both Euclidean distance measure as well MD measure. The experimental results reveal that maximin LHDS obtained by ILS are much better than maximin LHDS obtained by other approaches regarding Euclidian distance measure. Moreover maximin LHDS obtained by ILS are comparable with the maximin LHDS obtained by other approaches regarding MD measure.

Keywords: *Euclidean & Manhattan distance, ILS approach, Latin Hypercube design, Space-filling.*

1. INTRODUCTION

The design of computer experiments has much recent interest and this is likely to grow as more and more simulation models are used to carry out research and also made it clear that many simulation models involve several hundred factors or even more. Computer simulation experiments are used in a wide range of application to learn about the effect of input variables x on a response of interest y . Among the several experimental designs, Latin Hypercube Design (LHD) is one of the most chosen experimental designs in the field of application. Due to the important properties of experimental design, non-collapsing property posses in LHDS inherently. The definition of LHD is given below:

Consider a set of N points in a uniform k -dimensional grid $\{0, 1, \dots, N-1\}^k$. A configuration

$$X = \begin{pmatrix} x_1 \\ \vdots \\ x_N \end{pmatrix} = \begin{pmatrix} x_{11} & \cdots & x_{1k} \\ \vdots & \cdots & \vdots \\ x_{N1} & \cdots & x_{Nk} \end{pmatrix} \quad \forall x_{ij} = \{0, 1, \dots, N-1\}$$

Then X be a LHD if $x_{pj} \neq x_{qj} \quad \forall j, p, q \in \{0, 1, \dots, N-1\} \exists p \neq q$ i.e. each column has no duplicate entries.

Though LHDS have good non-collapsing property but randomly generated LHDS often show poor space-filling property as well as strong multi-co-linearity property. It is worthwhile to mention that a good experimental design should have good space-filling property as well as poor multi-co-linearity property along with non-collapsing property. Figure 1 displays randomly generated LHDS A: $(N, k) = (10, 2)$ and B: $(N, k) = (30, 3)$. It is observed in the Figure 1 that there is no any design point on a huge amount of space of the LHD (left upper corner as well as right lower corner) of both the LHDS – A and B. On the other hand Figure 2 displays the optimal (maximin) LHD measured in Euclidian measure and obtained by ILS approach proposed by Grosso *et al.* (2009). It is observed in the Figure 2 that design points are spread out all over the design space for the both LHDS – C and D.

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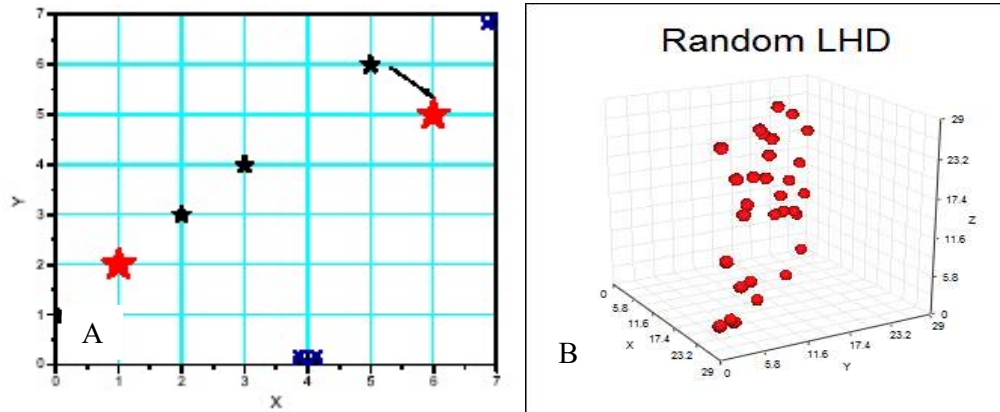


Figure 1: Randomly generated LHDS: (A) $(N, k) = (8, 2)$ and (B) $(N, k) = (30, 3)$

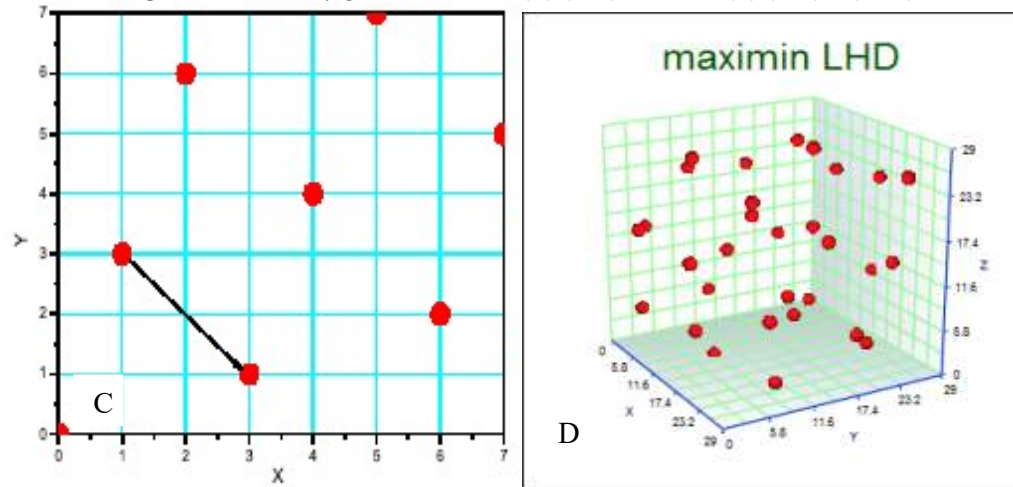


Figure 2: (after ILS approach) Maximin LHDS: (C): $(N, k) = (8, 2)$ and (D): $(N, k) = (30, 3)$

Iterated Local Search (ILS) is a heuristics approach (Grosso *et al.*, 2009). ILS is successfully implemented for finding optimal (maximin) Latin Hypercube Design (LHD) based on Euclidian distance measure. Huge number of improved maximin LHDS, measured in Euclidian distance measure, are obtained by ILS approach which are now available in the regularly updated web portal www.spacefillingdesigns.nl. Not only these maximin LHDS are optimal in the sense of space-filling property on the basis of Euclidian distance measure, but also the multi-co-linearity property of the LHDS are negligible (Jamali *et al.*, 2010; Dey, 2012). Joseph and Hung (2008) showed that maximin criterion and multi-co-linearity criterion need not necessarily agree with each other. Anyway, several authors search optimal experimental measured in MD measure rather than Euclidean distance measure too.

It is worthwhile to mention here that MD measure is also one of the important issues considered in several fields like. MD matrix for a rectangular grid arises frequently from communications and facility locations and is known to be among the hardest discrete optimization problems. 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. Mittelman and Pengy (2001) estimated bounds for quadratic assignment problems associated with hamming and MD matrices based on semi definite programming. Felipe (2013) showed that a new precision-weighted MD 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 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. Husslage *et al.* (2011)

considered MD measure for the optimization of LHD. They considered Φ_p optimal criteria as an objective function and simulated Annealing (SA) as optimization algorithm. It is noted that Morris and Mitchell (1995) first proposed Φ_p optimal criteria for finding maximin LHD. In (Morris and Mitchell, 1995), they obtained maximin LHDs by using modified simulated Annealing (MSA) in which inter-site distances are calculated by Euclidean distance measure. It is worthwhile to mention here that the maximin LHDs obtained by SA and MSA in either MD and/or Euclidean distance are available in the web portal (Morris and Mitchell, 1995). Moreover the best results of maximin LHD obtained by the ILS also available in that web portal. For the application of optimal experiments, it is requested to see (Ye, 1998; Fang *et al.*, 2000). Anyway as mentioned earlier Grosso *et al.* (2009) considered Euclidean distance measure for maximin LHDs by ILS approach. What about the optimality of maximin LHDs are obtained by ILS regarding MD measure? Recently, Jamali and Alam (2017) presented some partial results regarding the comparison between SA and ILS approach regarding MD measure. In this article we have investigated the optimality in perspective of MD measure as well as Euclidean distance measure to analysis the performance of ILS approach regarding Maximin LHDs.

2. METHOD

As our main attention is to study the performance of Iterated Local Search (ILS) approach (Grosso *et al.*, 2009), so we would like to present briefly the ILS approach for finding maximin LHD. For the details of ILS approach readers are requested to see (Lourenco, 2002; Grosso *et al.*, 2009). The pseudo-code of the proposed ILS heuristic for maximin LHD problems is given below:

The pseudo-code (ILS)

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

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There are four main ingredients in ILS approach namely (i) Initialization, (ii) Local Search (iii) Perturbation Move and (iv) Stopping Rule (S_R). The Initialization operator generates a random LHD which, no doubt, has poor space-filling property. The Local Search operator finds out the local optimal solution by heuristic local movement. The perturbation operator perturbs the local optimal solution, obtained previously by Local search operation, to search probably new unsearched feasible space for finding better local optimal solution. Stopping Rule consists of predefine heuristic criteria to stop the algorithm so that it will be able to find optimal/approximate solution. Anyway, the objective function of maximin LHD is given below:

$$\text{Min } \Phi_p(X) \quad (1)$$

Subject to X be a LHD, where

$$\Phi_p(X) = \left[\sum_{i=1}^N \sum_{j=i+1}^N \frac{1}{d_{ij}^p} \right]^{\frac{1}{p}} \quad (2)$$

d_{ij} is the inter-site pair-wise distance between two design points i and j measured and p is any integer (in the experiment p is set to 20).

3. EXPERIMENTAL RESULTS

At first two typical examples are considered namely LHD of $(N, k) = (5, 3)$ and LHD of $(N, k) = (9, 3)$. Now we have performed experiments through both ILS approach and SA (Simulated Annealing) method regarding maximin optimal criteria, Eq. (1). But for the calculation of inter-site distance among design points during optimization process former used L^2 whereas later considered L^1 distance measure respectively. It is also noted that the values of L^2 given in the following tables are the square of actual values if otherwise not specified. The detail results of the experiments for $(N, k) = (5, 3)$ and $(N, k) = (9, 3)$ are shown in the Table 1 and Table 2 respectively. In the tables the optimal LHD obtained by the SA approach is denoted as MLH-SA (Husslage *et al.*, 2011) and the optimal LHD obtained by the ILS approach is indicated as MLS-ILS (Grosso *et al.*, 2009). Moreover D_1 denotes minimum pair-wise inter-site distance of design points among all design points of a LHD; J_1 denotes number of D_1 in that

LHD. Superscript (1) and (2) indicate Manhattan and Euclidean distance measures respectively. Moreover in this article the $D_1^{(2)}$ values is the square of actual value regarding Euclidean measure.

It is observed in the both tables that for both $D_1(J_1)^{(2)}$ and $\Phi_p^{(2)}$, minimum pair-wise distance of MLH-ILSs and Φ_p value of MLS-ILSs design are significantly better than that of MLS-SAs regarding L^2 distance measure. On the other hand, though both MLS-SAs are optimized regarding L^1 distance measure and both MLS-ILSs are optimized regarding L^2 distance measure, for both $D_1(J_1)^{(1)}$ and $\Phi_p^{(1)}$ values of MLS-SAs are not significantly better but rather comparable to MLS-ILSs regarding L^1 distance measure.

Table 1: Comparison among optimal LHDs for
(N, k) = (5, 3)

Table 2: Comparison among optimal LHDs for
(N, k) = (9, 3)

	MLH-SA	MLH-ILS		MLH-SA	MLH-ILS
Optimal design matrix	1 1 2	1 3 5	Optimal Design matrix	1 3 3 4	1 5 8 4
	2 5 3	2 2 2		2 5 8 8	2 7 4 9
	3 2 5	3 5 1		3 8 6 2	3 2 1 6
	4 3 1	4 4 4		4 7 1 6	4 8 3 3
	5 4 4	5 1 3		5 2 9 3	5 1 5 1
				6 9 5 9	6 3 7 8
Dist.M.	L^1	L^2	Dist. M.	L^1	L^2
$D_1(J_1)^{(1)}$	5(3)	5(6)	$D_1(J_1)^{(1)}$	11(3)	10(4)
$\Phi_p^{(1)}$	0.2170	0.21879	$\Phi_p^{(1)}$	0.105	0.108
$D_1(J_1)^{(2)}$	9(1)	11(6)	$D_1(J_1)^{(2)}$	33(2)	42(6)
$\Phi_p^{(2)}$	0.1113	0.09956	$\Phi_p^{(2)}$	0.031	0.026

Table 3: Comparison of $D_1(X)$ values for (N, k) design points in MD measure

N	$k=3$		$k=4$		$k=5$		$k=6$		$k=7$		$k=8$		$k=9$	
	(ILS)	MSA	(ILS)	MSA	(ILS)	MSA	(ILS)	(MSA)	(ILS)	(MSA)	(ILS)	(MSA)	(ILS)	(MSA)
4	4	4	6	6	8	8	10	10	11	11	13	13	14	14
5	5	5	7	7	10	10	11	12	13	13	16	16	17	18
6	6	6	8	8	10	11	14	14	15	15	18	18	20	20
7	6	6	8	10	12	12	14	16	18	18	19	20	22	24
8	7	7												
9	8	8												
10	7	8												
11	8	8												
12	8	9												
13	9	10												
14	9	10												
15	10	11												
16	9	11												

Now we have performed further experiments for the comparison between MLH-ILS and MLS-SA in perspective of MD measure and also Euclidean distance measure. The experimental results are displayed in Table 3 and Table 4 respectively. It is worthwhile to mention here that the maximin LHD obtained by SA regarding MD measure are available in the web portal <http://www.spacefillingdesigns.nl/> but only few design points corresponding to each number of factors are given. Anyway the comparison between MLS-ILS and MLS-SA where the minimal pair-wise distance (D_1) is calculated in L^1 distance measure is shown in Table 3. On the other hand Table 4 have shown the comparison between MLS-ILS and MLS-SA where the minimal pair-wise distance (D_1) is calculated in L^2 distance

measure. It is observed in the Table 3 that regarding L^1 distance measure maximin LHDs obtained by MSA approach and maximin LHDs obtained by ILS approach are comparable. Though objective function of maximin LHDs obtained by MSA was calculated by L^1 measure during optimization procedure and the objective function of maximin LHDs obtained by ILS was calculated by L^2 measure optimization procedure.

On the other hand in the Table 4 where the distances of maximin LHDs (after optimized) are calculated by L^2 measure, it is observed that maximin LHDs obtained by ILS approach are significantly better than maximin LHDs obtained by MSA. It is also observed that these differences are significantly increasing more and more clearly with increasing of factors/and design points.

Table 4: Comparison of $D_1(X)$ values for (N, k) design points in Euclidean distance measure

N	$k=3$		$k=4$		$k=5$		$k=6$		$k=7$		$k=8$		$k=9$	
	(ILS)	MSA	(ILS)	MSA	(ILS)	MSA	(ILS)	(MSA)	(ILS)	(MSA)	(ILS)	(MSA)	(ILS)	(MSA)
4	6	6	12	12	14	14	20	18	21	19	26	23	28	26
5	11	11	15	13	24	22	27	24	32	27	40	36	43	40
6	14	14	22	18	32	27	40	36	47	37	54	48	61	54
7	17	12	28	26	40	32	52	52	62	56	71	54	80	72
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												

From this experimental study it may conclude that maximin LHDs obtained by ILS approach in which inter-site distances were calculated through Euclidean distance measure are not only significantly better than that of SA approach but also comparable with maximin LHDs obtained by the SA approach, regarding MD measure where inter-site distances were calculated through MD measure.

Now we will compare the ILS approach (Grosso *et al.*, 2009) with SA (Husslage *et al.*, 2011) and MSA (Morris and Mitchell, 1995) regarding maximin LHDs measure where the objective functions (for all cases) are measured by Euclidean distance measure. Table 5 displays the comparison of the ILS approach among other well-known methods available in the literature. It is noted that in all the maximin LHDs obtained by ILS, SA and MSA, the objective function is same i.e. Φ_p and algorithm considered L^2 distance measure during the optimization procedures. In the Table the best MLHs available in the web portal are denoted as MLH-Web. It is observed in the Table 5 that MLH-ILS always better than other two MLH regarding L^2 distance measure. More over except dimension 3 and 4 MLH-ILS are the best LHDs according to the MLS-Web. For dimension 3 and 4, the performance of ILS better than other two approaches considered but 65 and 47 MLHs respectively are not best LHDs according to the MLH-Web. From the experiments it is also observed that except $k=3$, for the larger values of N the performance of ILS are much more better than the performance of ILS increases with the increase of k values.

4. FURTHER ANALYSIS OF THE EXPERIMENTAL RESULT

It is worthwhile to mention here that it not possible to direct compare the distance values of two methods namely Euclidean distance measure and MD measure. But it is known that for the distance of any two particular points, the value of Euclidean distance measure is always less or equal to the value of the MD measure which is illustrate by the Tables 6 and 7. Table 6 displays the D_1 values (both in L^2 and L^1 measures) of maximin LHDs which are optimized regarding L^2 by the ILS approach. On the

other hand Table 7 displays the D_1 values (both in L^2 and L^1 measures) of maximin LHDS which are optimized regarding L^1 by the SA/MSA approaches.

Table 5: Comparison among different approaches with ILS approach for all $N=3, \dots, 100$ in each k regarding L^2 measure.

k	Number of best solutions (maximin LHD)			MLH-ILS Worse than web MLH
	SA	MSA	ILS	MLH-ILS < MLH-Web
3	0	0	32	65
4	0	0	50	47
5	0	0	86	11
6	0	0	97	00
7	0	0	97	00
8	0	0	97	00
9	0	0	97	00
10	0	0	97	00

Table 6: Comparison between L^1 and L^2 of D_1 values of Maximin LHDS optimized regarding Euclidean distance measure

N	k=3		k=7		k=9	
	D_1 in L^2	D_1 in L^1	D_1 in L^2	D_1 in L^1	D_1 in L^2	D_1 in L^1
4	2.44949	4	4.582576	11	5.291503	14
5	3.316625	5	5.656854	13	6.557439	17
6	3.741657	6	6.855655	15	7.81025	20
7	4.123106	6	7.874008	18	8.944272	22
8	4.582576	7				
9	4.690416	8				
10	5.196152	7				
11	5.477226	8				
12	6	8				
13	6.403124	9				
14	6.480741	9				
15	6.928203	10				
16	7.071068	9				

Table 7: Comparison between L^1 and L^2 for D_1 values of Maximin LHDS optimized regarding MD measure

N	k=3		k=7		k=9	
	D_1 in L^1	D_1 in L^2	D_1 in L^1	D_1 in L^2	D_1 in L^1	D_1 in L^2
4	4	2.44949	11	4.358899	14	5.09902
5	5	3.316625	13	5.196152	18	6.324555
6	6	3.741657	15	6.082763	20	7.348469
7	6	3.464102	18	7.483315	24	8.485281
8	7	4.582576				
9	8	4.690416				
10	8	4.690416				
11	8	4.690416				
12	9	5.196152				
13	10	6				
14	10	5.830952				
15	11	6.403124				
16	11	6.403124				

So for any two points, if the value of Euclidean distance measure is greater than the value of MD measure, then two points whose distance is measured by Euclidean distance measure is sparser rather than the two points whose distance is measured by MD measure. Exploiting this idea we would want to compare the maximin LHDS optimized regarding Euclidean distance measure and MD measure

respectively. For the comparison of two different measures, we transform the data by using following formulas:

- (a) Relative value of D_1 of an LHD X in L^2 measured = $\{(D_1 \text{ value calculated in } L^2 \text{ measured and } X \text{ is optimized regarding } L^2) - (D_1 \text{ value calculated in } L^2 \text{ measured and } X \text{ is optimized regarding } L^1)\} / (D_1 \text{ value calculated in } L^2 \text{ and } X \text{ is optimized regarding } L^1) \times 100$. In notation it may expressed as follow:

$$R_D1(X)_{L2} = \{D_1^{L2}(X^{\text{opt}L2}) - D_1^{L2}(X^{\text{opt}L1})\} / D_1^{L2}(X^{\text{opt}L1}) \times 100$$

- (b) Relative value of D_1 of an LHD X in L^1 measured = $\{(D_1 \text{ value calculated in } L^1 \text{ measured and } X \text{ is optimized regarding } L^2) - (D_1 \text{ value calculated in } L^1 \text{ measured and } X \text{ is optimized regarding } L^1)\} / (D_1 \text{ value calculated in } L^1 \text{ and } X \text{ is optimized regarding } L^1) \times 100$. In notation it may expressed as follow:

$$R_D1(X)_{L1} = \{D_1^{L1}(X^{\text{opt}L2}) - D_1^{L1}(X^{\text{opt}L1})\} / D_1^{L1}(X^{\text{opt}L1}) \times 100$$

Table 8: Comparison between Euclidean distance Measure and MD Measure regarding Maximin LHDs

N	k=3		k=7		k=9	
	$R_D1(X)_{L2}$	$R_D1(X)_{L1}$	$R_D1(X)_{L2}$	$R_D1(X)_{L1}$	$R_D1(X)_{L2}$	$R_D1(X)_{L1}$
4	0	0	5.131497	0	7.692308	0
5	0	0	8.866211	0	7.5	-5.55556
6	0	0	12.70627	0	12.96296	0
7	19.02381	0	5.220856	0	11.11111	-8.33333
8	0	0				
9	0	0				
10	10.78234	-12.5				
11	16.77484	0				
12	15.47005	-11.1111				
13	6.718737	-10				
14	11.14379	-10				
15	8.200356	-9.09091				
16	10.43153	-18.1818				
Total	98.54545	-70.8838	31.92483	0	39.26638	-13.8889
Avr.	7.580419	-5.4526	7.981208	0	9.816595	-3.47222

Finally we have counted the total relative better of D_1 regarding L^1 as well as L^2 measures. We have also find out the average relative better of D_1 regarding L^1 as well as L^2 measures. The comparison results are displayed in the Table 8. It is observed in the Table 8 that except few LHDs the (absolute) $R_D1(X)_{L2}$ values are better than that of $R_D1(X)_{L1}$. Moreover the (absolute) average values of $R_D1(X)_{L2}$ are always larger than $R_D1(X)_{L1}$ for all k values namely dimension 3, 7 and 9. Therefore it may conclude from this comparison study that the maximin LHDs optimized regarding L^2 measure are more space-filling rather than maximin LHDs optimized regarding L^1 measure.

It is also worthwhile to mention here that the all most all the Maximin LHDs considered here are optimal either Euclidean distance measure (obtained by ILS) or MD measure (given in the WEB obtained by SA or MSA approaches).

5. CONCLUSION

In this article we have studied the MLH obtained by ILS where the objective function is Φ_p criteria and for the calculation of Φ_p during optimization procedure, the algorithm considered Euclidean distance measure. The main task of this research works was to investigate the minimal inter-site distance i.e. D_1 value as well as Φ_p value of the optimized LHD namely MLH-ILS in perspective to MD measure as well as Euclidean distance measure. For the comparison, we have first considered the MLS obtained by ILS in which the objective function is Φ_p criteria but for the calculation of Φ_p during optimization procedure, the algorithm considered Euclidean distance measure. Secondly for the comparison we have considered the MLS obtained by SA as well as MSA in which the objective function is Φ_p criteria but for the calculation of Φ_p during optimization procedure, the algorithm considered MD measure too. The experimental results reveal that for Euclidean distance measure, the maximin LHDs obtained by ILSs are not only significantly better than other two approaches but also state-of-the-arts. On the other hand regarding MD measure, the D_1 values of maximin LHDs obtained by ILS are comparable though during the optimization procedure – ILS considered Euclidean distance measure and other approaches

(SA/MSA) considered MD measure. Moreover, experimental results also reveals that maximin LHDS optimized regarding Euclidean distance measure are on average more space-filling compared to maximin LHDS optimized regarding MD measure.

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