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AN INTEGER PROGRAMMING ALGORITHM FOR CONSTRUCTING MAXIMIN DISTANCE DESIGNS FROM GOOD LATTICE POINT SETS

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Abstract: Computer experiments can build computationally cheap statistical models to study complex computer models. These experiments are commonly conducted using maximin distance Latin hypercube designs (LHDs), generated using heuristic algorithms or algebraic methods in the literature. However, the performance of these algorithms deteriorates as the number of factors increases, and the algebraic methods work only for numbers of runs that are of a special kind, say, a prime number. To overcome these limitations, we introduce an integer programming algorithm to construct maximin distance LHDs of flexible sizes. Our algorithm leverages recent advances in the field of optimization, as implemented in commercial optimization solvers. Moreover, it benefits from the attractive algebraic structures given by good lattice point sets and the Williams transformation. Using comprehensive numerical experiments, we show that, with a few exceptions, our proposed algorithm outperforms benchmark algorithms and methods for constructing LHDs with up to 113 runs.

Key words and phrases: Exact algorithm, Gaussian process, Gurobi, L_1-distance, level permutation, space-filling design.

1. Introduction

Computer experiments enable us to study complex systems that are simulated using computer models (Fang, Li and Sudjianto (2006); Santner, Williams and Notz (2018)). A computer model uses algorithms and sets of mathematical equations to provide the best representation possible of the link between the input factors and the responses of the system. However, many of these models are computationally expensive, because they require solving complicated partial differential equations numerically. Therefore, one of the main goals of a computer experiment is to build an efficient, computationally cheap surrogate model that approximates the computer model well. To this end, they demand cost-effective experimental designs that gather high-quality data from the computer model, using a limited number of runs.

Space-filling designs are attractive for computer experiments because their runs are conducted at points that fill the experimental region evenly. A space-

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