DOCTORAL THESIS

Some New Developments of Experimental Designs and Their Applications

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Abstract

Experimental design is an important branch in statistics and has been widely applied to various fields of industry, system engineering, and others. There are diverse design and modeling methods for different purposes. Among them, the orthogonal design (OD), optimal regression design including the D-optimal design (DOD) and uniform design (UD) have been widely employed. However, there are various open problems involving these designs. My research during the doctor study period tries to solve several problems. Most of the new results have been published in several international journals (see the list of my publications). My dissertation is based on some of these publications.

The orthogonal design is the most popular method having a long history. It based on some additive ANOVA models incorporating main effects, interaction effects and random error. A good orthogonal design is able to obtain an efficient estimation for requested effects with a small number of experimental runs. The effects that are less important according to the hierarchical ordering principle can be confounded for saving the number of runs. There are various criteria including the minimum aberration and the uniformity measure for evaluating the orthogonal designs in the literature. To evaluate and avoid the confounding situation of projected saturated symmetric orthogonal designs, we (Lin and Fang (2019)) proposed a criterion "the main effect confounding pattern" (MECP). The new criterion MECP is consistent with other criteria including discrepancies, and the generalized word-length pattern. In the meanwhile, MECP can provide more information about statistical performances in the classification for projection designs than the other criteria, providing an approach to finding the best main effect arrangement for the experimenter. I also participated in the projects "New non-isomorphic detection methods for orthogonal designs" and "Detecting non-isomorphic orthogonal designs" for developing more techniques of the identification and detection of non-isomorphic orthogonal designs. In conservative view, isomorphic orthogonal designs ought to have the same statistical performance. However, MECP indicates that the isomorphism does not imply the equivalence of orthogonal designs.

A good design for experiments should consider both effectiveness and robustness. Each design method is based on a given model. The OD is based on ANOVA models, whereas the D-optimal regression design is based

on regression models, and the uniform design is on the overall mean model. These models have many unknown parameters to be estimated. A design is effective if it provides a more accurate (or even the best) estimate for the unknown model parameters. If the underlying model is not completely known, the robustness requests the design to perform at the same level when the model changes. If the underlying regression model is known, the D-optimal design (DOD) is the most effective on parameter estimation, but DOD is not robust against the model change. The uniform design is robust against the model change, but they are less efficient if the underlying model is completely known and more accurate than the overall mean model. The orthogonal design has good performance in both of efficiency and robustness, but it has a large space for improvements. To incorporate both robustness and effectiveness, we (Fang, Lin and Peng (2022)) proposed a new type of composite designs. According to the performances on prediction mean square error in selected practical models, the recommendation of designs is addressed. Many case studies are investigated, and the application to the chemometrics is mentioned.

With the development of science and technology, computer experiments have gained more and more attention in past decades. Engineers and scientists have implemented computer simulations on physical systems due to the complex relationships between the inputs and outputs. Many space-filling designs including the latin hypercube design and the uniform design have been proposed and widely used in real case studies. Fang, Li, and Sudjianto (2005) gave a comprehensive introduction to the design and modeling of computer experiments. Due to the computational complexity of constructing UDs, the current widely used the uniform designs (UD) are constructed over a discrete (lattice points) space. If the factors of interest are continuous and involved in a computer experiment, we wish the levels of factors are allowed to be continuous in the design since the corresponding experimental cost is not affected. In the literature, most of UDs are constructed by a stochastic heuristic, threshold accepting algorithm. However, this algorithm is not suitable on the continuous domain. Note that constructing UD is minimizing a given discrepancy and is an optimization problem. We (Lai, Fang, Peng, Lin (2021)) proposed an approach to searching UDs on a continuous domain by coordinate descent methods. Several case studies show that the UDs on the continuous domain can improve the experimental achievement compared to the UDs on the discrete domain.