A Mixed Integer Optimization Approach for Model Selection in Screening Experiments

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KU LEUVEN

Outline

1. Motivating Example

2. Mixed Integer Optimization (MIO) Approach
    1. Basic idea
    2. Constraints on the model search
    3. Create a list of best models

3. Results and Discussion

Vazquez, Schoen and Goos (2018). A mixed integer optimization approach for model selection in screening experiments. Technical report 2018007. University of Antwerp. Available upon request.

Decolorization experiment

- Investigate the electrochemical decolorization of the RV5 compound on a textile surface (Fidaleo et al., 2016).
- 9 continuous factors at three levels.
- A 21-run definitive screening design was used.
- Response is the % of color removal.

Goal: Detect the influential linear effects, two-factor interactions and quadratic effects.

Data analysis via model selection

Run	A	B	C	D	E	F	G	H	I	Y
1	0	1	1	1	1	1	1	1	1	3.26
2	0	-1	-1	-1	-1	-1	-1	-1	-1	-3.29
3	1	0	-1	-1	-1	-1	1	1	1	4.70
4	-1	0	1	1	1	1	-1	-1	-1	-2.53
5	1	-1	0	-1	1	1	-1	-1	1	-2.68
6	-1	1	0	1	-1	-1	1	1	-1	3.44
7	1	-1	-1	0	1	1	1	1	-1	4.25
8	-1	1	1	0	-1	-1	-1	-1	1	-1.80
9	1	-1	1	1	0	-1	-1	1	-1	-0.37
10	-1	1	-1	-1	0	1	1	-1	1	1.11
11	1	-1	1	1	-1	0	1	-1	1	0.42
12	-1	1	-1	-1	1	0	-1	1	-1	0.40
13	1	1	-1	1	-1	1	0	-1	-1	2.72
14	-1	-1	1	-1	1	-1	0	1	1	1.67
15	1	1	-1	1	1	-1	-1	0	1	1.14
16	-1	-1	1	-1	-1	1	1	0	-1	-0.14
17	1	1	1	-1	-1	1	-1	1	0	0.00
18	-1	-1	-1	1	1	-1	1	-1	0	0.49
19	1	1	1	-1	1	-1	1	-1	-1	-0.69
20	-1	-1	-1	1	-1	1	-1	1	1	-0.70
21	0	0	0	0	0	0	0	0	0	-0.38

Y: *logit* of the percentage of color removal.

Information:

- 54 potential effects, 21 observations.
- Effect heredity.
- Screening design.

Desirable properties of a model selection method for screening

Property 1: Creates a list of models that are compatible with the data.

Property 2: Reveals the aliasing present in the screening design.

Property 3: Provides a framework to specify restrictions on the model search.

Available Model Selection Methods

Method	P1: List	P2: Aliasing	P3: Restrictions
LASSO and Extensions (Yuan et al., 2006; Choi et al., 2010; Bien et al., 2016)	✓	✗	✗
Dantzig Selector (Phoa et al., 2009)	✓	✗	✗
LARS and Extensions (Yuan et al., 2007, 2009)	✓	✗	✓
Forward Selection (Westfall et al., 1998)	✓	✗	✗
Simulated Annealing Model Search (Wolters et al., 2011)	✓	✓	✗

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MIO approach

<u>Basic Idea:</u> Best-subset selection

$$\min_{\widehat{\boldsymbol{\beta}}} \sum_{i=1}^{n} \left(y_i - \sum_{u=1}^{p} x_{iu} \hat{\beta}_u \right)^2$$

Subject to:

$$\sum_{u=1}^{p} I\left(\hat{\beta}_u \neq 0\right) = k$$

Indicator function

$\widehat{\boldsymbol{\beta}} = \left(\hat{\beta}_1, \hat{\beta}_2, \ldots, \hat{\beta}_p\right)^T$: Parameter estimates.

k: Subset size.

MIO problem

Bertsimas et al. (2016) formulated the best-subset selection problem as a mixed integer optimization problem.

Parameter estimates

$$\widehat{\boldsymbol{\beta}} = \begin{pmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \vdots \\ \hat{\beta}_p \end{pmatrix}$$

Binary decision variables $z_u \in \{0,1\}$

$$\begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_p \end{pmatrix} = \mathbf{z}$$

Link between $\hat{\beta}_u$ and z_u:

$$\hat{\beta}_u(1 - z_u) = 0.$$

If $z_u = 0$, then $\hat{\beta}_u = 0$.

If $z_u = 1$, $\hat{\beta}_u$ can be different from zero.

Standard MIO problem

$$\min_{\hat{\boldsymbol{\beta}},\mathbf{z}} \sum_{i=1}^{n} \left(y_i - \sum_{u=1}^{p} x_{iu} \hat{\beta}_u \right)^2$$

Subject to:

$$\hat{\beta}_u (1 - z_u) = 0$$

$$\sum_{u=1}^{p} z_u = k$$

$$z_u \in \{0,1\}$$

$$\hat{\beta}_u \in \mathbb{R}$$

Framework to specify constraints on the model search.

Solvers: GUROBI, CPLEX, BARON, SCIP.

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Constraints on the model search

Effect heredity

z_u: linear effect of factor u.

z_{uv}: two-factor interaction between u and v.

- Strong effect heredity:

$$z_{uv} \leq z_u \text{ and } z_{uv} \leq z_v$$

- Weak effect heredity:

$$z_{uv} \leq z_u + z_v$$

- Effect heredity for quadratic effects:

$$z_{uu} \leq z_u$$

Final MIO problem

$$\min_{\hat{\boldsymbol{\beta}},\mathbf{z}} \sum_{i=1}^{n} \left(y_i - \sum_{u=1}^{p} x_{iu} \hat{\beta}_u \right)^2$$

Subject to:

$$\hat{\beta}_u (1 - z_u) = 0$$

$$\sum_{u=1}^{p} z_u = k$$

$$z_u \in \{0,1\}, \hat{\beta} \in \mathbb{R}$$

$$z_{uu} \leq z_u$$

$$z_{uv} \leq z_u + z_v$$

Categorical factors and heredity,

factor sparsity,

$\vdots$

Standard MIO problem.

- **Property 3: Search restrictions.**
- Output: The optimal feasible model of size k.

User-specified constraints.

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A sequential algorithm to list the best models

For a given model size k:

1. Solve MIO problem → Find optimal model S_1.
2. Solve MIO problem + extra constraint to exclude S_1 → Find second-best model S_2.
3. Solve … nts to excluc … model S_3.

Extra constraint:

$$\sum_{u \in S_1} z_u \leq k - 1$$

Ext

$\sum_{u}$ … $k - 1$

4. So … ex … S_M.

Output: List of the M best models of size k.

List of models

Repeat the sequential algorithm for several model sizes, $k = 1, 2, \ldots, k_0$.

Construct a list of the best models of different sizes. **Property 1: Compatible models with data.**

Study the list using raster plots. **Property 2: Visualize aliasing.**
Wolters and Bingham (2011)

The effects that appear consistently in the best feasible models are declared active.

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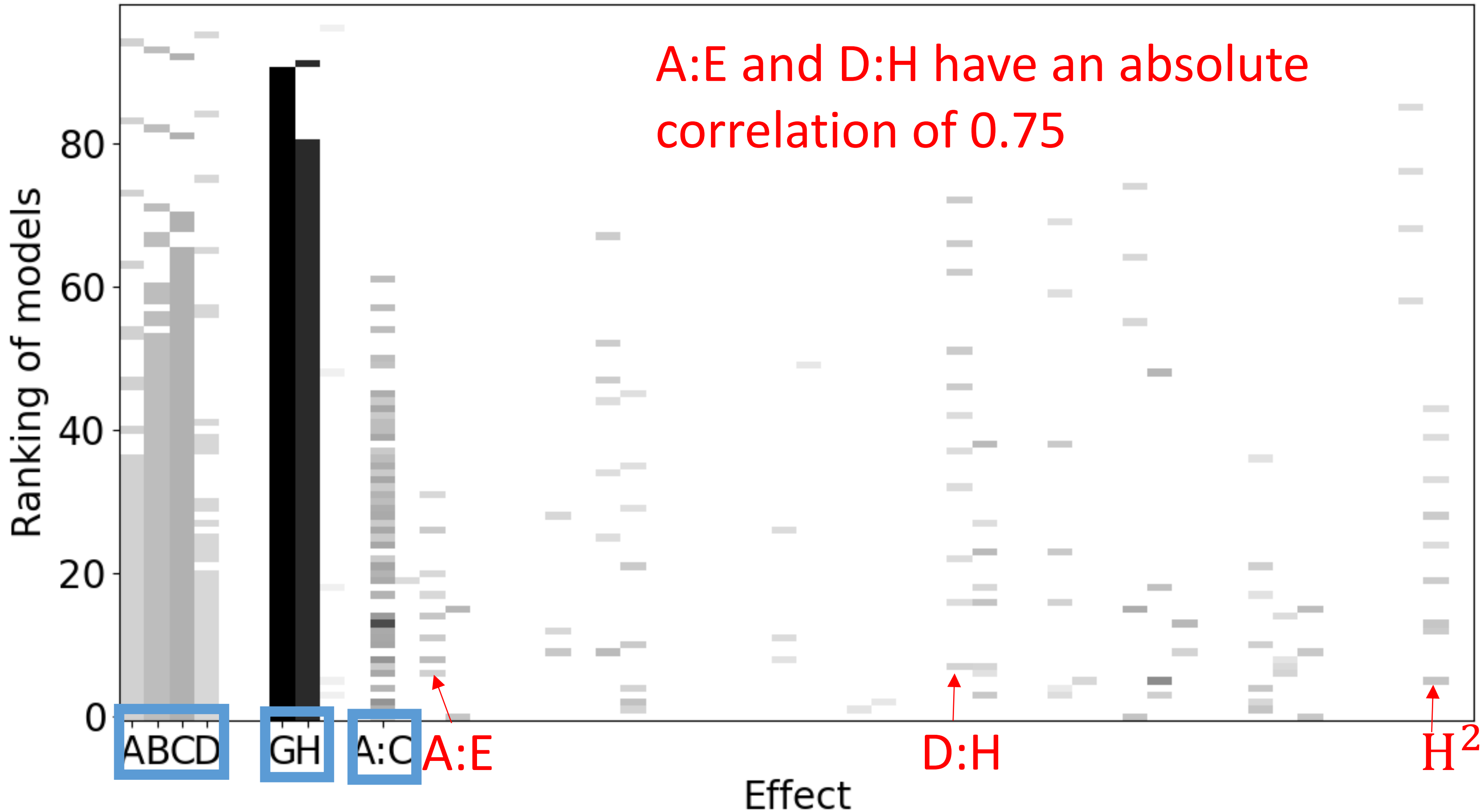
Decolorization experiment

The 10 best models of sizes 1, 2, ..., 10.



The models follow weak effect heredity.

Discussion

- We developed a MIO approach to analyze data from screening designs.

- Unlike the benchmark methods, MIO has all the desirable properties of a good model selection method for screening.

- The MIO approach is deterministic and guarantees that the best-fitting models will be found.

- A Python/Gurobi implementation is available.

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Appendix A: Computing times MIO approach

Specifications:

- Standard CPU: Intel(R) Core(TM) i7-4770 CPU @ 3.4 GHz, 16 GB.

- Python and Gurobi v7.5

Instance	(Runs, Effects)	Max. k	Additional Constraints	Time
Decolorization Experiment	(21, 54)	10	Heredity	3 m
TNO	(48, 91)	11	Heredity	30 m
DSD	(21, 65)	11	Heredity	10 m
Supersaturated	(24, 138)	6	None	> 1h 10m