LHD: An R package for efficient Latin hypercube designs with flexible sizes

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Abstract

Efficient Latin hypercube designs (LHDs), including maximin distance LHDs, maximum projection LHDs and orthogonal LHDs, are widely used in computer experiments, yet their constructions are challenging. In the current literature, various algebraic methods and searching algorithms have been proposed to construct different kinds of efficient LHDs, each having its own pros and cons. In this paper, we develop the R package LHD that integrates and improves various algebraic and searching methods to construct efficient LHDs with flexible design sizes. We summarize and compare different methods aiming to provide guidance for practitioners on how to choose the right designs. Moreover, many of the designs found in this paper are better than the existing ones. The designs generated by our R package can also be used as benchmarks for the future developments on constructing efficient LHDs.

Keywords: Computer Experiments; Simulated Annealing; Particle Swarm Optimization; Genetic Algorithms; Space-filling design; Orthogonality; Maximum Projection.

1 Introduction

Computer experiments are widely used in both scientific researches and industrial productions to simulate real-world problems with complex computer codes Sacks et al. (1989); Fang et al. (2005). Different from physical experiments, computer experiments are deterministic and subject to no random errors, and hence replications should be avoided Santner et al. (2003). The most popular experimental designs for computer experiments are Latin hypercube designs (LHDs) by McKay et al. (1979), which has uniform one-dimensional projections and avoids replications on every dimension. According to practical needs, there are various types of efficient LHDs (aka. optimal LHDs), including space-filling LHDs, maximum projection LHDs and orthogonal LHDs. There is rich literature on how to construct such designs, but it is still very challenging to find efficient ones for moderate or large design sizes Ye (1998); Fang et al. (2005); Joseph et al. (2015); Xiao & Xu (2018).

An LHD with \( n \) runs and \( k \) factors is an \( n \times k \) matrix with each column being a random permutation of \( 1, \ldots, n \). A space-filling LHD has its sampled region as scattered-out as possible and its unsampled region as minimal as possible, which considers the uniformity of all dimensions. Different criteria were proposed to measure designs’ space-filling property, including the maximin and minimax distance criteria Johnson et al. (1990); Morris & Mitchell (1995),
the discrepancy criteria \cite{Hickernell1998, Fang1998, Fang2002, Fang2005} and the entropy criterion \cite{Fang2002}. Since there are as many as $(n!)^{k-1}$ candidate LHDs for a given design size, it is nearly impossible to find the space-filling one via enumeration when $n$ and $k$ are moderate or large. In the current literature, both the searching algorithms \cite{Morris1995, Leary2003, Joseph2008, Ba2015, Kenny2000, Jin2005, Liefvendahl2006, Grosso2009, Chen2013} and algebraic constructions \cite{Zhou2015, Xiao2017, Wang2018} are proposed to find space-filling LHDs.

The searching algorithms can lead to space-filling LHDs with flexible sizes. Specifically, \cite{Morris1995} proposed a simulated annealing algorithm (SA) which can avoid being trapped at local optima and find the global best design. Following their work as well as \cite{Tang1993}, \cite{Leary2003} proposed to construct orthogonal array-based LHDs (OALHDs) using the SA algorithm. \cite{Joseph2008} proposed a multi-objective criterion and developed an adapted SA algorithm, which seeks both orthogonality and space-filling property. \cite{Ba2015} extended the work of sliced Latin hypercube designs (SLHD) by \cite{Qian2012} and proposed a two-stage SA algorithm. In addition to the SA based algorithms, there are various other searching algorithms for efficient designs. \cite{Kenny2000} proposed the column-wise pairwise (CP) algorithm to search for efficient symmetric LHDs. \cite{Jin2005} proposed the enhanced stochastic evolutionary algorithm (ESE), which is a combination of exchange procedure (inner loop) and threshold determination (outer loop). \cite{Liefvendahl2006} proposed to use genetic algorithm (GA), and implemented a strategy that focused on the global best directly during the searching process. \cite{Grosso2009} proposed to use Iterated Local Search heuristics where local searching and perturbation are considered. \cite{Chen2013} proposed a version of particle swarm optimization algorithm (PSO) whose searching process is to gradually reduce the Hamming distances between each particle and global best (or personal best) via exchanging elements. Generally speaking, the searching algorithms are often computationally expensive for moderate or large designs. For certain design sizes, algebraic constructions can generate efficient LHDs at nearly no cost. For example, \cite{Xiao2017} adopted Costas’ arrays to obtain space-filling saturate LHDs or Latin squares with run sizes $n = p - 2, p - 1$ or $p$ where $p$ is any prime power. \cite{Wang2018} proposed to apply the Williams transformation to linearly permuted GLP sets to construct maximin LHDs when the factor size is no greater than the number of positive integers that are co-prime to the run size.

Most space-filling designs only consider full-dimensional projections. To guarantee the space-filling properties on all possible dimensions, \cite{Joseph2015} proposed the maximum projection designs. From two to $k - 1$ projections, maximum projection LHDs (MaxPro LHDs) are generally more space-filling compared to the maximin distance LHDs. The construction of MaxPro LHDs is also challenging, and \cite{Joseph2015} proposed to use an SA algorithm. In this paper, we further propose a new GA framework that can lead to many better MaxPro LHDs.

Different from space-filling LHDs which minimize the similarities among rows, orthogonal LHDs (OLHDs) are another popular type of efficient designs which consider the similarities among
columns. All searching algorithms introduced above can also be used to obtain OLHDs which have zero column-wise correlations, and algebraic constructions are available for certain design sizes. Specifically, Ye (1998) proposed an algebraic construction of OLHDs with run sizes \( n = 2^m + 1 \) and factor sizes \( k = 2m - 2 \) with \( m \) being any integer no less than 2, and Cioppa & Lucas (2007) further extended this approach to accommodate more factors. Sun et al. (2010) extended their earlier work Sun et al. (2009) to construct OLHDs with \( n = r2^{c+1} \) or \( n = r2^{c+1} + 1 \) and \( k = 2^c \) where \( c \) and \( r \) are any two positive integers. Yang & Liu (2012) proposed to use generalized orthogonal designs to construct OLHDs and nearly orthogonal LHDs (NOLHDs) with \( n = 2^{r+1} \) or \( n = 2^{r+1} + 1 \) and \( k = 2^r \) where \( r \) is any positive integer. Steinberg & Lin (2006) developed a construction method based on factorial design and group rotations with \( n = 2^{2m} \) and \( k = 2^m t \), where \( m \) is any positive integer and \( t \) is the number of rotation groups. Georgiou & Efthimiou (2014) proposed a construction method based on orthogonal arrays and their full fold-overs with \( n = 2ak \) runs and \( k \) factors, where \( k \) is the size of orthogonal matrix and \( a \) is any positive integer. Additionally, inheriting the properties of orthogonal arrays, various types of efficient LHDs can be constructed. Tang (1993) proposed to construct OALHDs by deterministically replacing elements from orthogonal arrays, which tend to have better space-filling proprieties with low column-wise correlations. Lin et al. (2009) proposed to use OLHDs or NOLHDs as starting designs and then couple them with orthogonal arrays for constructing OALHDs. Their method requires less runs to accommodate large numbers of factors with \( n^2 \) runs and \( 2fp \) factors, where \( n \) and \( p \) are designs sizes of the OLHDs or NOLHDs and \( 2f \) is the number of columns in the coupled orthogonal array. Butler (2001) implemented the Williams transformation Williams (1949) to construct OLHDs under a second-order cosine model with \( n \) being odd primes and \( k \leq n - 1 \).

In this paper, we develop an R package LHD available on the Comprehensive R Archive Network [https://cran.r-project.org/web/packages/LHD/index.html], which integrates and improves current popular searching and algebraic methods for constructing maximin distance LHDs, Maxpro LHDs and orthogonal LHDs. With this package, users having few background on design theory can easily generate efficient LHDs with flexible sizes according to their practical needs. We also summarize and compare different methods to provide more guidance for practitioners. Moreover, many new designs that are better than the exiting ones are discovered using the developed package.

2 Conclusion

In this paper, we discussed the package LHD along with three types of Latin hypercube designs, namely, maximin distance Latin hypercube designs, maximum projection Latin hypercube designs, and orthogonal Latin hypercube designs. For the discussion of maximin distance Latin hypercube designs, we demonstrated and compared different searching algorithms such as simulated annealing algorithm, particle swarm optimization algorithm, and genetic algorithm. Since different algorithms perform differently, simulations of discussed algorithms in terms of \( \phi_p \) criterion were conducted and comparisons were made. For the discussion of maximum projection Latin Hypercube designs, we proposed to use the framework of particle swarm optimization algorithm and genetic algorithm due to the similarities between \( \phi_p \) and \( \psi \) criteria. The proposed
framework would be able to generate Latin Hypercube designs with better maximum projection properties than existing algorithm in the literature. For the discussion of orthogonal Latin hypercube designs, we summarized popular construction methods. Since all these methods yield orthogonal designs, only flexibility in terms of run sizes and the number of factors were focused in the discussion. We proposed to use the core functions in the package to identify OLHDs and NOLHDs with flexible sizes, and simulation results show that they are capable of identifying good NOLHDs for the sizes where construction method is not an option.

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