An Efficient Algorithm for Constructing Optimal Design of Computer Experiments

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Abstract

The long computational time required in constructing optimal designs for computer experiments has limited their uses in practice. In this paper, a new algorithm for constructing optimal experimental designs is developed. There are two major developments involved in this work. One is on developing an efficient global optimal search algorithm, named as enhanced stochastic evolutionary (ESE) algorithm. The other is on developing efficient methods for evaluating optimality criteria. The proposed algorithm is compared to existing techniques and found to be much more efficient in terms of the computation time, the number of exchanges needed for generating new designs, and the achieved optimality criteria. The algorithm is also very flexible to construct various classes of optimal designs to retain certain desired structural properties.

Key words: optimal design, computer experiments, stochastic evolutionary algorithm

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1. INTRODUCTION

Building surrogate models (or called metamodels) based on computer experiments has been widely used in engineering design due to the high computational cost of using high-fidelity simulations. Design of computer experiments, or called sampling (for simulations) has a considerable effect on the accuracy of a metamodel. To improve the space-filling property as well as to maintain a good computational efficiency in sampling, some researchers proposed to search an optimal design within a class of designs that have desirable structural properties, e.g., the Latin hypercube designs (LHD) (McKay, et al., 1979) with good one-dimensional projective property. Morris and Mitchell (1995) introduced optimal LHDs based on the ϕ_p criterion (a variant of the maximin distance criterion, see Johnson, et. al., 1990); Park (1994) introduced optimal LHDs based on either the maximum entropy criterion or the integrated mean squared-error (IMSE) criterion; Fang, et al (2002) introduced optimal LHDs based on the Centered L_2 discrepancy criterion.

Searching the optimal design of experiments within a class of designs, even though more tractable than searching in the entire sample space without any restrictions, is still difficult to solve exactly. An exhaustive search method is computationally prohibitive even for a small problem. For example, for optimizing 10×4 LHDs (10 runs, 4 factors), the number of distinct designs is more than 10^{22}. It is more practical to solve optimal design (of experiments) problems approximately. Toward this effort, Morris and Mitchell (1995) adapted a version of simulated annealing (SA) algorithm for constructing optimal LHDs; Park (1994) developed a rowwise element exchange algorithm for constructing optimal LHDs; Ye, et al (2000) used the columnwise-pairwise (CP) algorithm (Li and Wu, 1997) for constructing optimal symmetrical LHDs; Fang, et al (2002) adapted the threshold accepting (TA) algorithm (essentially a variant of SA) in constructing optimal LHD. The optimal designs constructed by these algorithms have been shown to have a good space-filling property. However, the computational cost of these existing algorithms is generally high. For example, Ye, et al (2000) reported that generating an optimal 25×4 LHDs using CP could take several hours on a Sun SPARC 20 workstation. For a design as large as 100×10, the computational cost could be formidable; thus, search processes often stop before finding a good design.

In this paper, we propose an algorithm that is not only able to quickly construct a good design of experiments given a limited computational resource but also capable of moving away from a locally optimal design. The proposed method is especially useful for constructing median to large-sized design of experiments. For example, for a 100×10 LHD, the proposed algorithm is able to find a good design within minutes, if not within seconds. Furthermore, the algorithm is able to work on different classes of designs and maintain desirable special structural properties, e.g., the balance property of LHDs and the orthogonality of OA (Owen, 1992; Hedayat et al., 1999) and OA-based LHDs (Tang, 1993). In this paper, we only show how it is used to optimize LHDs. The extensions to optimizing other classes of designs can be found in Jin 2003.

2. THE TECHNOLOGICAL BASE

An experimental design with n runs and m factors is usually written as an $n\times m$ matrix $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2,\ldots,\mathbf{x}_n]^T$, where each row $\mathbf{x}_i^T = [x_{i1}, x_{i2},\ldots, x_{im}]$ stands for an experimental run and each column stands for a factor or a variable. The optimal experimental design problem we are interested is to search a design $\mathbf{X}^*$ in a given design class $\boldsymbol{Z}$, which optimizes (for simplicity, minimization is considered) a given optimality criterion f, i.e,

$$\min_{\mathbf{X}\in \boldsymbol{Z}} f(\mathbf{X}) . \tag{1}$$

2.1. Optimality Criteria

Optimal criteria are used to achieve the space-filling property in design of computer experiments. Three widely used optimality criteria are considered in this work.

Maximin Distance Criterion and ϕ_p Criterion

A design is called a maximin distance design (Johnson, et al, 1990) if it maximizes the minimum inter-site distance:

$$\min_{1\le i, j\le n, i\ne j} d(\mathbf{x}_i, \mathbf{x}_j) , \tag{2}$$

where $d(\mathbf{x}_i, \mathbf{x}_j)$ is the distance between two sample points $\mathbf{x}_i$ and $\mathbf{x}_j$:

$$d(\mathbf{x}_i, \mathbf{x}_j) = d_{ij} = \left[\sum_{k=1}^{m} \left|x_{ik} - x_{jk}\right|^t\right]^{1/t}, t = 1 \; or \; 2 . \tag{3}$$

Morris and Mitchell (1995) proposed an intuitively appealing extension of the maximin distance criterion. For a given design, by sorting all the inter-sited distance d_{ij} ($1\le i, j \le$n, $i \neq j$), a distance list (d_1, d_2, ..., d_s) and an index list (J_1, J_2,..., J_s) can be obtained, where d_i's are distinct distance values with $d_1<d_2<...<d_s$, J_i is the number of pairs of sites in the design separated by d_i, s is the number of distinct distance values. A design is called a ϕ_p-optimal design if it minimizes:

$$\phi_p = \left[\sum_{i=1}^{s} J_i d_i^{-p} \right]^{1/p}, \tag{4}$$

where p is a positive integer. With a very large p, the ϕ_p criterion is equivalent to the maximin distance criterion.

Entropy Criterion

Shannon (1948) used entropy to quantify the "amount of information": the lower the entropy, the more precise the knowledge is. Minimizing the posterior entropy is equivalent to finding a set of design points on which we have the least knowledge. It has been further shown that the entropy criterion is equivalent to minimizing the following (see, e.g., Koehler and Owen, 1996):

$$-\log|\mathbf{R}|, \tag{5}$$

where $\mathbf{R}$ is the correlation matrix of the experimental design matrix $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_n]^T$, whose elements are:

$$R_{ij} = \exp\left(-\sum_{k=1}^{m} \theta_k \left| x_{ik} - x_{jk} \right|^t \right), 1 \le i, j \le n; 1 \le t \le 2, \tag{6}$$

where θ_k (k=1,..,m) are correlation coefficients.

Centered L_2 Discrepancy Criterion

The L_p discrepancy is a measure of the difference between the empirical cumulative distribution function of an experimental design and the uniform cumulative distribution function. In other words, the L_p discrepancy is a measure of non-uniformity of a design. Among L_p discrepancy, L_2 discrepancy is used most frequently since it can be expressed analytically and is much easier to compute. Hickernell (1998) proposed three formulas of

L_2 discrepancy, among which the centered L_2-discrepancy (CL_2) seems the most interesting.

$$CL_2(\mathbf{X})^2 = \left(\frac{13}{12}\right)^2 - \frac{2}{n}\sum_{i=1}^{n}\prod_{k=1}^{m}(1+\frac{1}{2}\left|x_{ik}-0.5\right| - \frac{1}{2}\left|x_{ik}-0.5\right|^2) \\ + \frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}\prod_{k=1}^{m}(1+\frac{1}{2}\left|x_{ik}-0.5\right| + \frac{1}{2}\left|x_{jk}-0.5\right| - \frac{1}{2}\left|x_{ik}-x_{jk}\right|). \tag{7}$$

A design is called uniform design if it minimizes the centered L_2 discrepancy (Fang, et al, 2000).

2.2. Updating Operations and Search Algorithms

A typical experiment-constructing algorithm is repeated in the following procedure:

1. Start from a randomly chosen starting design $\mathbf{X_0}$;

2. Construct a new design (or a set of new designs) by some kinds of *updating operations* on the current design;

3. Compute the criterion value of the new design and decide whether to replace the current design with the new one.

There are two major types of *updating operations*, i.e., *rowwise* operations and *columnwise* operations (Li and Wu, 1997). We are interested in columnwise operations since they are particularly easier to keep the structure properties of a design in relation to columns, such as the balance and orthogonality properties. In this study, we focus on a particular type of columnwise operation, called *element-exchange*, which interchanges two distinct elements in a column and guarantee to retain the balance property. Take a 5×4 LHD for example:

$$\begin{matrix} 1 & 2 & 4 & 0 \\ 3 & \colorbox{lightgray}{$\mathbf{4}$} & 0 & 3 \\ 2 & 1 & 3 & 4 \\ 4 & \boxed{\mathbf{0}} & 1 & 2 \\ 0 & 3 & 2 & 1 \end{matrix} \quad \xrightarrow[\text{second column}]{\text{Exchange two elements in the}} \quad \begin{matrix} 1 & 2 & 4 & 0 \\ 3 & \boxed{\mathbf{0}} & 0 & 3 \\ 2 & 1 & 3 & 4 \\ 4 & \colorbox{lightgray}{$\mathbf{4}$} & 1 & 2 \\ 0 & 3 & 2 & 1 \end{matrix}$$

Figure 1. Element-exchange in a 5×4 LHD

Obviously, after the element-exchange, the balance property of 2nd column is retained, while the design is still a LHD. Another advantage of using element-exchange, as to be shown in Section 3.2, is that the evaluation of an optimal criterion of a new design induced by an element-exchange can be very efficient.

The three existing optimization search algorithms for optimal DOEs are reviewed here with the highlights of their differences. The *CP algorithm* (Li and Wu, 1997) starts from an $n \times m$ randomly chosen design $\mathbf{X}$. Each iteration in the algorithm is divided into m steps. At the ith step, the CP algorithm compares all possible distinct designs and selects the best design $\mathbf{X}_{try}$ from all those designs. If after an iteration, $\mathbf{X}_{try}$ is better than $\mathbf{X}$, i.e., $f(\mathbf{X}_{try}) < f(\mathbf{X})$, the procedure will be repeated; if no improvement is achieved at an iteration, the search will be terminated. The CP algorithm could quickly find a locally optimal design. However, depending on the starting design, the optimal design obtained could be of low quality. In practice, with the CP algorithm, the optimization process needs to repeat for N_s cycles from different starting designs and the best design is selected. Because CP algorithm compares all possible exchange within a column to select the best element exchange, the computational requirement can be excessively large when n is large. Li and Nachtsheim (2000) proposed the *restricted* CP algorithm as an improvement of the original CP algorithm. In that algorithm, only a fraction of all pair exchanges in a column is considered. The approach can be applied to reduce the number of element exchange candidates for general factorial designs but not space filling design such as LHD.

With the SA algorithm (Morris and Mitchell, 1995), a new design $\mathbf{X}_{try}$ replaces $\mathbf{X}$ if it leads to an improvement. Otherwise, it will replace $\mathbf{X}$ with probability of $\exp\{-[f(\mathbf{X}_{try}) - f(\mathbf{X})]/T\}$, where T is a parameter called “temperature” in the analogous physical process of annealing of solids. Initial set to T_0, T will be monotonically reduced by a *cooling schedule*. Morris and Mitchell used $T' = \alpha T$ as the cooling schedule, where α is a constant called cooling factor here. SA usually converges slowly to a high quality design. The TA algorithm (Winker and Fang, 1998) is essentially a variant of the SA, with a simple deterministic acceptance criterion:

$f(\mathbf{X}_{try}) - f(\mathbf{X}) \le T_h$, where T_h is called “threshold”. T_h is monotonically reduced based on a cooling schedule. TA has been used for constructing uniform designs (c.f., Fang 2000; Fang, et al, 2002).

3. PROPOSED ALGORITHM FOR CONSTRUCTING OPTIMAL EXPERIMENTAL DESIGN

To overcome the difficulties associated with the existing methods and to achieve much improved efficiency, our proposed method adapts and enhances a global search algorithm, i.e., the stochastic evolutionary algorithm (Section 3.1), and utilizes efficient methods for evaluating different optimality criteria (Section 3.2) to significantly reduce the computational burden.

3.1. Enhanced Stochastic Evolutionary (ESE) Algorithm

The enhanced stochastic evolutionary (ESE) algorithm is adapted and enhanced from the stochastic evolutionary (SE) algorithm, which was originally developed by Saab and Rao (1991) for general combinatorial optimization applications. With SE, whether to accept a new design is decided by a threshold-based acceptance criterion, but its strategy (or schedule) to change the value of threshold is different from that of TA or SA. It is shown (Saab and Rao, 1991) that SE can converge much faster than SA. SE is also capable of moving away from low quality local optimum to find a high quality solution. However, adjusting the initial threshold T_{h0} and the warming schedule for different problems is still quite troublesome with the original SE. The ESE algorithm developed in this work uses a sophisticated combination of warming schedule and cooling schedule to control T_h so that the algorithm can be self-adjusted to suit different experimental design problems (i.e., different classes of designs, different optimality criteria, and different sizes of designs).

The ESE algorithm, as shown in Fig 2, consists of double loops, i.e., the inner loop and the outer loop. While the inner loop constructs new designs by element-exchanges and decides whether to accept them based on an acceptance criterion, the outer loop controls the entire optimization process by adjusting the threshold T_h in the acceptance criterion. In the entire process, $\mathbf{X}_{best}$ is used to keep track of the updated best design.

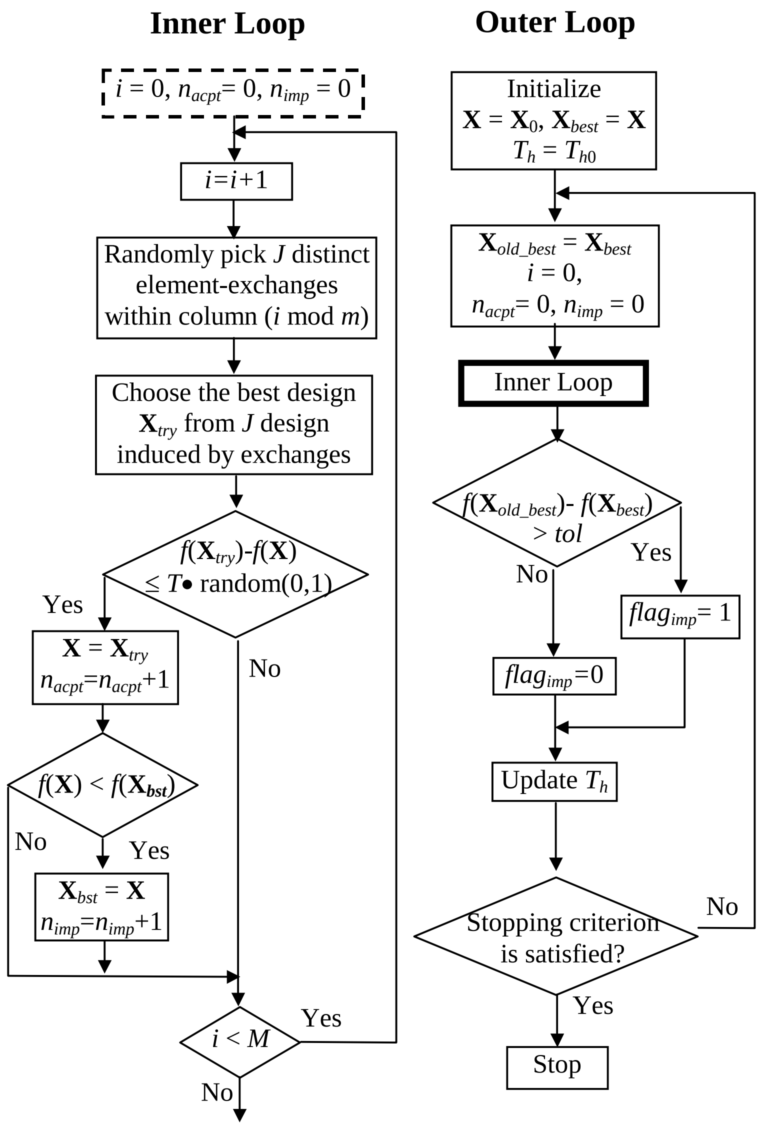

Inner Loop
Outer Loop
i = 0, n_acpt = 0, n_imp = 0
i=i+1
Randomly pick J distinct element-exchanges within column (i mod m)
Choose the best design X_try from J design induced by exchanges
f(X_try)-f(X) ≤ T• random(0,1)
Yes
No
X = X_try
n_acpt=n_acpt+1
f(X) < f(X_bst)
No
Yes
X_bst = X
n_imp=n_imp+1
i < M
Yes
No
Initialize
X = X_0, X_best = X
T_h = T_h0
X_old_best = X_best
i = 0,
n_acpt= 0, n_imp = 0
Inner Loop
f(X_old_best)- f(X_best) > tol
Yes
No
flag_imp= 1
flag_imp=0
Update T_h
Stopping criterion is satisfied?
No
Yes
Stop

Figure 2. Flowchart of the ESE Algorithm

3.1.1. Inner Loop

The inner loop has M iterations. Generally, at iteration i, the algorithm randomly picks J distinct element-exchanges in i (mod m) column of the current design $\mathbf{X}$ and chooses the best design $\mathbf{X}_{try}$ based on the values of optimal criterion. If $\mathbf{X}_{try}$ is better than the current design **X**, it will be accepted to replace **X**; otherwise, $\mathbf{X}_{try}$ will be accepted to replace **X** if it satisfies the following acceptance criterion:

$$\Delta f \leq T_h \cdot \text{random}(0,1)\,, \tag{8}$$

where $\Delta f = f(\mathbf{X}_{try}) - f(\mathbf{X})$, random(0,1) is a function that generates uniform random numbers between 0 and 1 and $T_h > 0$ is a control parameter, which is called threshold here. If $\Delta f \geq T_h$, $\mathbf{X}_{try}$ will never be accepted and if $0 < \Delta f < T_h$, let S = random(0,1), then $\mathbf{X}_{try}$ will be accepted with probability:

$$P(S \geq \Delta f / T_h) = 1 - \Delta f / T_h\ . \tag{9}$$

With this acceptance criterion, a temporarily worse design could be accepted and a slightly worse design (i.e., a small Δf) is more likely to replace the current design than a significantly worse design (i.e., a large Δf). In addition, a given increase in criterion value is more likely to be accepted if T_h has a relatively high value. The setting of T_h will be discussed later.

The values of parameters involved in the inner loop, i.e., *J* and *M*, are pre-specified. Unlike CP, which compares all possible distinct designs induced by exchanges, our algorithm only randomly picks *J* distinct designs resulted from exchanges. Based on our testing experience, too large of *J* may make it more possible to be stuck in a locally optimal design for small-sized designs and lead to low efficiency for large-sized designs. Based on our tests, we set *J* to be $n_e/5$ but no large than 50, where n_e is the number of all possible distinct element-exchanges in a column ($\binom{n}{2}$ for a LHD and $\binom{q_i}{2} \times (n/q_i)^2$ for a balanced design). For mixed-level balanced designs, the values of *J* will be different for different columns. The parameter *M* is the number of iterations in the inner loop, i.e., the number of tries the algorithm will make before going on to the next threshold T_h. It seems reasonable that *M* should be larger for larger problems. In our test, we set *M* to be $2n_e m / J$ but no larger than 100.

3.1.2. Outer Loop

The outer loop controls the optimization process by updating the value of the threshold T_h. At the beginning of the optimization process, T_h is set to be a small value, i.e., T_{h0} = 0.005×criterion value of the initial design. Later on it will be adjusted and maintained based on whether the search is within the so-called *improving process* or *exploration process*. A search process is turned to the improving process ($flag_{imp}$ = 1) if the criterion is improved after a cycle (an inner loop). Once turning to the improving process, T_h is adjusted to rapidly find a locally optimal design. If no improvement is made after a cycle, the search process will be turned to the exploration process ($flag_{imp}$ = 0), during which T_h is adjusted to help the algorithm escape from a locally optimal design. The maximum number of cycles is used as the stopping criterion.

Based on our tests, the following proposed schedules for controlling T_h is found to work very well for different experimental design problems:

1. In the *improving process,* T_h is maintained on a small value so that only better design or slightly worse design will be accepted. Unlike the original SE, the value of T_h will not be fixed to $T_{h0.}$ Instead, T_h will be updated based on the acceptance ratio n_{acpt}/M (number of accepted design versus the number of tries in the inner loop) and the improvement ratio n_{imp}/M (number of improved design versus the number of tries in the inner loop). Specifically, T_h will be decreased if the acceptance ratio is larger than a small percentage (e.g., 10%) and the improvement ratio is less than the acceptance ratio; T_h will be maintained in the current value if the acceptance ratio is larger than the small percentage and the improvement ratio is equal to the acceptance ratio (meaning that T_h is so small that only improving designs are accepted by the acceptance criterion); T_h will be increased otherwise. The following equations are used in our algorithm to decrease and increase T_h, respectively, $T' = \alpha_1 T$ and $T' = T / \alpha_1$, where $0 < \alpha_1 < 1$. The setting of α_1 = 0.8 appears to work well in all tests.

2. In the *exploration process,* T_h will fluctuate within a range based on the acceptance ratio. If the acceptance ratio is less than a small percentage (e.g., 10%), T_h will be rapidly increased until the acceptance ratio is larger than a large percentage (e.g. 80%). If this happens, T_h will be slowly decreased until the acceptance ratio is less than the small percentage. This process will be repeated until an improved design is found. The following equations are used to decrease and increase T_h, respectively, $T' = \alpha_2 T$ and

$T' = T / \alpha_3$, where $0 < \alpha_3 < \alpha_2 < 1$. Based on our experience, we set α_2 = 0.9 and α_3 = 0.7. T_h is increased rapidly (so that more worse designs could be accepted) to help moving away from a locally optimal design. T_h is decreased slowly for searching better designs after moving away from the local optimal design.

3.2. Efficient Methods for Evaluating Optimality Criteria

As an optimality criterion is repeatedly evaluated whenever a new design of experiments is constructed, the efficiency of this evaluation becomes critical for optimizing the design of experiment within a reasonable time frame. In this work, we propose efficient evaluation methods that take into account the feature of our updating operation, i.e., when using columnwise element-exchanges for generating new designs, only two elements in the design matrix are involved each time. The evaluations of optimal criteria, such as ϕ_p criterion, the entropy criterion, and the CL_2 criterion, involve different types of matrices (e.g., the inter-distance matrix **D**, the correlation matrix **R**, and the discrepancy matrix **C**, respectively). Re-evaluating all the elements in the matrices each time is not affordable, especially if the matrix size is large (determined by the number of experiments and number of factors).

ϕ_p Criterion

The re-evaluation of ϕ_p based on Eq. 4 includes three parts, i.e., the evaluation of all the inter-site distances, the sorting of those inter-site distances to obtain a distance list and index list, and the evaluation of ϕ_p. The evaluation of all the inter-site distances will take O(mn^2), the sorting will take O($n^2\log_2(n)$) (c.f. Press, et al, 1997), and the evaluation of ϕ_p will take O($s^2\log_2(p)$) (since p is an integer, p-powers can be computed by repeated multiplications). In total, the computational complexity will be O(mn^2)+O($n^2\log_2(n)$)+O($s^2\log_2(p)$). Therefore, re-evaluating ϕ_p will be very time-consuming.

Before introducing the new method, a new equation of ϕ_p is first provided, which helps develop an efficient evaluation algorithm by avoiding the sorting required by Eq. 4. Let $\mathbf{D} = [d_{ij}]_{n \times n}$ be a symmetric matrix, whose elements are the inter-site distances of the current design **X**, the new equation, called p-norm form here, is expressed by:

$$\phi_p = \left[\sum_{1 \le i < j \le n} \left(1/d_{ij}\right)^p \right]^{1/p} = \left[\sum_{1 \le i < j \le n} d_{ij}{}^{-p} \right]^{1/p} . \quad (10)$$

The equivalence between this form and Eq. 4 can be easily proved, which is omitted here.

Our new algorithm takes into account the fact that after an exchange ($x_{i_1k} \leftrightarrow x_{i_2k}$), only elements in rows i_1 and i_2 and columns i_1 and i_2 are changed in **D** matrix. For any $1 \le j \le n$ and $j \ne i_1, i_2$, let:

$$s(i_1, i_2, k, j) = \left|x_{i_2k} - x_{jk}\right|^t - \left|x_{i_1k} - x_{jk}\right|^t , \quad (11)$$

then:

$$d_{i_1j}' = d_{ji_1}' = \left[d_{i_1j}{}^t + s(i_1, i_2, k, j)\right]^{1/t} \quad (12)$$

and

$$d_{i_2j}' = d_{ji_2}' = \left[d_{i_2j}{}^t - s(i_1, i_2, k, j)\right]^{1/t} . \quad (13)$$

With the above representation, the computational complexity of updating the elements in **D** matrix is O(n). The new ϕ_p is now computed by:

$$\phi_p{}' = \left[\phi_p{}^p + \sum_{1 \le j \le n, j \ne i_1, i_2} \left[(d_{i_1j}')^{-p} - d_{i_1j}{}^{-p}\right] + \sum_{1 \le j \le n, j \ne i_1, i_2} \left[(d_{i_2j}')^{-p} - d_{i_2j}{}^{-p}\right] \right]^{1/p} , \quad (14)$$

of which the computational complexity is O(n $\log_2(p)$). The total computational complexity of the new algorithm is O(n)+O(n $\log_2(p)$). This results in significant reduction of computation compared to re-evaluating ϕ_p.

Entropy Criterion

Since the correlation matrix $\mathbf{R} = [r_{ij}]_{n \times n}$ in Eq. 6 is positive-definite, it can be expressed by Cholesky decomposition:

$$\mathbf{R} = \mathbf{U}^T * \mathbf{U} , \quad (15)$$

where, $\mathbf{U} = [u_{ij}]_{n \times n}$ is an upper triangle matrix, i.e., $u_{ij} = 0$ if $i < j$.

Therefore,

$$|\mathbf{R}| = \prod_{i=1}^{n} u_{ii}{}^2 . \quad (16)$$

The computational complexity of Cholesky factorization (or decomposition) is O(n^3). In addition, the calculation of the elements of **R** costs O(mn^2), and therefore the computational complexity for totally re-evaluating the entropy will be O(mn^2)+O(n^3) .

While the determinant of the new **R** matrix cannot be directly evaluated based on the determinant of the old **R** matrix, by modifying the Cholesky algorithm, some improvement in efficiency is achievable. Let n_1=min(i_1,i_2), then **R** can be written as:

$$\mathbf{R}_{n\times n} = \begin{bmatrix} (\mathbf{R}_1)_{n_1\times n_1} & (\mathbf{R}_2)_{n_1\times(n-n_1)} \\ (\mathbf{R}_2{}^T)_{n_1\times(n-n_1)} & (\mathbf{R}_3)_{(n-n_1)\times(n-n_1)} \end{bmatrix}. \tag{17}$$

If the Cholesky factorization of $\mathbf{R}_1$ is known, i.e., $\mathbf{R}_1 = \mathbf{U}_1{}'{*}\mathbf{U}_1$, the Cholesky factorization **U** of **R** can be computed based on $\mathbf{U}_1$:

$$\mathbf{U} = \begin{bmatrix} (\mathbf{U}_1)_{n_1\times n_1} & (\mathbf{U}_2)_{n_1\times(n-n_1)} \\ 0 & (\mathbf{U}_3)_{(n-n_1)\times(n-n_1)} \end{bmatrix} \tag{18}$$

where $\mathbf{U}_3$ is also an upper triangle matrix. Therefore, the elements of **U** with index $1 \le i \le j \le n_1$ are kept unchanged. The rest of the elements in the upper triangle matrix **U** can be calculated by following a modified Cholesky factorization algorithm (see Jin, 2003 for details).

The computational complexity of the modified Cholesky factorization algorithm will depend on both n and n_1. For example, if n_1=n-1, the computational complexity will be O(n^2). On the other hand, if n_1=1, the computational complexity will be still O(n^3). In average, the computational complexity will be smaller than O(n^3) but larger than O(n^2). The total computational complexity of the new mthod will be between O(n) + O(n^2) and O(n) + O(n^3), which is not dramatically better than O(n^3)+O(mn^2).

CL

Evaluating the CL_2 criterion employs a similar idea as that for the ϕ_p criterion. Let $\mathbf{Z} = [z_{ik}]_{n\times m}$ be the centered design matrix of **X**, i.e., $z_{ik} = x_{ik} - 0.5$. Let $\mathbf{C} = [c_{ij}]_{n\times n}$ be a symmetric matrix, whose elements are:

$$c_{ij} = \begin{cases} \frac{1}{n^2}\prod_{k=1}^{m}\frac{1}{2}(2+|z_{ik}|+|z_{jk}|-\left|z_{ik}-z_{jk}\right|) & if\ i \neq j \\ \frac{1}{n^2}\prod_{k=1}^{m}(1+|z_{ik}|)-\frac{2}{n}\prod_{k=1}^{m}(1+\frac{1}{2}|z_{ik}|-\frac{1}{2}{z_{ik}}^2) & otherwise \end{cases} \tag{19}$$

Let $g_i = \prod_{k=1}^{m}(1+|z_{ik}|)$ and $h_i = \prod_{k=1}^{m}(1+\frac{1}{2}|z_{ik}|-\frac{1}{2}{z_{ik}}^2) = \prod_{k=1}^{m}\frac{1}{2}(1+|z_{ik}|)(2-|z_{ik}|)$, then,

$$c_{ii} = g_i / n^2 - 2h_i / n\ . \tag{20}$$

It can be easily proved that: $CL_2(\mathbf{X})^2 = \left(\frac{13}{12}\right)^2 + \sum_{i=1}^{n}\sum_{j=1}^{n} c_{ij}$ (21)

The computational complexity of totally re-evaluating CL_2 discrepancy is O(mn^2).

After an exchange $x_{i_1k} \leftrightarrow x_{i_2k}$, only elements in i_1 and i_2 rows and i_1 and i_2 columns of **C** are changed. For any $1 \le j \le n$ and $j \neq i_1, i_2$, let

$$\gamma(i_1,i_2,k,j) = (2+|z_{i_2k}|+|z_{jk}|-\left|z_{i_2k}-z_{jk}\right|)\Big/(2+|z_{i_1k}|+|z_{jk}|-\left|z_{i_1k}-z_{jk}\right|)\ , \tag{22}$$

then,

$$c_{i_1j}' = c_{ji_1}' = \gamma(i_1,i_2,k,j)c_{i_1j} \tag{23}$$

and

$$c_{i_2j}' = c_{ji_2}' = c_{i_2j} / \gamma(i_1,i_2,k,j)\ . \tag{24}$$

Let $\alpha(i_1,i_2,k) = (1+|z_{i_2k}|)\big/(1+|z_{i_1k}|)$ and $\beta(i_1,i_2,k) = (2-|z_{i_2k}|)\big/(2-|z_{i_1k}|)$, then:

$$c_{i_1i_1}' = \alpha(i_1,i_2,k)g_{i_1} / n^2 - 2\alpha(i_1,i_2,k)\beta(i_1,i_2,k)h_{i_1} / n\ , \tag{25}$$

and

$$c_{i_2i_2}' = g_{i_2} / [n^2\alpha(i_1,i_2,k)] - 2h_{i_2} / [n\alpha(i_1,i_2,k)\beta(i_1,i_2,k)]\ . \tag{26}$$

The computational complexity of updating the **C** matrix is O(n).

The new CL_2 can be computed by:

$$({CL_2}^2)' = {CL_2}^2 + c_{i_1i_1}' - c_{i_1i_1} + c_{i_2i_2}' - c_{i_2i_2} + 2\times\sum_{1\le j\le n,\, j\neq i_1,i_2}^{n}(c_{i_1j}' - c_{i_1j} + c_{i_2j}' - c_{i_2j})\ , \tag{27}$$

whose computational complexity is O(n). The total computational complexity is also O(n), which is much less than O(mn^2).

A comparison of the computational complexity of totally re-evaluating all elements in matrices and those of our new methods are summarized in Table 1. From the table, we find that for the ϕ_p criterion and the CL_2 criterion, with the new algorithms, the efficiency can be significantly improved. The new computational complexity is close to O(n) in both cases. However, for the entropy criterion, because of the involvement of matrix determinant calculation, the efficiency is not improved dramatically (complexity larger than O(n^2)).

Table 1. Computational Complexity of Criterion Evaluation

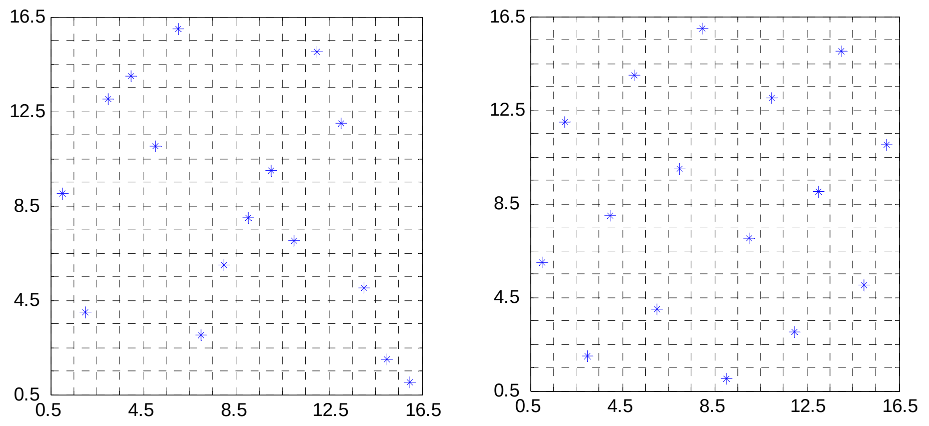
	ϕ_p	CL_2	**Entropy**
Re-evaluating Methods	$O(mn^2)+O(n^2\log_2(n))+O(s^2\log_2(p))$	$O(mn^2)$	$O(n^3)+O(mn^2)$
New Methods	$O(n)+O(n\log_2(p))$	$O(n)$	$O(n^2)+O(n)$ ~ $O(n^3)+O(n)$

4. TEST RESULTS AND COMPARATIVE STUDIES

In this section, we first provide an illustrative example of optimal LHD obtained using our proposed algorithm. The improved efficiency is evaluated by comparative studies in two separate categories, those associated with criteria evaluation, and those associated with ESE search algorithm only. An example is presented at the end to show how fast the combined algorithm will work on today's computers.

4.1. Illustrative Example of Optimal DOE

Our proposed algorithm can be used for optimizing various classes of designs of experiments, including but not limited to LHDs, general balanced designs, OAs, and OLs. Here we provide one example of optimal LHD based on the CL_2 criterion. As shown in Figure 3, before optimization, the initial LHD is a random design with good one-dimensional projective property but not so good space-filling property. After optimization, the projective property is maintained while the space filling property is much improved.



(Before Optimization) **(After Optimization)**

Figure 3. Optimized LHD (CL$_2$ Criterion)

4.2. Improvement through New Methods for Criteria Evaluation

We use the ratio between the time (T_r) necessary to totally re-evaluating all matrix elements and the time (T_n) required by our new criteria evaluation methods (Section 3.2) to show the improvement achieved by the new evaluation methods, not considering the improvement achieved by the ESE optimization search algorithm. The empirical results in Table 2 match well with our analytical examinations earlier (see Table 1). We find that the larger the size of an experimental design, the more savings our methods will make. For example, for 100x10 LHDs, our new method for evaluating CL$_2$ criteria only requires 1/82.1 of the computation effort compared to re-evaluating the whole matrix. Compared to other two criteria, the entropy criterion is much less efficient. It is also observed that with the new algorithms, the computing time for the ϕ_p criterion is 2.3~3.0 times as much as that for the CL_2 criterion.

Table 2. Computing Time (in seconds) of Criterion Values for 500,000 LHDs

T_r stands for the time needed to totally re-evaluating the matrix of a LHD for 500,000 times. T_n stands for the time needed to construct 500,000 different LHDs by element-exchanges and compute their criterion values by our method. T_r/T_n is the ratio of T_r and T_n.

	ϕ_p (p = 50, t =1)			**CL_2**			**Entropy (θ = 5, t =2)**		
	T_r	T_n	T_r/T_n	T_r	T_n	T_{rt}/T_n	T_r	T_n	T_r/T_n
12× 4 LHDs	12.2	5.5	2.2	10.7	2.4	4.5	16.6	14.2	1.2
25 × 4 LHDs	53.0	10.1	5.2	41.5	3.4	12.1	75.3	39.8	1.9
50 × 5 LHDs	239	19.8	12.1	197	6.5	30.3	347	167	2.1
100 × 10 LHDs	1378	45.2	30.5	1305	15.9	82.1	2116	1012	2.1

4.3. Improvement through the ESE Search Algorithm

To verify the improved efficiency of the proposed ESE search algorithm, we compare its performance with two other well known search algorithms, CP and SA, used respectively by Li and Wu (1997) and Morris and Mitchell (1995) for optimizing DOEs. In all test runs, the optimality criterion is evaluated using our proposed methods (Section 3.2) instead of re-evaluating all matrix elements. The tests are conducted on two sets of LHDs of relatively small sizes, i.e., 12×4 and 25×4, and two sets of LHDs of relatively large sizes, i.e., 50×5 and 100×10. As randomness is involved in all constructing algorithms, we repeat the same test 100 times starting from different initial LHDs. On each set of LHDs, two types of comparison are made, i.e.,

Type-I: Comparing the performance of ESE with that of SA and CP in terms of the average of criterion values of optimal designs with nearly the same numbers of exchanges. This group of tests for ESE is denoted as ESE (I)

Type-II: Comparing the efficiency of ESE with that of SA and CP in terms of numbers of exchanges needed for ESE to achieve optimal designs with the average of criterion values slightly better than that of SA or CP. This group of tests for ESE is denoted as ESE (II)

In both types of comparison, *t*-test is used to statistically compare the average criterion value of the optimal designs generated by ESE with those generated by SA or CP. The *p*-value is used to measure the level at which the observed difference (< 0) between the average criterion values is statistically significant. We use a tighter standard that the *p*-value should be smaller than 0.001%. For type-I comparison, this standard is not that critical since virtually all the *p*-values in the comparison are much smaller than 0.001%; for type-II comparison, however, this standard is used to judge whether optimal designs generated by ESE are close to but still statistically significantly better than those generated by SA or CP.

4.3.1. Results of Small Sizes of Designs

For small-sized LHDs, relatively large number of exchanges is affordable. For example, with 2,865,600 exchanges, it takes ESE about 57 seconds to construct an optimal 25×4 LHDs based on the ϕ_p criterion. The tests for small-sized problems are therefore focused on the capability of moving away from locally optimal designs and finding better experimental designs given a large number of exchanges.

The results of using the ϕ_p criterion are shown in Table 4. For each algorithm, two sets of tests with different numbers of exchanges are conducted. For SA, the two sets of tests correspond to two different values for cooling factor α suggested by Morris and Mitchell (1995), i.e., $\alpha = 0.90$ (faster cooling) and 0.95 (slower cooling), respectively. In a particular set of tests, the numbers of exchanges of SA for constructing optimal designs will differ test by test. For instance, for 12×4 LHD and $\alpha = 0.95$, the numbers of exchanges could be anywhere between 362,384 and 1,192,482. The numbers of exchanges of SA shown in the table are the average numbers. CP is terminated at a cycle number N_s, which is selected so that the average number of exchanges is close to that of SA. The numbers of exchanges shown are also the average of 100 tests. The results of SA are used to determine when to stop ESE.

Table 3. Results of optimal 12×4 LHDs and 25×4 LHDs (ϕ_p criterion, p =50 and t =1)
For SA, Sets 1 &2 correspond to $\alpha = 0.90$ and $\alpha = 0.95$, respectively. N_e (shown in thousands) stands for the average numbers of exchanges of 100 tests in each set of tests. For CP, cycle numbers N_s are given in the parentheses following the average numbers of exchanges.

ϕ_p criterion		Set 1		Set 2	
		Exchange Number	Mean (STD)	Exchange Number	Mean (STD)
12×4 LHD	SA	289,360	0.8569 (0.0131)	523,432	0.8505 (0.0133)
	CP	292,150 (154)	0.8581 (0.0082)	530,452 (280)	0.8546 (0.0096)
	ESE (I)	286,000	0.8384 (0.0057)	520,000	0.8362 (0.0041)
	ESE (II)	96,200	0.8483 (0.0114)	174,200	0.8426 (0.0084)
25×4 LHD	SA	1,416,175	1.1205 (0.0101)	2,724,318	1.1149 (0.0103)
	CP	1,442,076 (65)	1.1495 (0.0078)	2,743,920 (124)	1.1455 (0.0070)
	ESE (I)	1,416,000	1.1051 (0.0060)	2,724,000	1.0989 (0.0051)
	ESE (II)	470,400	1.1150 (0.0072)	840,000	1.1072 (0.0072)

For type-I comparison, error-bar plots (Figs. 4 and 5) are used to display the mean and variability of achieved ϕ_p values from 100 tests. The error bars (thick vertical lines) are each drawn a distance of one STD above and below the mean value. For each algorithm, a mean-line links the middles (i.e., the means) of error-bars. The dash error-bars and mean-lines are for the results of SA. From the figures, it is found that with similar number of exchanges, on average the proposed ESE always achieves better designs than both SA and CP with respect to the ϕ_p criterion. This is also confirmed statistically by the p-values in t-tests, which are all smaller than 1.0e-15. Furthermore, ESE is more efficient than both SA and CP. Table 4 shows that to obtain a statistically significantly better design for both 12×4 and 25×4 LHDs, ESE needs less than 1/3 of exchanges used in SA and in CP.

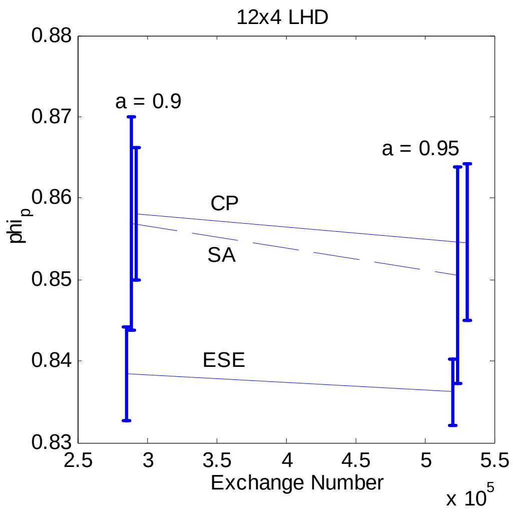


Figure 4. Type-I Comparison for 12 ×4 LHDs (ϕp criterion)

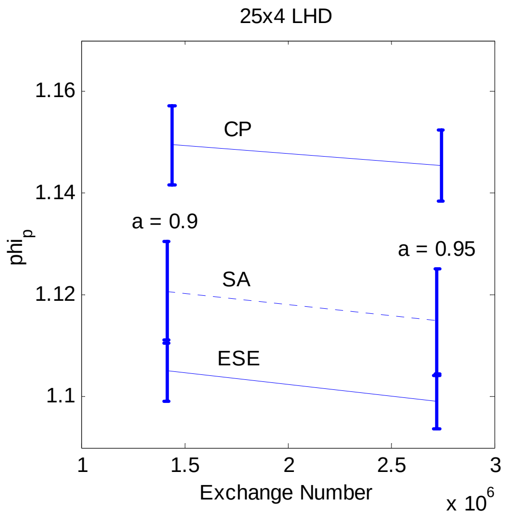


Figure 5. Type-I Comparison for 25 ×4 LHDs (ϕp criterion)

When using the CL_2 criterion, it is found that ESE uses around 1/3 ~ 1/2 exchanges used in CP for 12×4 LHDs and around 1/6 ~ 1/2 of exchanges used in CP for 25×4 LHDs to achieve statistically significantly better designs.

4.3.2. Results for Large Sizes of Designs

The computational cost of constructing an optimal design of large sizes is much larger than that of small sizes. Our comparison focuses on how efficient our algorithm is compared to others by using the same amount of reasonable numbers of exchanges, which are considered as small in relative to the size of the LHDs.

For large-sized designs, SA in general converges much more slowly than CP and ESE. Therefore with the numbers of exchanges that are small relative to the size of design, the SA search process will not be able to converge before the maximum number of exchanges is reached. As the result, the design generated by SA could be much inferior to those generated by CP and ESE. For instance, for 50×5 LHDs based on the ϕ_p criterion, with around 1,520,000 exchanges, the average criterion value of SA ($\alpha = 0.9$) is 1.4658 in comparison with 0.9875 for ESE and 1.0322 for CP. Therefore for large problems, SA may not be suitable since it needs excessive numbers of exchanges. Our test for large-sized designs only focuses on CP and ESE.

CP provides baselines for determining when to stop ESE in both types of comparisons. For large-sized problems, the computational cost could be too high for CP to even finish a single cycle. For instance, a single cycle of CP for 100×10 LHD with ϕ_p criterion could take 31,482,000 exchanges (2,758 seconds). Therefore, the tests of CP for large-sized LHDs have been restricted to at most several cycles for 50×5 LHDs and one cycle for 100×10 LHDs. Table 5 shows the maximum numbers of exchanges and the computing time. From the table we find that the computing time has been close to merely several minutes (if not seconds).

Table 4. Maximum Exchange Number and Computing Time for Constructing Optimal LHDs

	ϕ_p		CL_2	
	Max Exchange Number	**Max Computing Time (seconds)**	**Max Exchange Number**	**Max Computing Time (seconds)**
50×5 LHDs	1,945,000	77	2,960,000	35
100×10 LHDs	2,500,000	219	7,685,000	198

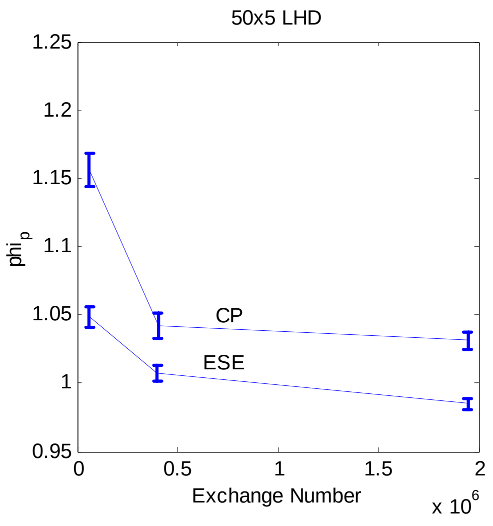
As shown in Table 5, for each algorithm, three sets of tests with different numbers of exchanges are performed. For 50×5 LHDs, the numbers of exchanges of the first set of tests are not sufficient to finish one cycle; the second set of tests involves exactly one cycle and the numbers of exchanges are the average of the 100 tests; likewise, the third set of tests involves exactly 5 cycles. For 100×10 LHDs, even though large numbers of exchanges are used for CP in all three sets of tests, they are not sufficient to finish the first cycle.

Table 5. Test Results of optimal 50×5 LHDs and 100×10 LHDs based on ϕ_p criterion (p =50, t =1)
For CP, the cycle numbers are provided in the parentheses following the exchange numbers. If there are no cycle numbers marked, it means that CP is stopped within the first cycle

ϕ_p criterion		Set 1		Set 2		Set 3	
		Exchange Number	**Mean (STD)**	**Exchange Number**	**Mean (STD)**	**Exchange Number**	**Mean (STD)**
50×5 LHD	**CP**	61,250	1.1564 (0.0121)	403,638 (1)	1.0420 (0.0097)	1,947,811 (5)	1.0311 (0.0068)
	ESE (I)	60,000	1.0486 (0.0072)	400,000	1.0076 (0.0059)	1,945,000	0.9850 (0.0038)
	ESE (II)	10,000	1.1264 (0.0099)	80,000	1.0348 (0.0069)	110,000	1.0248 (0.0063)
100×10 LHD	**CP**	297,000	0.5381 (0.0044)	544,500	0.5059 (0.0024)	2,524,500	0.4660 (0.0014)
	ESE (I)	280,000	0.4562 (0.0012)	500,000	0.4525 (0.0014)	2,500,000	0.4440 (0.0010)
	ESE (II)	10,000	0.5214 (0.0031)	20,000	0.4996 (0.0025)	140,000	0.4634 (0.0015)

The means and variability of the achieved ϕ_p values for 50×5 LHDs and 100×10 are shown in Figs. 6 and 7 for types-I comparison. From the figures, it is found that ESE consistently outperforms CP, which is also confirmed by *t*-tests (*p*-values are all smaller than 1.0e-15). From Table 5, it is observed that ESE is much more efficient than CP. To reach statistically significantly better designs than CP, ESE needs only around 1/17~ 1/5 of exchanges used in CP for 50×5 LHDs and 1/29 ~ 1/18 of exchanges used in CP for 100×10 LHDs.

Similar tests to the above have been carried out for the CL_2 criterion. It is found that ESE consistently outperforms CP, which is confirmed by *t*-tests (*p*-values are all smaller than 1.0e-15). It is observed that ESE is much more efficient than CP. To reach statistically significantly better designs than CP, ESE needs only around 1/23 ~ 1/4 of exchanges used in CP for 50×5 LHDs and 1/33 ~ 1/10 of exchanges used in CP for 100×10 LHDs.



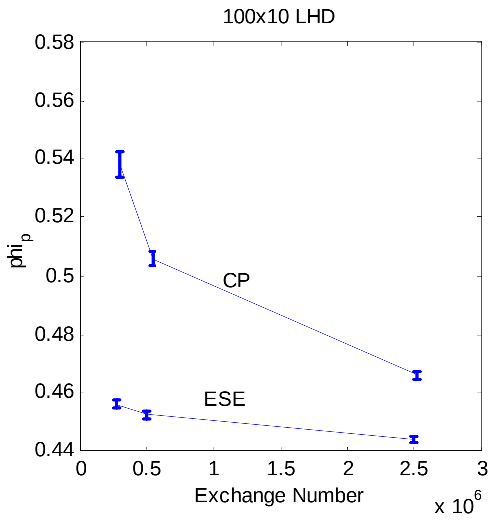


Figure 6. Type-I Comparison for 50 ×5 LHDs (ϕp criterion)

Figure 7. Type-I Comparison for 100 ×10 LHDs (ϕp criterion)

4.4. Total Savings in Computing Time

The achieved savings from our combined algorithms are illustrated by comparing the computation time of our combined algorithms (ESE algorithm and algorithms for evaluating optimality) with that of other methods reported in literature, in particular, the results of the CP algorithm presented in Ye, et al, 2000. The comparison is for optimal

25×4 LHDs constructed based on the ϕ_p criterion (p = 50 and t = 1). It should be noted that even though Ye, et al used the ϕ_p criterion (with the same parameter settings as in our tests) as the optimality criterion in constructing optimal LHDs, their results were reported in the form of (maximizing) the minimum L_1 distance (the larger the better), which, as discussed before, is strongly related to but not totally in accord with the ϕ_p value (the smaller the better). To be consistent, the results of our proposed ESE are also in the form of minimum L_1 distance in Table 7.

Table 7. ESE vs. CP for Constructing Optimal 25×4 LHDs Based on ϕ_p Criterion (p = 50 and t = 1)
N_e stands for number of exchanges (shown **in thousands**). The results for CP are from Ye, et al (2000, based on Sun SPARC 20 Workstation). In the CP test, 100 cycles (shown in the parentheses following the exchange numbers) are used. ESE is tested on a PC with a Pentium III 650 MHZ CPU.

	Exchanges Number	**Min L_1 Distance**	**Computing Time**
CP	2,241,900 (100)	0.8750	10.63 hr
ESE	120,000	0.9167	2.5 sec

In the work of Ye, et al, the optimization process was repeated for 100 cycles starting from different random LHDs and the design with the largest minimum L_1 distance of the 100 constructed optimal designs was reported as the final optimal design. The number of exchanges or computing time of CP is the total number or time used in the 100 cycles. From the results, it is found that the designs constructed by our ESE with less than 2.5 seconds is better than those constructed by CP with around 10.63 hours. In fact, ESE is tested for many times and the minimum distances are consistently larger than or equal to 0.9167. The saving of computing time is dramatic even if the difference between the computing platforms is considered. As introduced earlier, such a good efficiency is achieved by:

- Improving the efficiency of criterion evaluation (5 times faster than totally re-evaluating for the example test case; more significant improvement for larger size designs, see Table 2);
- Using fewer exchanges with ESE to search an optimal design (120,000 with ESE versus 2,241,900 with CP).

5. SUMMARY

In this study, we develop a very efficient and flexible algorithm for constructing optimal experimental designs. Our method includes two major elements: the use of ESE algorithm for controlling the search process and the employment of efficient methods for evaluating the optimality criteria. Our proposed algorithm has shown great efficiency compared to some algorithms in the literature. Specifically, it has cut the computation time from hours to minutes and seconds, which makes the just-in-time generation of large size optimal designs possible. In comparison, we have the following observations:

- With the same number of exchanges, the optimal designs generated by ESE is generally better than those generated by SA and CP.
- To obtain a design statistically significantly better than those generated by SA and CP, ESE needs far less number of exchanges (typically around 1/6 ~ 1/2 of exchanges needed by SA or CP for small-sized designs and 1/33~ 1/4 of exchanges needed by CP for large-sized designs).
- For small-size problems (a relatively large number of exchanges are affordable), SA often has better performance than CP. However, for large-size problems, SA may converge very slowly and require a tremendous number of exchanges.

While our focus in this paper is on optimizing LHDs, the ESE algorithm can be used to optimize other classes of designs such as OAs and OLs. Furthermore, while the algorithm works on the ϕ_p criterion, the entropy criterion, and the CL_2 criterion, it can be conveniently extended to other optimality criteria.

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