Abstract

BENKOVÁ, Eva. *Algorithms for computing optimal designs of experiments under constraints* [dissertation thesis]. Comenius University in Bratislava. Faculty of Mathematics, Physics and Informatics; Department of Applied Mathematics and Statistics. Supervisor: doc. Mgr. Radoslav Harman, PhD. Bratislava 2022, 111 pages.

In this dissertation thesis, we study several problems of finding the optimal experimental design under various design constraints. First, we introduce a multiplicative algorithm for constructing D-optimal approximate size- and cost-constrained designs, that is, designs restricted on the number of trials and, simultaneously, on the total cost of the experiment. The proposed method is a non-trivial specification of the "barycentric" algorithm introduced in [31], which includes also reducing the design space by removal of unnecessary design points. We analytically prove its convergence and demonstrate its performance in comparison to the competing methods.

A different type of linearly constrained designs are space-filling designs frequently used in computer experiments. We propose a general exchange-type heuristic framework for computing exact designs, which is based on the notion of "privacy sets" and can be adapted for various space-filling restrictions. Our specification of the framework for the so-called Bridge designs significantly outperforms the state-of-the-art method. Moreover, we implemented the general framework for the so-called Minimum-distance designs by the use of Voronoi diagrams and their generalizations - power diagrams. We explain the role of these diagrams in constructing efficient Minimum-distance designs by deriving some crucial theoretical properties. Performance of the heuristic for both kinds of constraints is compared against competing algorithms in numerical studies.

Key words: design of experiments, optimal design, linearly constrained design, D-optimality criterion, multiplicative algorithm, exchange algorithm, Voronoi diagram.