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Computational Experiment of Iterated Local Search for Higher Dimensions for Optimizing Latin Hypercube Designs

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Abstract: *Latin Hypercube Designs (LHDs) almost always show poor space-filling properties. On the other hand, maximin distance designs have very well space-filling properties but often show poor projection properties under the Euclidean or the Rectangular distance. It is shown that the Iterated Local search(ILS) approach not only able to obtain good LHDs in the sense of space-filling property but the correlations among the factors are acceptable i.e. multi-collinearity is not high. When number of factors or number of design points is large then it requires hundreds of hours by the brute-force approach to find out the optimal design. So when numbers of factors as well as number of experimental points are large, the heuristic approaches also require a couple of hours or even more to find out a simulated optimal design. So time complexity is an important issue for a good algorithm. In this research some experiments have been performed for higher dimension namely dimensions k >10. Some new maximin LHDs value are obtained from these experiments, as there are few maximin LHDs value available in the literatures for higher dimension, k >10. From these experiments, multi-collinearity property, maximin LHDs in Rectangular distance, mimimal Φ values, maximum pair-wise distance value of LHDs etc. are represented in this thesis.*

Keywords: *Iterated Local search, Latin Hypercube design, multi-collinearity, optimal criterion.*

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I. Introduction:

Latin Hypercube Designs (LHDs) fulfill the *non-collapsing* property. Such design, firstly introduced in 1979 by McKay and his colleagues has proved to be a popular choice for experiments run on computer simulators [Levy et al. (2010)] and in global sensitivity analysis [Helton and Davis (2000), Steinberg and Dennis (2006)]; Assume that *N* design points have to be placed and that there are *k* distinct parameters. It would be done such that the points will uniformly spread when projected along each single parameter axis. It is also assumed that each parameter range is normalized to the interval [0, *N*-1]. Then, a LHD is made up by *N* points, [Audze P., and V. Eglais, 1997] each of which has *k* integer coordinates with values in 0, 1, . . . , *N*-1 and such that there do not exist two points with one common coordinate value. This allows a non-collapsing design because points are evenly spread when projected along a single parameter axis. Note that the number of possible LHDs is huge: there are $(N!)^k$ possible LHDs (where *N* is number of design points and *k* is number of factors). Anyway the main attraction of these designs is the one-dimensional projective property. The 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** designs, proposed by [Jonson et al. (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 (1997) suggested to search for **maximin LHDs** when looking for "optimal" designs. In the literature the optimal criterion for maximin LHD are defined in several ways [Grosso et al. (2008)] but the main objective is identical i.e. searching the LHD with the maximizing the minimum pair-wise distance.

Though finding the optimal LHD in brute-force approach is $(N!)^k$, but we expected, in ILS approach, this will be polynomial time with low order. It will be worthwhile to mention here that the solution obtained by the ILS approach must not be guaranteed to be optimal one rather it may be approximately optimal. It is also expected that function based approach also work well. Finally it is expected that structural analysis as well as theoretical analysis may build the method as well as experimental design much more stronger. Besides some complexity analysis, several experiments will be performed for dimension $k \rangle$ 10. Then the results will be compared available one in the literature.

II. 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.

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 lead 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:

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

III. Maximin Latin Hypercube Designs:

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

$$d_{ij}=\|x_i - x_j\|_s$$

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

3.1 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) X, where each column of X consists of a permutation of integers $0, 1, \cdots, N-1$ (note that each factor range is normalized to the interval $[0, N-1]$) [Ye, K. Q., 1998] so that for each dimension j all x_{ij}, $i = 0, 1, \cdots, N-1$ are distinct. We will refer to each row of X as a (discrete) design point and each column of X as a factor (parameter) of the design points.
We can represent $\boldsymbol{X}$ as follows

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

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 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 $D_r(X)$ as the r-th minimum distance in D, and $J_r(X)$ as the number of pairs $\{x_i, x_j\}$ having $d(x_i, x_j) = D_r(X)$ in X.

The maximin LHD problem aims at finding a LHD X^* such that $D_1(X)$ 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.

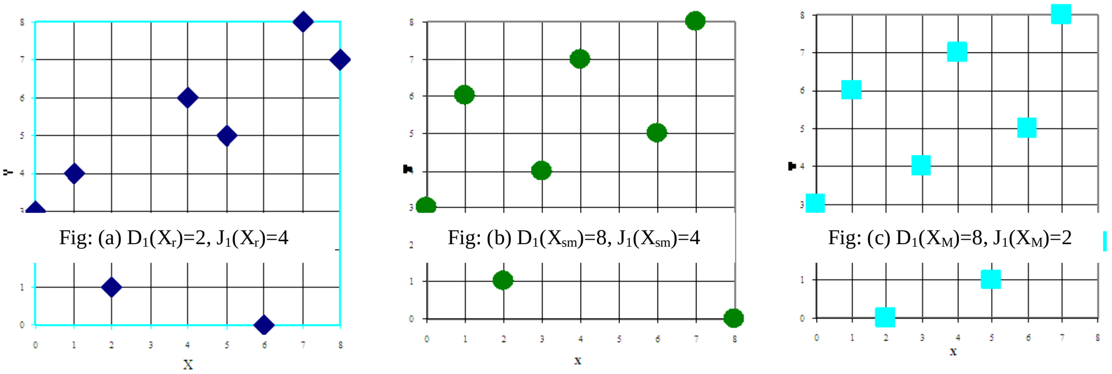

Figure 3.1: Some LHDs and their corresponding (D_1, J_1) values

IV. Computational experiment of iterated local search for higher dimensions:

We have performed several experiments to find out the time complexity in experimental domain. Grosso et al. (2008) have shown that, for finding maximin LHDs, ILS approach outperforms when number of dimensions (k) are less than 11. The outperforms results are available in the well-known website http://www.spacefillingdesigns.nl/. But they could not performed experiments higher than 10 dimension. It is also noted that few results (in the cases of dimensions greater than 10) are available in the literatures which are reported in the website http://www.spacefillingdesigns.nl/ . Here we will perform several experiments for higher dimensions typically k greater than 10 regarding ILS approaches. Also the results are compared with available one in the literature i.e. in the above mentioned website.

Table 4.1: The setting of number of runs for the ILS approach

k	***N***	***R***
11 – 15	3-25	2

For ILS approach, we set RP local moves with BI acceptance rule in local search, SPC. perturbation and MaxNonImp=100. We also consider the Opt(Φ) optimality criterion i.e. we consider ILS(Φ) approach. the value of p is equal to 20 as well. In what follows the approach will be simply denoted as ILS(Φ). For what concerns the number of runs for each LHD, we considered is given in Table 4.1. In the table R denotes the number of runs (trials) for each experiment $(k, N): k = 11, 12, \cdots, 15;\ N = 3, 4, \cdots, 25;$. It is noted that for dimension k = 11, besides R = 2 we have also considered R = 5 and 10. The experimental results are reported in the Table 4.2(a), Table 4.2(b) and Table 4.2(c) where the distances are measured in Euclidian measure and the values are the best maximin squared distance rather than actual distances each for (k,N). It is noted that the 2nd column of the tables 4.2(a), 4.2(b) and 4.2(c) denotes the maximin LHDs values available in the website

Table 4.2 (a): Comparison of maximin LHD values for dimensions k = 11

Points(*N*)	**Web Value**	**ILS Value**		
		Trial 2	**Trial 5**	**Trial 10**
3		20	20	20
4	35	34	34	35
5	54	52	54	54

6	74	73	74	74
7		98	98	98
8		125	125	126
9		156	157	158
10		190	190	191
11		227	229	229
12		270	270	272
13		306	306	309
14		350	350	350
15		393	397	397
16		445	445	448
17		501	501	501
18		560	560	561
19		619	620	623
20		685	691	692
21		760	767	767
22		844	851	857
23		848	857	857
24		907	925	925
25		967	974	984

http://www.spacefillingdesigns.nl/. In the tables we have observed that few web values (maximin LHDs values available in the web) are available for higher dimensions. It is observed that the ILS values are identical with Web values. It worthwhile to mention here that these values are analytically global optimal rather than approximate optimal. Moreover The ILS approaches able to obtain some new maximin LHDs value for $6<N<26$ which are reported in the tables 4.2(a), 4.2(b) and 6.2(c). There is another observed in the table 4.2(a) that the increasing of number of trials do not significantly increasing the maximum LHDs values. From this observation it may conclude that for higher dimensions, few trials of ILS approach able to find approximate optimal LHDs.

Table 4.2 (b): Comparison of maximin LHD values for dimensions k = 12 and 13

k = 12			k = 13		
Point(N)	Web Value	ILS Value	Point(N)	Web Value	ILS Value
3		24	3		25
4	40	40	4	41	41
5	60	60	5	64	64
6	82	82	6	89	89
7		107	7		117
8		137	8		150
9		172	9		187
10		209	10		229
11		251	11		274
12		296	12		322

13		347	13		376
14		351	14		434
15		438	15		605
16		495	16		669
17		550	17		487
18		611	18		540
19		684	19		745
20		758	20		823
21		830	21		910
22		908	22		997
23		999	23		1083
24		1105	24		1179
25		1230	25		1290

Table 4.2 (c): Comparison of maximin LHD values for dimensions k = 14 and 15

k = 14			k = 15		
Point(N)	Web Value	ILS Value	Point(N)	Web Value	ILS Value
3		26	3		30
4	46	46	4	48	48
5	70	70	5	74	74
6		95	6		103
7		127	7		136
8		162	8		173
9		202	9		217
10		249	10		266
11		293	11		319
12		349	12		374
13		404	13		436
14		464	14		504
15		537	15		574
16		595	16		653
17		660	17		721
18		731	18		797
19		815	19		883
20		897	20		969
21		987	21		1064
22		1079	22		1063
23		1183	23		1271
24		1284	24		1376
25		1397	25		1502

It is also noted that the ILS (Φ) approach proposed by Grosso et al. (2008) does not consider the LHD with corresponding optimal (minimum) Φ value but tracking the optimal maximin LHD (whose minimum pair-wise distance is maximum) during minimizing Φ value. Here several experiment are performed to analyze the above discussion. For these experiments we consider k = 11 , N = 3, 4, …, 25 and number of trials R = 2, 5, 10. Other parameter setting are same. The experimental results displayed in table 4.3. It is observed form the table that though increasing of number of trials causes monotonic increasing of maximin LHDs values but corresponding Φ values do not necessarily monotonic decreasing. In the table we also observed that some time lower trial may better results. This implies that initial solution may affect the final output.

Table 4.3: Comparison of maximin LHD values and Φ values for dimensions *k* = 11

N	LHD values				Φ values		
	R **=2**	***R*** **=5**	***R*** **=10**		***R*** **=2**	***R*** **=5**	***R*** **=10**
3	20	20	20		0.456287	0.456287	0.456287
4	34	35	35		0.546794	0.513469	0.513469
5	54	54	54		0.565956	0.60572	0.60572
6	74	74	74		0.653762	0.653762	0.653762
7	97	97	99		0.690905	0.690839	0.690505
8	126	125	125		0.721167	0.721102	0.721102
9	154	154	156		0.747052	0.746939	0.746679
10	189	193	193		0.768803	0.768375	0.768375
11	226	225	225		0.787288	0.787281	0.787281
12	272	272	272		0.803762	0.803513	0.803513
13	309	309	309		0.824438	0.824438	0.824438
14	341	341	341		0.842359	0.842359	0.842359
15	383	383	390		0.857904	0.857904	0.857816
16	443	443	436		0.871477	0.871477	0.871336
17	495	495	504		0.882531	0.882531	0.882233
18	557	557	554		0.893106	0.893106	0.892659
19	625	625	625		0.901792	0.901792	0.901792
20	683	682	684		0.910757	0.910681	0.910578
21	750	768	748		0.918572	**0.918509**	*0.918449*
22	848	848	848		0.924703	0.924703	0.924703
23	850	850	850		0.942046	0.942046	0.942046
24	901	908	908		0.952664	0.95243	0.95243
25	958	958	950		0.965299	0.965299	0.965077

It is worthwhile to mention here that for all experiments performed earlier all the distances measured in L^2 measure. But when maximize the minimum pair-wise distance in L^2 measure might causes L^1 measure too. That is in any experimental design when the minimum pair-wise distance is increasing in L^2 measure, then the minimum pair-wise distance in L^1 measure should be increase but not necessarily monotonic. The experimental results are reputed in the table 4.4. It is noted that the L^1 value reputed in the table 4.4 are measured from the LHDs which are maximin LHD in L^2 measure by the ILS approach but not maximin LHDs in L^1 measure. Since there are no any value available in the literatures, so we could not compare the results.

Table 4.4: Experimental results of maximin L^1 values corresponding to optimized LHD values measured in L^2 measure for *k* = 11 - 15

N	***k*** **= 11**	***k*** **= 12**	***k*** **= 13**	***k*** **= 14**	***k*** **= 15**
3	14	16	17	18	20
4	17	20	21	23	24
5	22	24	26	28	30
6	23	27	28	31	34
7	27	29	32	34	36
8	30	32	36	39	42
9	32	37	39	41	44

10	36	41	41	47	51
11	40	42	46	50	55
12	43	45	49	56	59
13	44	50	55	59	61
14	45	54	57	59	66
15	47	55	60	64	70
16	51	56	64	68	74
17	56	58	68	72	76
18	60	62	71	78	80
19	59	67	74	82	85
20	61	70	76	84	88
21	68	73	80	87	96
22	66	77	85	89	96
23	71	80	87	96	103
24	76	86	86	95	106
25	76	83	96	97	105

Table 4.5: Experimental results of maximum average coefficient of correlation of the co-factors of the maximin LHDs for $k = 11 - 15$

N	*k* = 11	*k* = 12	*k* = 13	*k* = 14	*k* = 15
3	0.953463	0.953463	0.960769	0.963624	0.963624
4	0.738549	0.738549	0.748331	0.751263	0.758445
5	0.592376	0.603023	0.612896	0.620174	0.627163
6	0.490927	0.505309	0.517086	0.526916	0.535017
7	0.409534	0.427894	0.441798	0.453797	0.463749
8	0.340129	0.362158	0.379442	0.393168	0.404955
9	0.27707	0.30364	0.324707	0.341046	0.35451
10	0.215443	0.249506	0.273677	0.294027	0.309932
11	0.14771	0.193683	0.226577	0.250427	0.268747
12	0.038924	0.134783	0.177042	0.207415	0.229611
13	0.135165	0.036809	0.124208	0.163625	0.191376
14	0.154653	0.121373	0.030303	0.113747	0.151578
15	0.162267	0.148942	0.114768	0.029532	0.104976
16	0.157082	0.154097	0.134213	0.105412	0.026695
17	0.149606	0.148493	0.144009	0.127823	0.097976
18	0.136881	0.139549	0.14477	0.135268	0.121348
19	0.118659	0.134324	0.134428	0.137081	0.131929
20	0.096469	0.125651	0.137371	0.142735	0.133814
21	0.07354	0.10854	0.127346	0.1344	0.13852
22	0.018811	0.090604	0.114545	0.12536	0.135415

23	0.046038	0.068007	0.10028	0.116373	0.129211
24	0.075818	0.018534	0.082387	0.107147	0.117659
25	0.089355	0.044584	0.060996	0.093726	0.109148

It is also remarks that multicollinearity is another important properties of an experimental design. A good experimental design should minimum multicollinearity among the factors along with other two properties. Then the measure the multicollinearity among the factors can be defined by the following measure of average pair-wise correlations

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

Where ρ_{ij} denotes the product-moment correlation between the *i*-th and *j*-th factors. Note that this definition is frequently used in literature [Fang et al. (2000b), Joseph and Hung (2008)]. Whereas the definition of maximum pair-wise correlation is given below:

$$\rho_{\max} = \max_{1 \le i, j \le k} \rho_{ij}$$

Now another experiment is performed by considering the same setting as considered above. The experimental results are plotted in the table 4.5. It is observed that when the number of design points (i.e N) is small the maximum coefficient of correlation is high. Whereas the coefficient of correlation is negligible as well as decreasing when increasing the N values.

It is noted that in any experimental design when the minimum pair-wise distance is increasing, then the maximum pair-wise distance should be decreasing but not necessarily monotonic. So minimizing the maximum pair-wise distance may be the another optimal criterion for optimal the experimental design. So another experiments is performed by considering the same setting as considered above. The experimental results are plotted in the table 4.5. In the table 4.6, L_M^1 and L_M^2 denote the maximum pair-wise distance of the maximin LHDs measured in L^1 and L^2 distance measure respectively. As there are no value available in the literature, so we could not compare the experimental results.

Table 4.6: Experimental results of maximum pair-wise distance value (L_M^1 and L_M^2) of the maximin LHDs for *k* = 11 - 15

N	L_M^1					L_M^2				
	***k* = 11**	***k* = 12**	***k* = 13**	***k* = 14**	***k* = 15**	***k* = 11**	***k* = 12**	***k* = 13**	***k* = 14**	***k* = 15**
3	15	16	18	19	20	23	24	28	29	30
4	20	20	24	24	27	42	40	48	47	55
5	22	24	26	28	30	56	60	66	70	76
6	27	29	32	34	36	80	87	96	101	108
7	32	35	37	39	43	108	118	125	137	148
8	36	39	42	46	48	146	152	162	176	188
9	40	44	47	50	55	174	192	208	222	234
10	45	48	53	56	60	218	238	248	270	290
11	48	53	57	60	67	256	279	307	327	347
12	52	58	63	66	70	305	332	359	380	408

1 3	85	62	67	72	79	695	395	416	461	482
1 4	87	94	74	78	82	787	866	482	526	553
1 5	89	99	107	82	87	887	991	1075	604	628
1 6	94	104	110	125	93	968	1103	1194	1297	721
1 7	100	111	120	129	146	1088	1204	1348	1451	1572
1 8	105	118	127	134	143	1221	1356	1481	1612	1747
1 9	109	117	134	144	153	1339	1463	1615	1783	1940
2 0	117	129	137	149	160	1481	1619	1781	1920	2109
2 1	122	135	140	155	168	1650	1781	1937	2081	2241
2 2	127	145	151	167	177	1795	1962	2131	2291	2466
2 3	134	146	158	169	187	1948	2126	2328	2511	2700
2 4	143	154	169	181	195	2011	2348	2512	2717	2914
2 5	144	160	169	190	203	2139	2497	2743	2969	3152

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