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Iterated local search for the construction of D-optimal experimental designs

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Outline

- Introduction to experimentation and screening experiments
- Design of experiments
- Coordinate exchange algorithm
- New orthogonality-based selection strategy
- Iterated local search
- Iterated local search vs. Coordinate exchange algorithm
- Conclusions

Experimentation

Purpose:

To quantify the relationship between a response variable and the settings of several factors that are assumed to affect it, using linear regression techniques

Example:

- Response variable: Corn yield ($\mathbf{y}$)
- Factors: Amount of fertilizer ($\mathbf{x_1}$) and type of seed ($\mathbf{x_2}$)
- Models that can be estimated:
  - $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon$
  - $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \epsilon$
  - $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \epsilon$

Screening experiments

Purpose:

To carry out an experiment with several factors in order to determine those that affect the response variable most

Characteristics:

- Large number of factors
- Two levels per each factor. Usually coded using -1 and $+1$
- Estimation of main-effects models (with only first-order terms)

Example (extended):

- Factors: Amount of fertilizer ($\mathbf{x_1}$), type of seed ($\mathbf{x_2}$), amount of water ($\mathbf{x_3}$) and soil structure ($\mathbf{x_4}$)
- Model to be estimated: $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \epsilon$

Design of experiments

- **Main idea:** Fix the settings of the factors to be used in each observation
- **Objective:** To maximize information produced by the experiment

Example (extended):

Obs.	Fertilizer	Type of seed	Water	Soil
1	$+1$	$+1$	-1	-1
2	$+1$	$+1$	$+1$	-1
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
7	$+1$	-1	$+1$	-1

Design of experiments

Traditional approach: Adapt the experiment in order to fit one of the experimental designs available in the literature

- Often infeasible in practice due to complications that arise in real-life experimentation
- The available number of observations is not a power of two (full factorial and fractional factorial designs)

Optimal design of experiments approach: Attempt to find the best possible design for each particular scenario

- Complex combinatorial optimization problem!
- D-optimality criterion

Design of experiments - Optimization Problem

- **Model matrix of the design:**

$$X = \begin{bmatrix} 1 & \overbrace{+1 & +1 & -1 & -1}^{\text{Design matrix}} \\ 1 & +1 & +1 & +1 & -1 \\ 1 & +1 & -1 & -1 & +1 \\ 1 & -1 & -1 & +1 & -1 \\ 1 & +1 & +1 & +1 & -1 \\ 1 & -1 & +1 & -1 & +1 \\ 1 & +1 & -1 & +1 & -1 \end{bmatrix}$$

- **Objective function to maximize:** $|X'X|$
- If the number of observations (n) is multiple of 4, then $100 \times |X'X|^{\left(\frac{1}{f+1}\right)}/n = 100$

Coordinate exchange algorithm (CEA)

- In each iteration, the algorithm considers possible exchanges for every element of the design matrix

$$\begin{bmatrix} 1 & +1 & +1 & -1 & -1 \\ 1 & {\color{red}+1} & +1 & +1 & -1 \\ 1 & +1 & -1 & -1 & +1 \\ 1 & -1 & -1 & +1 & -1 \\ 1 & +1 & +1 & +1 & -1 \\ 1 & -1 & +1 & -1 & +1 \\ 1 & +1 & -1 & +1 & -1 \end{bmatrix} \Rightarrow \begin{bmatrix} 1 & +1 & +1 & -1 & -1 \\ 1 & {\color{red}-1} & +1 & +1 & -1 \\ 1 & +1 & -1 & -1 & +1 \\ 1 & -1 & -1 & +1 & -1 \\ 1 & +1 & +1 & +1 & -1 \\ 1 & -1 & +1 & -1 & +1 \\ 1 & +1 & -1 & +1 & -1 \end{bmatrix}$$

$|X'X| = 3840$ $\qquad$ $|X'X| = 4096$

CEA - Selection strategy

- In which order should the algorithm explore the elements of the matrix?
  - Column
  - Row
  - Prediction variance of each row
- Which element should be exchanged?
  - Best improvement
  - Worst improvement
  - First improvement

$$\begin{bmatrix} 1 & +1 & +1 & -1 & -1 \\ 1 & -1 & +1 & +1 & -1 \\ 1 & +1 & -1 & -1 & +1 \\ 1 & -1 & -1 & +1 & -1 \\ 1 & +1 & +1 & +1 & -1 \\ 1 & -1 & +1 & -1 & +1 \\ 1 & +1 & -1 & +1 & -1 \end{bmatrix}$$

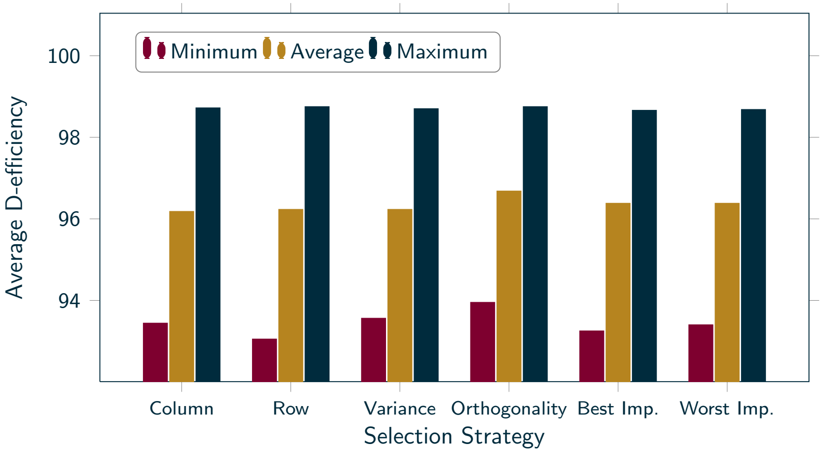
CEA - Orthogonality-based selection strategy

- **Foundation:** The orthogonality (measure) of the columns is a very good indicator of a design's quality
- **Strategy:** To first explore the columns of the design matrix that are less orthogonal (relative to the other columns) and where an exchange is more likely to produce an improvement

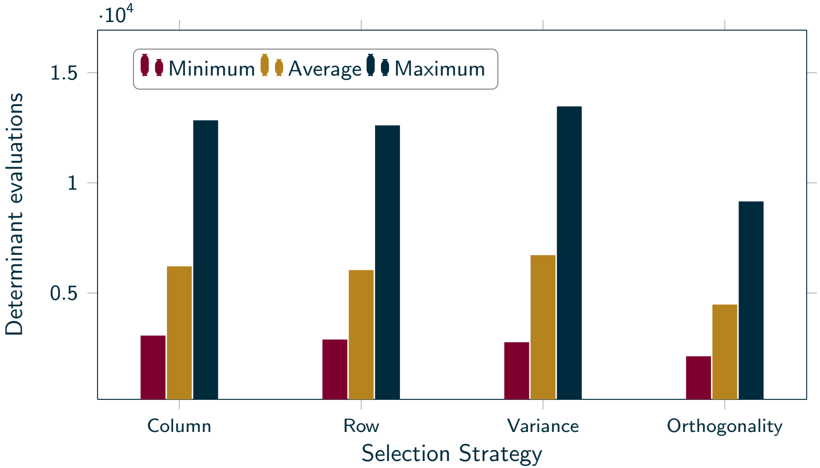
$$X = \begin{bmatrix} 1 & +1 & +1 & -1 & -1 \\ 1 & -1 & +1 & +1 & -1 \\ 1 & +1 & -1 & -1 & +1 \\ 1 & -1 & -1 & +1 & -1 \\ 1 & +1 & +1 & +1 & -1 \\ 1 & -1 & +1 & -1 & +1 \\ 1 & +1 & -1 & +1 & -1 \end{bmatrix} \qquad X'X = \begin{bmatrix} 7 & 1 & 1 & 1 & -3 \\ 1 & 7 & -1 & -1 & -1 \\ 1 & -1 & 7 & -1 & -1 \\ 1 & -1 & -1 & 7 & -5 \\ -3 & -1 & -1 & -5 & 7 \end{bmatrix}$$

$$\begin{bmatrix} 13 & 11 & 11 & 15 & 17 \end{bmatrix}$$

Strategy comparison - Design quality



Strategy comparison - Execution time



Strategy comparison - CEA limitation

	Average D-efficiency		
Selection Strategy	Min.	Avg.	Max
Small experiments (3 to 10 factors)			
Row	88.94	95.03	99.96
Variance	89.42	95.03	99.93
Orthogonality	**90.71**	**96.43**	99.96
Medium experiments (11 to 20 factors)			
Row	92.97	96.24	98.85
Variance	93.92	96.25	98.69
Orthogonality	93.98	96.37	98.80
Large experiments (21 to 30 factors)			
Row	96.43	97.19	97.68
Variance	96.50	97.18	97.73
Orthogonality	96.53	97.20	97.70

Iterated Local Search (ILS)

- **Common solution to CEA limitation:** Execute the algorithm several times starting from different initial designs and select the overall best design found
- **Assumption:** Better solutions can be found in the space surrounding locally optimal solutions but cannot be reached by the structure of the local search
- **ILS Strategy:** Apply a perturbation operator in each iteration in order to better explore the surrounding solution space

ILS - Construction of experimental designs

Algorithm 1: Iterated Local Search Pseudocode

Input: An initial design D_0

Design D_{best}, D_{pert}
$D_{best} \longleftarrow CEA(D_0)$
while $\neg$ *TerminationCondition* **do**
  $D_{pert} \longleftarrow Perturb(D_{best})$
  $D_{pert} \longleftarrow CEA(D_{pert})$
  if $determinant(D_{pert}) > determinant(D_{best})$ **then**
    $D_{best} \longleftarrow D_{pert}$
return D_{best}

ILS - Construction of experimental designs

Main features:

- **Probabilistic perturbation operator** in order to modify the design's worst portion with a higher probability
- **A reactive modification of the perturbation operator** in order to balance the intensification and the diversification phases of the search
  - When a better design is found, the intensity of the perturbation operator is set to the minimum
  - If no better design is found during the next iterations, the intensity is progressively increased

ILS vs. CEA

Algorithm	Avg. determinant evaluations	Average D-efficiency	Optimal designs found
CEA	6.16×10^6	98.73	8
ILS	6.27×10^6	**99.14**	**12**
CEA	6.17×10^7	98.90	9
ILS	5.78×10^7	**99.35**	**15**

Conclusions

What we propose:

- A new selection strategy for the CEA, the execution time of which is 20% lower than the other strategies
- A very competitive algorithm for the generation of optimal designs of screening experiments

Important insights about the problem:

- The poor performance of the best improvement selection strategy of the CEA compared to first improvement strategies
- The consideration of several initial designs is still recommended due to the large number of locally optimal designs