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A Method of Constructing Orthogonal Array-Based Latin Hypercube Designs for Computer Experiments

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Abstract

Orthogonal array-based Latin hypercube designs (OALHDs) were constructed for four input variables computer experiments. The proposed designs have some advantages over the random Latin hypercube designs in terms of better space-filling properties and maximin distance criterion employed in the construction. There is a link between Graeco-Latin squares and orthogonal arrays (OAs). Graeco-Latin squares are two mutually orthogonal Latin squares of the same order such that when one is superimposed on the other, each symbol in the body of one square appears together with each symbol in the body of the other exactly once. This method is fast and straightforward to implement. In this paper, orthogonal arrays, OA (25, 4, 5, 2) and OA (49, 4, 7, 2) were generated from Graeco-Latin square of orders 5 and 7 and the orthogonal arrays generated were used to construct OA(25, 4)LHD and OA(49, 4)LHD for use in a computer experiment that involves only four input variables. The OALHDs constructed have better space-filling properties. MATLAB 2012a package was used for the development of the program that constructs the OALHDs in this paper.

***Keywords**: Computer experiments, Graeco-Latin squares, Latin hypercube designs, Orthogonal array, Space-filling properties*

1. Introduction

Computer experiments are widely used in many areas of science and engineering. Some physical phenomena that are either complex or infeasible to investigate using conventional statistical experiments have been represented by mathematical models that are implemented in computer codes (simulators). The first computer experiment was performed by Enrico Fermi and colleagues, [18] at the Los Alamos Laboratory in 1953. Scientists in diverse fields have since then accepted computer experiments as a useful tool to understand their respective processes. For example, the author in [3] and [23] used computer experiments in the design of analog integrated circuit behaviour and author in [9] also used computer experiments to study the time it took a pendulum bob to return to rest in a simple pendulum experiment. The inputs to the computer model can be changed in order to determine the effect of various input variables on the output. The output of such computer models serves as a substitute for the real life experiment. A computer experiment is a collection of pairs of inputs and output from runs of a computer model. A Latin hypercube space-filling design has been greatly employed in the design of computer experiments [11]. In this work we are particularly interested in constructing space-filling design called OALHDs.

A space-filling design is a design that spreads design points evenly throughout the experimental region. Two mutually orthogonal Latin squares of the same order with the property that when one is superimposed on the other, each symbol in the body of one square appears together with each symbol in the body of the other square exactly once are called a Graeco-Latin square design. The second square allows us to add the fourth column to the orthogonal array, yielding an OA (s^2, 4, s,

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2). This technique is an improvement on the method employed by [10] in the construction of OALHDs for three input variables computer experiments. This method works perfectly for computer experiments with four factors.

2. Orthogonal Arrays

Orthogonal arrays (OAs) were originally introduced by [15] followed by [1]. Orthogonal arrays (OAs) are useful in designing statistical experiments and they are greatly important in all areas of human investigations. The use of orthogonal arrays provides more acceptable statistical information.

Mathematically, an orthogonal array of N runs, k factors, s levels, strength $t \geq 2$ and index λ is an N-by- k matrix with entries from a set of s levels, usually taken as 0. . . s -1 such that for every N-by-k matrix of s symbols, every subset of t columns from among the k columns, when considered alone must contain each of the possible s^t ordered rows the same number of times. The variables N, k, s, t and λ are the parameters of the OA and such an array is usually denoted by OA (N, k, s, t). The parameter $\lambda = N/s^t$ is referred to as the index of the orthogonal array and is determined by the remaining parameters. The most familiar examples of orthogonal arrays are regular fractional factorial designs discussed in [22]. The OA with $s_1 = s_2 = \cdots s_n = s$ is symmetric, otherwise, the OA is said to be asymmetric. The row of the array represents the experiment to be performed and the column corresponds to different variables whose effects are being analysed.

The construction of OALHDs is largely dependent on the existence of orthogonal arrays. Another important problem associated with OAs is to determine either the minimum number of rows N in any OA (N, k, s, t) for given values of k, s and t or the maximum number of columns k for given values N, s and t. The solution to this problem is adapted from the famous inequalities found by [16] for the construction of OAs.

Theorem 1. The Rao's Inequalities

The Rao's inequalities [Rao47] were governed by the following two inequality statements:

(i) $N \geq \sum_{i=0}^{u} \binom{K}{i} (s-1)^{i})^{i}$,if $t = 2u$ and

(ii) $N \geq \sum_{i=0}^{u} \binom{K}{i} (s-1)^{i} + \binom{k-1}{u} (s-1)^{u+1}$, if $t = 2u+1$ for $u \geq 0$

The use of these inequalities depends on whether t is even or odd. The proof of these theorems can be found in [2]. The method employed for the construction of OALHDs in this work is simple and straightforward as it generates OAs based on a mathematical theorem to construct the desired OALHDs.

3. Orthogonal Array-Based Latin Hypercube Designs (OALHDs)

Latin hypercube designs (LHDs) were originally proposed by [6] for developing computer experiments. A LHD guarantees maximum of the minimum distance between design points and it requires that the levels of each input variable be uniformly spaced. A LHD is an appropriate choice involving some useful criteria such as maximin distance and orthogonality which enhance better space-filling properties. The creation of experimental designs with as many design points as possible because of flexibility in terms of data density and location, non-collapsing and space-filling properties have made LHDs widely known in computer experiments. Maximin LHDs were considered by [7] to enhance the space-filling property of maximin distance designs. A LHD of size N has

$$L_{ij} = \frac{(d_{ij} - U_{ij})}{N}, i=1, \ldots, N, j = 1, \ldots, k \quad (1)$$

where d_{1j}, . . . , d_{Nj} are random permutations of the integers 1, . . . , N. $U_{ij} \sim U[0,1]$ with k permutations while the N_k uniform variates are mutually independent, [12]. Some literature discussed the simpler Lattice sample following [13] where

$$L_{ij} = \frac{(d_{ij}-0.5)}{N}, i=1,\ldots,N, j=1,\ldots,k \qquad (2)$$

Equations 1 and 2 are two methods of generating design points in the unit cube $[0, 1)^k$ based on a given Latin hypercube. The two methods have the property that one and only one of the N design points fall within each of the N small intervals defined by [0, 1/N), [1/N, 2/N), . . . , [(N − 1)/N, 1] when projected onto each of the *k* variables.

The first method gives the points that are distributed uniformly in their corresponding intervals while the second method gives the mid-points of these intervals. The variables (N, *k*, *s*, *t*) cannot be interpreted in the same way as we do for an orthogonal array since they do not all have a clear statistical interpretation, [19]. For example, *s* which refers to the number of levels of orthogonal array does not refer to the number of levels of the design since the design has N levels in this case. The other parameters N, k and t are interpreted in the same way as number of rows, columns and the strength of either OA or OALHD respectively.

An OALHD was proposed by [20]. A paper on the algorithm for constructing space-filling designs for Hadamard matrices of Orders 4λ and 8λ was presented by [8]. Similarly, a method for constructing space-filling designs for three input variables computer experiments was proposed by [10]. An OALHD was also constructed by the authors in [11] for developing borehole computer experiment. Several researchers have constructed designs that are space-filling in the low dimensional projection. Randomized orthogonal arrays and OALHDs were constructed by [13] and [20]. For an excellent review of design and analysis of computer experiments, the author in [4] and [17] can be consulted. Orthogonal arrays are used to construct LHDs in this study with the choice of a maximin distance criterion to achieve better space-filling property. The author in [21] provided a way of obtaining OALHDs based on single replicated full factorial designs and proved that if the underlying orthogonal array is optimal with respect to the maximin distance criterion, so is the corresponding OALHD. The paper written by [5] also considered searching for optimal OALHDs that minimize:

$$\sum_{i=1}^{N}\sum_{j\neq i}\frac{1}{d_{ij}^{2}}$$

where d_{ij} is the Euclidean distance, defined as:

$$d_{ij} = \frac{l_{ij} + {}^{(N-1)}\!/_{2} + u_{ij}}{N}, i=1,\ldots N, j=1,\ldots k \qquad (3)$$

with strength, t = 2, between the i_{th} and j_{th} design points.

4. Implementation

An algorithm was written in MATLAB based on various cell executions to construct the desired OALHDs. A Graeco-Latin square of order *s* where *s* is a prime power was employed to generate OA (s^2, 4, *s*, 2). The OA (25, 4, 5, 2) and OA (49, 4, 7, 2) were generated from Graeco-Latin square of order s for which s = 5 and *s* = 7 and these OAs were later used to construct the OA (25, 4) LHD and OA (49, 4) LHD using Equation 1. The upper case letters D and L stand for the OA and the corresponding OALHD respectively. The steps taken in the generation of OA from Graeco-Latin square of order s is illustrated with the aid of program flowchart as shown in Figure 1.

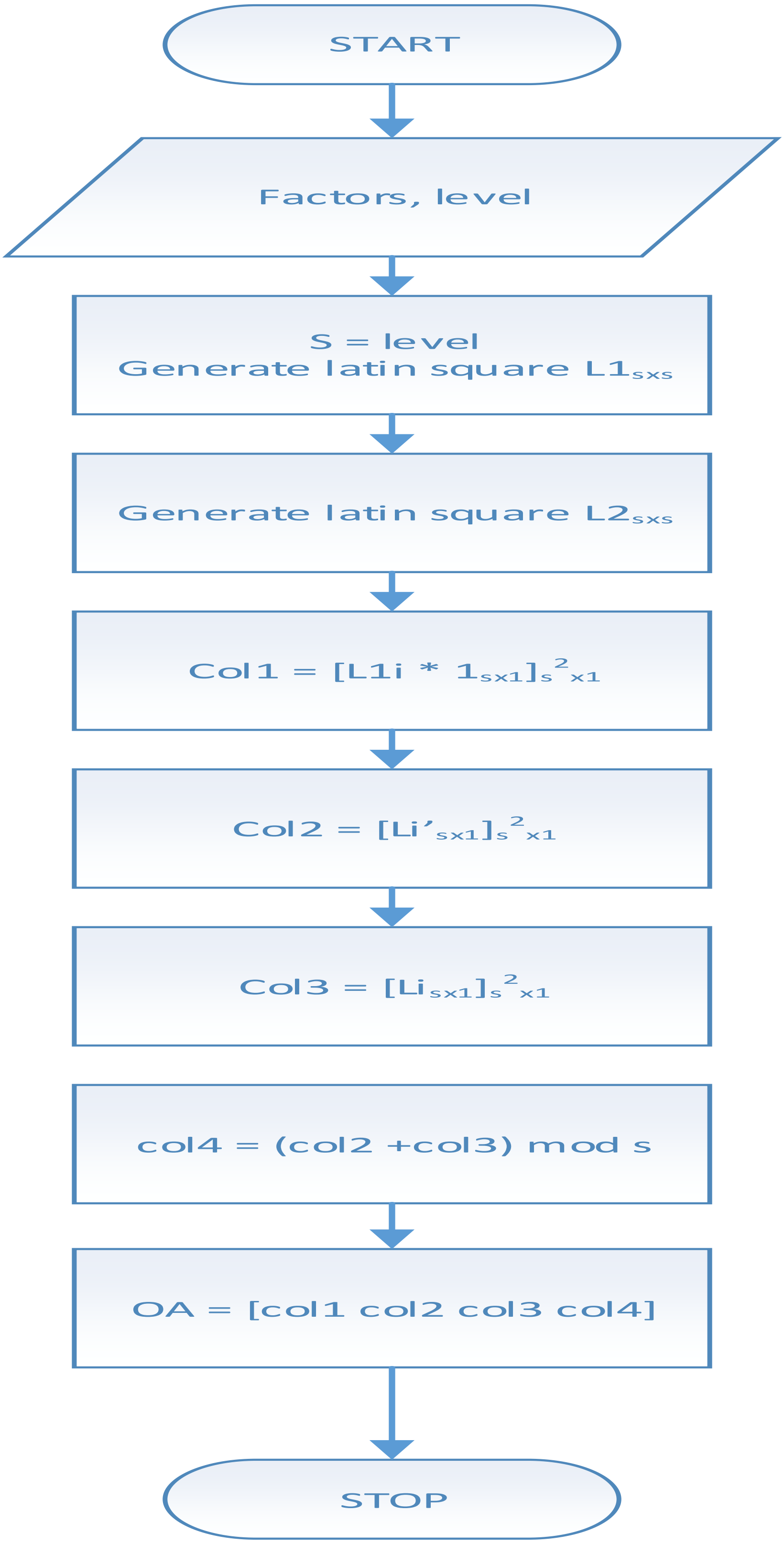

Figure 1. Program Flowchart for the Generation of OA

5. Results

Results of the OA (25, 4) LHD and OA (49, 4) LHD constructed from OA (25, 4, 5, 2) and OA (49, 4, 7, 2) and their plots for bivariate projections among the four input variables are provided in this section. The bivariate projections clearly showed the space-filling properties of the OALHDs constructed.

Table 1. OA (25, 4) LHD Constructed From Graeco-Latin Square of Order 5

Orthogonal Array (D)					**Design Points (L)**			
	x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
1	0	0	0	0	0.0200	0.0200	0.0200	0.0200
2	0	1	1	2	0.0600	0.2200	0.2200	0.4200
3	0	2	2	4	0.1000	0.4200	0.4200	0.8200
4	0	3	3	1	0.1400	0.6200	0.6200	0.2200
5	0	4	4	3	0.1800	0.8200	0.8200	0.6200
6	1	0	1	1	0.2200	0.0600	0.2600	0.2600
7	1	1	2	3	0.2600	0.2600	0.4600	0.6600
8	1	2	3	0	0.3000	0.4600	0.6600	0.0600
9	1	3	4	2	0.3400	0.6600	0.8600	0.4600
10	1	4	0	4	0.3800	0.8600	0.0600	0.8600
11	2	0	2	2	0.4200	0.1000	0.5000	0.5000
12	2	1	3	4	0.4600	0.3000	0.7000	0.9000
13	2	2	4	1	0.5000	0.5000	0.9000	0.3000
14	2	3	0	3	0.5400	0.7000	0.1000	0.7000
15	2	4	1	0	0.5800	0.9000	0.3000	0.1000
16	3	0	3	3	0.6200	0.1400	0.7400	0.7400
17	3	1	4	0	0.6600	0.3400	0.9400	0.1400
18	3	2	0	2	0.7000	0.5400	0.1400	0.5400
19	3	3	1	4	0.7400	0.7400	0.3400	0.9400
20	3	4	2	1	0.7800	0.9400	0.5400	0.3400
21	4	0	4	4	0.8200	0.1800	0.9800	0.9800
22	4	1	0	1	0.8600	0.3800	0.1800	0.3800
23	4	2	1	3	0.9000	0.5800	0.3800	0.7800
24	4	3	2	0	0.9400	0.7800	0.5800	0.1800
25	4	4	3	2	0.9800	0.9800	0.7800	0.5800

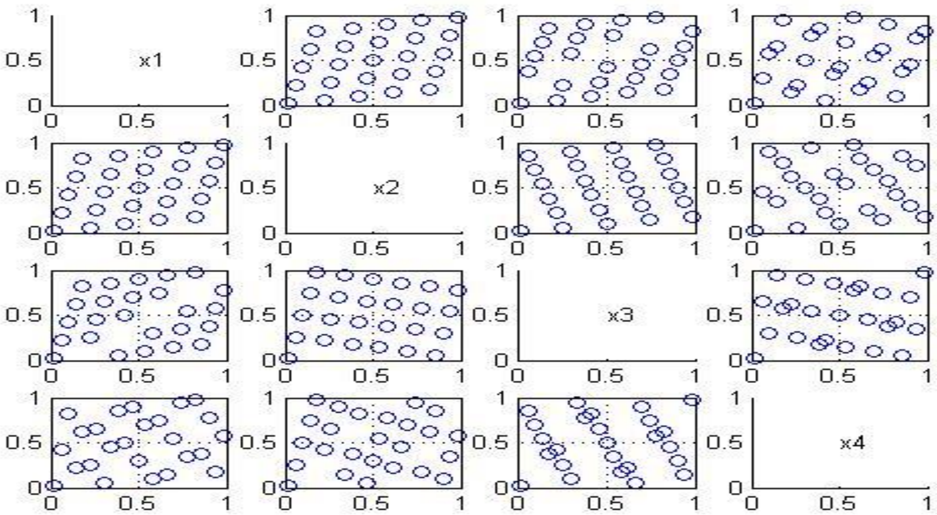

Figure 2. Bivariate Projections among 4 Factors of OA (25, 4) LHD Showing Space-Filling Properties of the Design

Similarly, the results of the OALHD constructed from Graeco-Latin Square of order 7 are presented in Table 2. The bivariate projections among the four factors of this design that clearly showed the space-filling property of the OALHD constructed is also provided in Figure 3.

Table 2. OA (49, 4) LHD Constructed from Graeco-Latin Square of Order 7.

Orthogonal Array (D)					**Design Points (L)**			
	x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
1	0	0	0	0	0.0100	0.0100	0.0100	0.0100
2	0	1	1	2	0.0300	0.1500	0.1500	0.3000
3	0	2	2	4	0.0500	0.3000	0.3000	0.5800
4	0	3	3	6	0.0700	0.4400	0.4400	0.8700
5	0	4	4	1	0.0900	0.5800	0.5800	0.1500
6	0	5	5	3	0.1100	0.7200	0.7200	0.4400
7	0	6	6	5	0.1300	0.8700	0.8700	0.7200
8	1	0	1	1	0.1500	0.0300	0.1700	0.1700
9	1	1	2	3	0.1700	0.1700	0.3200	0.4600
10	1	2	3	5	0.1900	0.3200	0.4600	0.7400
11	1	3	4	0	0.2100	0.4600	0.6000	0.0300
12	1	4	5	2	0.2300	0.6000	0.7400	0.3200
13	1	5	6	4	0.2600	0.7400	0.8900	0.6000
14	1	6	0	6	0.2800	0.8900	0.0300	0.8900
15	2	0	2	2	0.3000	0.0500	0.3400	0.3400
16	2	1	3	4	0.3200	0.1900	0.4800	0.6200
17	2	2	4	6	0.3400	0.3400	0.6200	0.9100
18	2	3	5	1	0.3600	0.4800	0.7700	0.1900
19	2	4	6	3	0.3800	0.6200	0.9100	0.4800
20	2	5	0	5	0.4000	0.7700	0.0500	0.7700
21	2	6	1	0	0.4200	0.9100	0.1900	0.0500
22	3	0	3	3	0.4400	0.0700	0.5000	0.5000
23	3	1	4	5	0.4600	0.2100	0.6400	0.7900

24	3	2	5	0	0.4800	0.3600	0.7900	0.0700
25	3	3	6	2	0.5000	0.5000	0.9300	0.3600
26	3	4	0	4	0.5200	0.6400	0.0700	0.6400
27	3	5	1	6	0.5400	0.7900	0.2100	0.9300
28	3	6	2	1	0.5600	0.9300	0.3600	0.2100
29	4	0	4	4	0.5800	0.0900	0.6600	0.6600
30	4	1	5	6	0.6000	0.2300	0.8100	0.9500
31	4	2	6	1	0.6200	0.3800	0.9500	0.2300
32	4	3	0	3	0.6400	0.5200	0.0900	0.5200
33	4	4	1	5	0.6600	0.6600	0.2300	0.8100
34	4	5	2	0	0.6800	0.8100	0.3800	0.0900
35	4	6	3	2	0.7000	0.9500	0.5200	0.3800
36	5	0	5	5	0.7200	0.1100	0.8300	0.8300
37	5	1	6	0	0.7400	0.2600	0.9700	0.1100
38	5	2	0	2	0.7700	0.4000	0.1100	0.4000
39	5	3	1	4	0.7900	0.5400	0.2600	0.6800
40	5	4	2	6	0.8100	0.6800	0.4000	0.9700
41	5	5	3	1	0.8300	0.8300	0.5400	0.2600
42	5	6	4	3	0.8500	0.9700	0.6800	0.5400
43	6	0	6	6	0.8700	0.1300	0.9900	0.9900
44	6	1	0	1	0.8900	0.2800	0.1300	0.2800
45	6	2	1	3	0.9100	0.4200	0.2800	0.5600
46	6	3	2	5	0.9300	0.5600	0.4200	0.8500
47	6	4	3	0	0.9500	0.7000	0.5600	0.1300
48	6	5	4	2	0.9700	0.8500	0.7000	0.4200
49	6	6	5	4	0.9900	0.9900	0.8500	0.7000

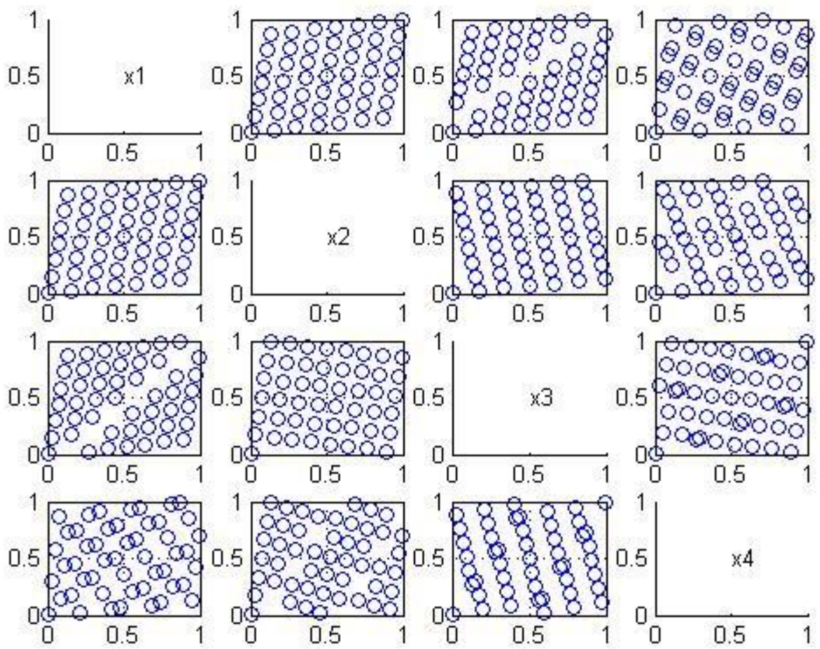

Figure 3. Bivariate Projections among 4 Factors of OA (49, 4) LHD Showing Space-Filling Properties of the Design

The computer snap-short of MATLAB code for the construction of various OALHDs in this work is presented in Figure 4.

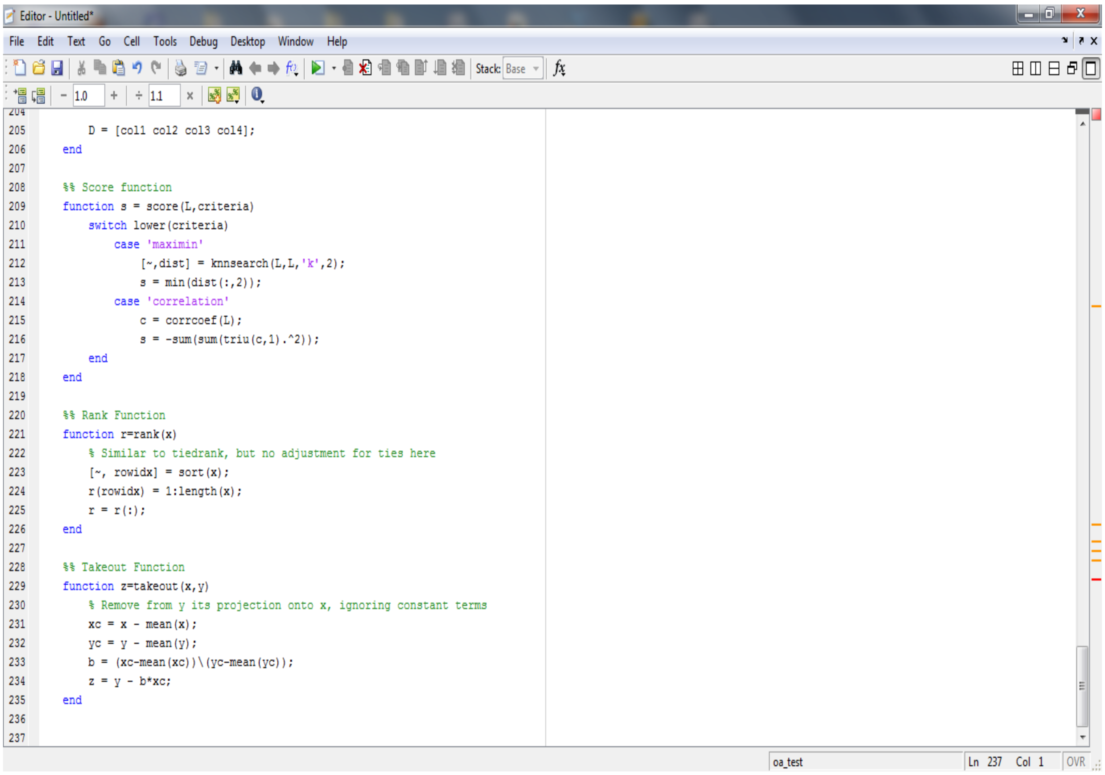

Figure 4. MATLAB Code for the Construction of OALHDs

6. Discussion of Results

The results of OALHDs given in Section 5 showed the construction of OA (25, 4) LHD and OA (49, 4) LHD from Graeco Latin square of orders 5 and 7 respectively. The OA (25, 4,) LHD contains 25 runs with 4 input variables while OA (49, 4) LHD has 49 runs with 4 input variables. In both cases we have been able to construct OALHDs for only 4 factors. The method employed in this paper can work for designs of various runs and different levels. This approach works for N = 25, 49, 81, 121, 169 … for OALHD with levels, s = 5, 7, 9, 11, 13 … from OA such that s is a prime number. The OALHDS constructed achieved better space-filling properties as shown in Figures 2 and 3.

7. Conclusion

A method for the construction of OALHDs from Graeco Latin square of order s where s is a prime number has been presented in this work. There are several techniques and criteria available for the construction of space-filling designs in the literature. This study simplifies the construction of OALHDs by using computer codes that employed the maximin criterion in k-Nearest Neighbour with Euclidean distance to produce results within seconds. Conclusively, the OALHDs constructed in this work can be used to develop computer experiments with four input variables.

References

[1] R.C. Bose and K.A. Bush, "Orthogonal Arrays of Strength Two and Three", Annals of Mathematical Statistics, vol. 23, **(1952)**, pp. 508-524.

[2] A.S. Hedayat, N.J.A. Sloane and J. Stufken, "Orthogonal Arrays: Theory and Applications", Springer-Verlag, New York, **(1999)**.

[3] J. Sacks, W.J. Welch, T.J. Mitchell and H.P. Wynn, "Design and Analysis of Computer Experiments", Statistical Science, vol. 4, **(1989)**, pp. 409-423.

[4] J. R. Koehler and A. B. Owen, "Computer Experiments: Handbook of Statistics: Edited by S. Ghosh and C.R. Rao", Elsevier, Amsterdam, **(1996)**.

[5] S. Leary, A. Bhaskar and A. Keane, "Optimal Orthogonal Array-Based Latin Hypercubes", Journal of Applied Statistics, vol. 30, **(2003)**, pp. 585-598.

[6] M.D. McKay, R.J. Beckman and W.J. Conover, "A Comparison of Three Methods for selecting Values of Input Variables in the Analysis of Output from a Computer Code", Technometrics, vol. 21, **(1979)**, pp. 239-245.

[7] M.D. Morris and T. J. Mitchell, "Exploratory Designs for Computer Experiments", Journal of Statistical Planning and Inference, vol. 43, **(1995)**, pp. 381-402.

[8] K.A. Osuolale , W.B. Yahya and B.L. Adeleke, "An Algorithm for constructing Space-Filling Designs for Hadamard Matrices of Orders 4λ and 8 λ", Proceedings of the 49th Annual Conference of the Science Association of Nigeria, Ilorin, Nigeria, **(2014a)** April 27-May 1.

[9] K.A. Osuolale , W.B. Yahya and B.L. Adeleke, "Performing a Simple Pendulum Experiment as a Demonstrative Example for Computer Experiments", Annals, Computer Science Series, vol. 12, no. 2, **(2014b)**, pp. 33-38.

[10] K.A. Osuolale , W.B. Yahya and B.L. Adeleke, "Construction of Space-filling Designs for Three Input Variables Computer Experiments", International Journal of Computer, Control, Quantum and Information Engineering, WASET, vol. 8, no.9, **(2014c),** pp. 1624-1628.

[11] K.A. Osuolale, W.B. Yahya and B.L. Adeleke, "Construction of Orthogonal Array-Based Latin Hypercube Designs for Deterministic Computer Experiments", Annals, Computer Science Series, vol. 13, no.1, **(2015)**, pp. 24-29.

[12] A. B. Owen, "A Central Limit Theorem for Latin Hypercube Sampling", Journal of Royal Statistical Society Ser. B, vol. 54, **(1992a)**, pp. 541-551.

[13] A. B. Owen, "Orthogonal Arrays for Computer Experiments, Integration and Visualization", Statistica Sinica, vol. 2, **(1992b)**, pp. 439-452.

[14] H.D. Patterson, "The Error of Lattice Sampling", Journal of Royal Statistical Society Ser. B, vol. 16, **(1954)**, pp. 140-149.

[15] C.R. Rao, "Hypercube of Strength 'd' leading to Confounded Designs in Factorial Experiments" Bull. Calcutta Math. Soc., vol. 38, **(1946)**, pp. 67-78.

[16] C.R. Rao, "Factorial Experiments Derivable from Combinatorial Arrangements of Arrays", Journal of the Royal Statistical Society (Suppl.), vol. 9, **(1947)**, pp. 128-139.

[17] T.J. Santner, B.J. Williams and W.I. Notz, "The Design and Analysis of Computer Experiments", Springer, New York, **(2014)**.

[18] S. Strogatz, "The Real Scientific Hero of 1953", New York Times, **(2003)** March 4.

[19] B. Tang, "Orthogonal Array-Based Latin Hypercubes", IIQP Research Report, **(1991)**, RR91-10.

[20] B. Tang, "Orthogonal Array-Based Latin Hypercubes", Journal of the American Statistical Association, vol. 88, **(1993)**, pp. 1392–1397.

[21] B. Tang, "A Theorem for selecting OA-Based Latin Hypercubes using a Distance Criterion", Comm. Statist., A Theory and Methods, vol. 23, **(1994)**, pp. 2047–2058.

[22] C. F. J. Wu and M. Hamada, "Experiments: Planning, Analysis and Parameter Design Optimization", Wiley, New York, **(2000)**.

[23] Y. K. Lo, W. J. Zhang and M. X. Han, "Applications of the Uniform Design to Quality Engineering", Journal of Chinese Statistical Association, vol. 38, **(2000)**, pp. 411-428.