Integer First-Order Methods for the Exact Design of Experiments Problem

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1 Introduction

We tackle the Optimal Experiment Design Problem, which consists in choosing experiments to run or observations to select from a finite set to estimate the parameters of a system. Each experiment $\mathbf{v} \in \mathbb{R}^n$ represents choices for the input of the system controlled by design parameters. The objective is to maximize some information criterion on the system from the observations, leading to a convex integer optimization problem. The constraints restrict the total number of experiments, and add potential lower and upper bounds on the number of times each experiment can be performed. If we concatenate all experiments as rows of a design matrix $A = \mathbf{v}_1 \ldots\ldots, \mathbf{v}_m \in \mathbb{R}^{m\times n}$ where each row represents an experiment, the resulting problem can be formulated as:

$$
\begin{aligned}
\text{(OED)}\ \ \min_{\mathbf{x}}\ & f(X(\mathbf{x})) \\
\text{s.t.}\ & \mathbf{l} \leq \mathbf{x} \leq \mathbf{u} \\
& \mathbf{x} \in \mathbb{Z}^n_+,
\end{aligned}
$$

with $X(\mathbf{x}) = A^\intercal \operatorname{diag}(x) A$ the information matrix. The function f is convex, differentiable on its domain but not necessarily Lipschitz-smooth, and represents an information criterion that summarizes the information of the matrix X.

2 Methods

We leverage `Boscia`, a recent algorithmic framework which is based on a nonlinear branch-and-bound with node relaxations solved to approximate optimality using Frank-Wolfe algorithms. One particular advantage of the method is its efficient utilization of the polytope formed by the original constraints of (OED) which remains preserved by the method, unlike in those relying on epigraph-based formulations. We assess our method against both generic and specialized convex mixed-integer approaches. Computational results highlight the performance of the proposed method, especially on large and challenging instances.

References

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