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Model Selection for Screening Experiments with Random Effects: An Adaptation of the SAMS Algorithm

Model selection in screening experiments is challenging when data arise from split-plot designs, multi-day industrial studies, or other settings that introduce correlation between observations. Standard approaches, including stepwise selection, LASSO, and mixed-integer optimisation (MIO), assume independent errors and may show degraded performance when this assumption is violated, limiting their applicability to a wide class of practically relevant experiments.

We present an adaptation of the Simulated Annealing Model Search algorithm (SAMS; Wolters and Bingham, 2011) that accounts for correlation induced by random effects. The core modification is a whitening step that transforms correlated observations prior to the model search, enabling computationally efficient exploration while preserving the key strengths of SAMS: a large collection of well-fitting models, visualisation of effect aliasing via raster plots, and identification of active effects through an entropy criterion. The method is implemented in the open-source Python package PyOptEx.

We evaluate the approach through a simulation study covering a range of experimental designs and variance structures. We compare the adapted SAMS against mixed-integer optimisation and backward selection, investigating in particular how performance differs between methods that correctly account for the correlation structure and those that do not. We further illustrate the method on data from a pilot-plant screening experiment on potato fry production to demonstrate practical applicability.

Special/ Invited session

Classification

Keywords

Screening experiments; random effects; split-plot designs

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