Abstracts of the Ninth Workshop on Simulation (2018) 1-2

A New Branch and Bound Algorithm for the D-optimal Design Problem

Selin Damla Ahipasaoglu[1] and Benjamin Tan [2]

1 Introduction

Calculating an exact D-optimal design over a finite set of points remains a very challenging task even though approximate designs can be found efficiently. We develop a new branch-and-bound framework for solving the exact D-optimal Design problem and discuss how it can be implemented efficiently. In each node of the branch-and-bound tree, we solve a generalization of D-optimal design problem via a simple yet effective first-order algorithm. We provide promising computational results.

2 Formulation of the problem

Given a set of regression points $\{x_1, \ldots, x_m\} \in \Re^n$ and the total number of experiments N, the exact D-optimal design can be calculated by solving the following program:

$$\begin{aligned} \max_u \ & ln\Big(det\big(XUX^T\big)\Big) \\ s.t. \quad & \sum_{i=1}^{m} u_i = 1, \\ & u_i \geq 0, \ \forall i, \\ & Nu_i \in \mathbb{Z}, \ \forall i, \end{aligned}$$

where X is an $n \times m$ matrix whose i^{th} column stores x_i and U is a diagonal matrix with components of $u \in \Re^m$ on its diagonal.

We solve the integer program by a branch-and-bound method. We start with solving a relaxation of the problem where the last constraint is ignored. This corresponds to the well-known approximate D-optimal design problem for which many efficient algorithms exist. (See [1] and references therein.) If the optimal solution u (of the relaxed problem) violates the omitted integrality constraints, then we "branch" on an index j (such that Nu_j is fractional) to generate two subproblems with additional constraints: $u_j \leq \frac{\lfloor Nu_j \rfloor}{N}$ and $u_j \geq \frac{\lceil Nu_j \rceil}{N}$. Therefore, in each node of the search tree, we solve the following generalization of the approximate D-optimal design problem:

[1]Engineering Systems and Design Pillar, Singapore University of Technology and Design, E-mail: ahipasaoglu@sutd.edu.sg

[2]Engineering Systems and Design Pillar, Singapore University of Technology and Design, E-mail: benjamin_tanwj@mymail.sutd.edu.sg

$$\max_{u} \; ln\Big(det\big(XUX^T\big)\Big)$$
$$s.t. \qquad \sum_{i=1}^{m} u_i = 1,$$
$$\alpha_i \leq u_i \leq \beta_i, \; \forall i,$$

where $\alpha_i, \beta_i \in [0,1], \forall i$. We solve the subproblems by a first-order algorithm that updates only two coordinates of the iterate at each iteration. This facilitates efficient calculation of the optimal step size and new objective function value at each iteration.

We compare our results to recent work provided by [2] and observe promising results for certain problem sizes.

References

[1] S D Ahipaşaoğlu and P Sun and M J Todd, Linear convergence of a Modified Frank-Wolfe algorithm for computing minimum-volume enclosing ellipsoids, Optimization Methods and Software, 23, 5–19 (2008)

[2] R Harman and L Filova, Computing efficient exact designs of experiments using integer quadratic programming, Computational Statistics & Data Analysis, 71 1159–1167 (2014)