
# Optimal design: getting more out of experiments with hard-to-change factors

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# Literature related to this webinar

- Reason why I deliver this webinar

  Jones, B., Goos, P., 2007. A candidate-set-free algorithm for generating D-optimal split-plot designs, Applied Statistics, 56, 347–364.

- Earlier work

  Goos, P., Vandebroek, M., 2003. D-optimal split-plot designs with given numbers and sizes of whole plots, Technometrics, 45, 235–245.

- Follow-up work

  Jones, B., Goos, P., 2009. D-optimal design of split-split-plot experiments, Biometrika, 96, 67–82.

  Arnouts, H., Goos, P., Jones, B., 2013. Three-stage industrial strip-plot experiments, Journal of Quality Technology, 45, 1-17

# Outline

- Motivating examples
  - Two-stage and three-stage experiments
  - Experiment with hard-to-change factors
  - Need for flexible experimental design methods
- Models
- Optimal experimental design
  - D-optimal experimental designs
  - I-optimal experimental designs
- Illustrations
- Recent work
- Future research

# Examples

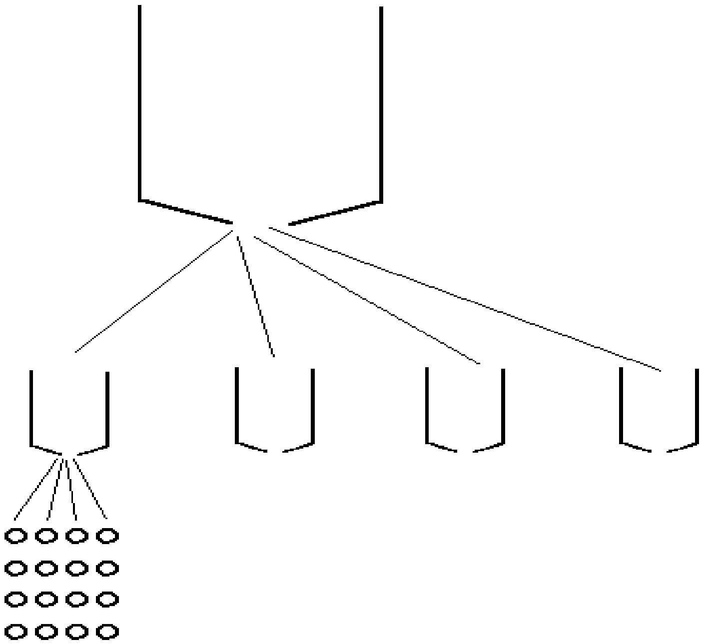
# Anti-bacterial surface treatments

- A 32-run experiment conducted to learn about the impact of 5 factors on the anti-bacterial properties of the lining of refrigerators
  - gap between electrode and isolator ($w$)
  - frequency ($s$)
  - power ($t_1$)
  - gas flow rate ($t_2$)
  - atomizer pressure ($t_3$)
- The first two factors were hard to change (technician required), while the other factors were easy to change
- Randomizing the experiment is therefore undesirable

# A split-plot design

| Run | WP | $w$ | $s$ | $t_1$ | $t_2$ | $t_3$ | Run | WP | $w$ | $s$ | $t_1$ | $t_2$ | $t_3$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | -1 | 1 | 1 | -1 | -1 | 17 | 5 | -1 | 1 | -1 | -1 | 1 |
| 2 | 1 | -1 | 1 | 1 | 1 | 1 | 18 | 5 | -1 | 1 | 1 | -1 | -1 |
| 3 | 1 | -1 | 1 | -1 | -1 | 1 | 19 | 5 | -1 | 1 | 1 | 1 | 1 |
| 4 | 1 | -1 | 1 | -1 | 1 | -1 | 20 | 5 | -1 | 1 | -1 | 1 | -1 |
| 5 | 2 | 1 | 1 | 1 | -1 | 1 | 21 | 6 | 1 | -1 | 1 | -1 | -1 |
| 6 | 2 | 1 | 1 | -1 | 1 | 1 | 22 | 6 | 1 | -1 | -1 | -1 | 1 |
| 7 | 2 | 1 | 1 | 1 | 1 | -1 | 23 | 6 | 1 | -1 | 1 | 1 | 1 |
| 8 | 2 | 1 | 1 | -1 | -1 | -1 | 24 | 6 | 1 | -1 | -1 | 1 | -1 |
| 9 | 3 | -1 | -1 | -1 | 1 | 1 | 25 | 7 | 1 | 1 | 1 | 1 | -1 |
| 10 | 3 | -1 | -1 | 1 | -1 | 1 | 26 | 7 | 1 | 1 | 1 | -1 | 1 |
| 11 | 3 | -1 | -1 | -1 | -1 | -1 | 27 | 7 | 1 | 1 | -1 | 1 | 1 |
| 12 | 3 | -1 | -1 | 1 | 1 | -1 | 28 | 7 | 1 | 1 | -1 | -1 | -1 |
| 13 | 4 | 1 | -1 | -1 | -1 | 1 | 29 | 8 | -1 | -1 | 1 | -1 | 1 |
| 14 | 4 | 1 | -1 | -1 | 1 | -1 | 30 | 8 | -1 | -1 | 1 | 1 | -1 |
| 15 | 4 | 1 | -1 | 1 | -1 | -1 | 31 | 8 | -1 | -1 | -1 | -1 | -1 |
| 16 | 4 | 1 | -1 | 1 | 1 | 1 | 32 | 8 | -1 | -1 | -1 | 1 | 1 |

# Cheese-making experiment
(Schoen, Journal of Applied Statistics 1999)



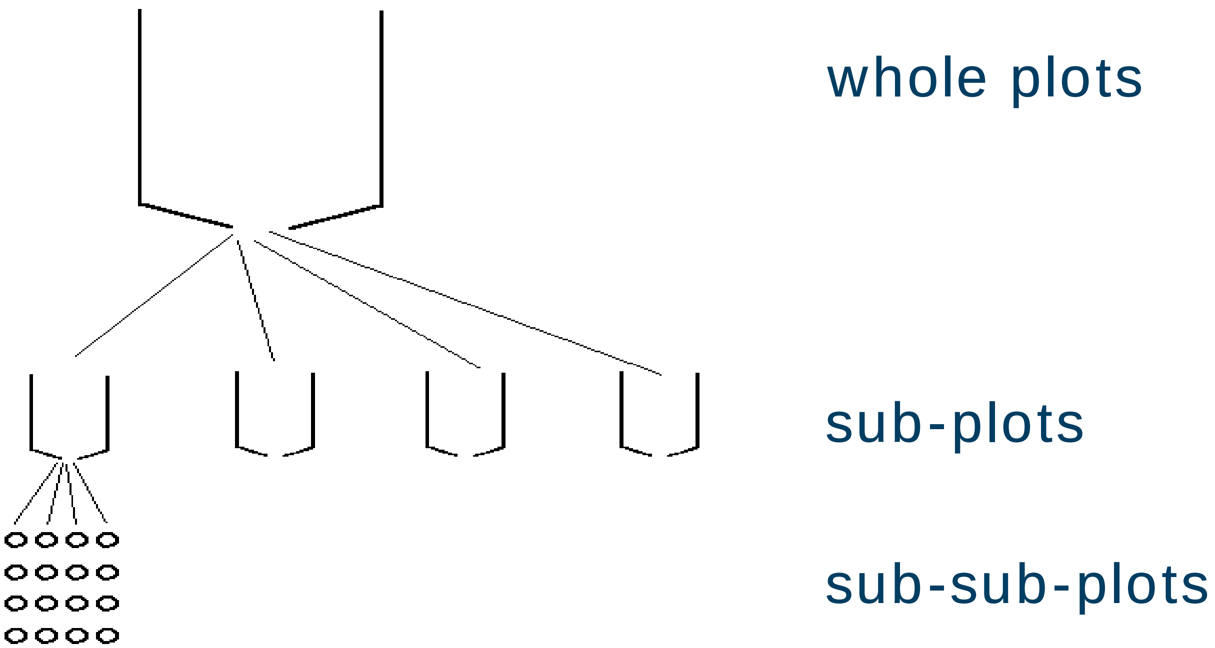
storage tanks / milk
(2 factors)

vats / curds (5 factors)

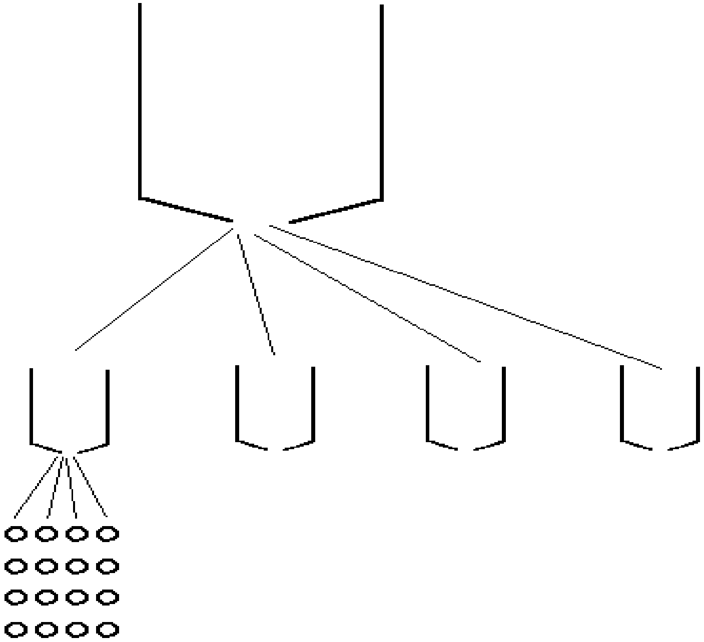
cheeses (3 factors)

# Cheese-making experiment

## (Schoen, Journal of Applied Statistics 1999)



# Cheese-making experiment
## (Schoen, Journal of Applied Statistics 1999)



whole-plot factors

(or very-hard-to-change factors)

sub-plot factors

(or hard-to-change factors)

sub-sub-plot factors

(or easy-to-change factors)

# Polypropylene experiment

- complex problem
  - 11 factors were investigated simultaneously
  - 7 factors related to polypropylene formulation
  - 4 factors related to gas plasma treatment
- goal: improve adhesion properties of polypropylene
  - water-based coatings
  - solvent-based coatings
- responses: total surface tension, lifetime, …

# Polypropylene experiment

- Stage 1:
  - 20 batches of different polypropylene formulations were prepared by Domo PPC
  - Each batch was a large box with many little polypropylene plates
- Stage 2:
  - 100 gas plasma treatments were tested by Europlasma on 100 different samples selected from the 20 initial batches
  - They could investigate about 5 plasma treatments for each batch
- Classical experimental designs were infeasible

# Stage 1

- 20 different polypropylene formulations
- 7 two-level factors
  - EPDM
  - homopolymer/copolymer (with/without ethylene)
  - talcum } never used together
  - mica }
  - lubricant
  - UV-stabiliser
  - EVA (colour)
- interest was in main effects and all 2-factor interactions involving EPDM

# Stage 2

- 4 factors
  - type of gas (2 activation gases, 1 etching gas)
  - gas flow rate
  - power
  - reaction time
- quantitative factors were investigated at 3 levels
- interest in
  - main effects, 2-factor interactions, and (for quantitative factors) quadratic effects
  - interactions between plasma treatment factors and ingredients of polypropylene formulation

# Factors and levels

| *Factor* | *Range or level* |
|---|---|
| EPDM ($w_1$) | 0–15% |
| Ethylene ($w_2$) | 0–10% |
| Talc ($w_3$) | 0–20% |
| Mica ($w_4$) | 0–20% |
| Lubricant ($w_5$) | 0–1.5% |
| UV stabilizer ($w_6$) | 0–0.8% |
| Ethylene vinyl acetate ($w_7$) | 0–1.5% |
| Flow rate ($s_1$) | 1000–2000 sccm |
| Power ($s_2$) | 500–2000 W |
| Reaction time ($s_3$) | 2–15 min |
| Gas type ($s_4$) | Etching gas<br>Activation gas 1<br>Activation gas 2 |

# Model with 66 parameters

1. the main effects of the seven additives
2. the six two-factor interactions involving EPDM and each of the other additives
3. the main effects of the gas type, the flow rate, the power and the reaction time
4. all two-factor interactions of these four factors
5. the quadratic effects of the flow rate, the power and the reaction time
6. all two-factor interactions between the seven additives and the four plasma treatment factors

# Need for flexible approach

- the presence of a multi-component constraint (mica and tallow cannot both be present)
- a categorical factor at three levels
- the use of 20 batches
- the interest in all the two-factor interactions involving EPDM
- the overall sample size of 100
- the need to estimate quadratic effects for flow rate, power and reaction time
- creating some nice orthogonal design that guarantees a simple analysis is out of the question here

# Design Stage 1

| *Whole plot* | $w_1$ | $w_2$ | $w_3$ | $w_4$ | $w_5$ | $w_6$ | $w_7$ | $k_i$ |
|---|---|---|---|---|---|---|---|---|
| 1 | −1 | −1 | −1 | −1 | −1 | −1 | 1 | 7 |
| 2 | −1 | −1 | −1 | 1 | 1 | −1 | −1 | 6 |
| 3 | −1 | −1 | 1 | −1 | −1 | 1 | −1 | 6 |
| 4 | −1 | −1 | 1 | −1 | 1 | 1 | 1 | 5 |
| 5 | −1 | 1 | −1 | −1 | 1 | 1 | −1 | 7 |
| 6 | −1 | 1 | −1 | 1 | −1 | 1 | 1 | 7 |
| 7 | −1 | 1 | 1 | −1 | −1 | −1 | −1 | 4 |
| 8 | −1 | 1 | 1 | −1 | 1 | −1 | 1 | 5 |
| 9 | 1 | −1 | −1 | −1 | −1 | −1 | 1 | 3 |
| 10 | 1 | −1 | −1 | −1 | 1 | 1 | 1 | 6 |
| 11 | 1 | −1 | −1 | 1 | −1 | −1 | −1 | 6 |
| 12 | 1 | −1 | −1 | 1 | 1 | 1 | 1 | 5 |
| 13 | 1 | −1 | 1 | −1 | −1 | 1 | −1 | 3 |
| 14 | 1 | −1 | 1 | −1 | 1 | −1 | −1 | 4 |
| 15 | 1 | 1 | −1 | −1 | −1 | 1 | −1 | 4 |
| 16 | 1 | 1 | −1 | −1 | 1 | −1 | −1 | 6 |
| 17 | 1 | 1 | −1 | 1 | −1 | −1 | 1 | 4 |
| 18 | 1 | 1 | −1 | 1 | 1 | 1 | −1 | 4 |
| 19 | 1 | 1 | 1 | −1 | −1 | 1 | 1 | 5 |
| 20 | 1 | 1 | 1 | −1 | 1 | −1 | 1 | 3 |

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# Design Stage 2

| Whole plot | $s_1$ | $s_2$ | $s_3$ | $s_4$ | Whole plot | $s_1$ | $s_2$ | $s_3$ | $s_4$ |
|---|---|---|---|---|---|---|---|---|---|
| 1 | −1 | 1 | 1 | C | 10 | 0 | 0 | 0 | C |
| 1 | 1 | −1 | −1 | C | 10 | 1 | 1 | −1 | C |
| 1 | −1 | 1 | −1 | B | 10 | −1 | −1 | 1 | B |
| 1 | 1 | −1 | 0 | B | 10 | 1 | −1 | −1 | B |
| 1 | −1 | −1 | 0 | A | 10 | −1 | 0 | −1 | A |
| 1 | 1 | 1 | −1 | A | 10 | 1 | 0 | 1 | A |
| 1 | 1 | 1 | 1 | A | 11 | 1 | 1 | 0 | C |
| 2 | −1 | 1 | −1 | C | 11 | −1 | −1 | 0 | B |
| 2 | 0 | −1 | 1 | C | 11 | 1 | 0 | −1 | B |
| 2 | 0 | 1 | 1 | B | 11 | −1 | 1 | −1 | A |
| 2 | 1 | −1 | 0 | B | 11 | 1 | −1 | −1 | A |
| 2 | −1 | −1 | 1 | A | 11 | 1 | 0 | 1 | A |
| 2 | 1 | 1 | 0 | A | 12 | −1 | 1 | 1 | C |
| 3 | −1 | 0 | 1 | C | 12 | 0 | −1 | −1 | C |
| 3 | 1 | −1 | −1 | C | 12 | −1 | 0 | 0 | B |
| 3 | 0 | −1 | 1 | B | 12 | 1 | 1 | 1 | B |
| 3 | 0 | 1 | −1 | B | 12 | 1 | 1 | −1 | A |
| 3 | −1 | −1 | −1 | A | 13 | 0 | 1 | 1 | C |
| 3 | 1 | 1 | 1 | A | 13 | 1 | −1 | 0 | B |
| 4 | 1 | 0 | 0 | C | 13 | 0 | 0 | 0 | A |
| 4 | −1 | −1 | −1 | B | 14 | −1 | −1 | 0 | C |
| 4 | 1 | 1 | 0 | B | 14 | −1 | 1 | 1 | B |

# Model and design selection

# Grouping of runs

- The presence of hard-to-change factors in the anti-bacterial surface treatment experiment results in a grouping of experimental tests for which the gap and the frequency were held constant
- In the cheese-making experiment, there are two kinds of grouping:
  - The milk tanks produce many cheeses with the same settings of the factors applied to milk storage tanks
  - The curds produce several cheeses from one setting of the factors applied to the vats
- In the polypropylene example, all the gas plasma treatments applied to samples from the same batch/box form a groupd

# Model

- Main-effects, interaction effects, quadratic effects, …
- Quantitative experimental factors
- Qualitative experimental factors
  - Two levels
  - More than two levels
- Random effects for the various kinds of grouping
  - Capture the correlation between the responses of the tests performed within the same group
  - Variance component for every kind of grouping
  - Random intercept model
  - Factor effects do not vary across groups

# Model

- Split-plot model for $j$-th observation in $i$-th whole plot

$$Y_{ij} = \mathbf{x}_{ij}^T \boldsymbol{\beta} + \gamma_i + \varepsilon_{ij}$$

- Split-split-plot model for $k$-th observation in the $j$-th sub-plot of the $i$-th whole plot

$$Y_{ijk} = \mathbf{x}_{ij}^T \boldsymbol{\beta} + \gamma_i + \delta_{ij} + \varepsilon_{ijk}$$

# Matrix notation

- Split-plot model

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma} + \boldsymbol{\varepsilon}$$

- Split-split-plot model

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}_1\boldsymbol{\gamma} + \mathbf{Z}_2\boldsymbol{\delta} + \boldsymbol{\varepsilon}$$

# Variance-covariance matrix

- Split-plot model

$$\mathbf{V} = \text{var}(\mathbf{Y}) = \sigma_\gamma^2 \mathbf{Z}\mathbf{Z}^T + \sigma_\varepsilon^2 \mathbf{I}$$

- Split-split-plot model

$$\mathbf{V} = \text{var}(\mathbf{Y}) = \sigma_\gamma^2 \mathbf{Z}_1\mathbf{Z}_1^T + \sigma_\delta^2 \mathbf{Z}_2\mathbf{Z}_2^T + \sigma_\varepsilon^2 \mathbf{I}$$

# Model estimation

- Generalized least squares estimator

$$\hat{\boldsymbol{\beta}} = \left(\mathbf{X}^T\mathbf{V}^{-1}\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{V}^{-1}\mathbf{Y}$$

- Variance-covariance matrix

$$\mathrm{var}\left(\hat{\boldsymbol{\beta}}\right) = \left(\mathbf{X}^T\mathbf{V}^{-1}\mathbf{X}\right)^{-1}$$

- Information matrix

$$\mathbf{M} = \mathbf{X}^T\mathbf{V}^{-1}\mathbf{X}$$

- **V** is estimated using restricted maximum likelihood

# Design optimality criteria

- D-optimality criterion
  - Criterion used in the 2007 Applied Statistics paper
  - Seeks a design that maximizes the determinant of the information matrix
  - Minimizes the generalized variance about the model parameters
- I-optimality criterion
  - Seeks a design that minimizes the average variance of prediction over all combinations of factor levels
  - Was not explored until Jones & Goos (Journal of Quality Technology, 2012)
- Assumption: $\sigma_{\varepsilon}^{2} = \sigma_{\gamma}^{2} \left(= \sigma_{\delta}^{2}\right)$



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# Candidate-set-free algorithm

a.k.a. coordinate-exchange algorithm

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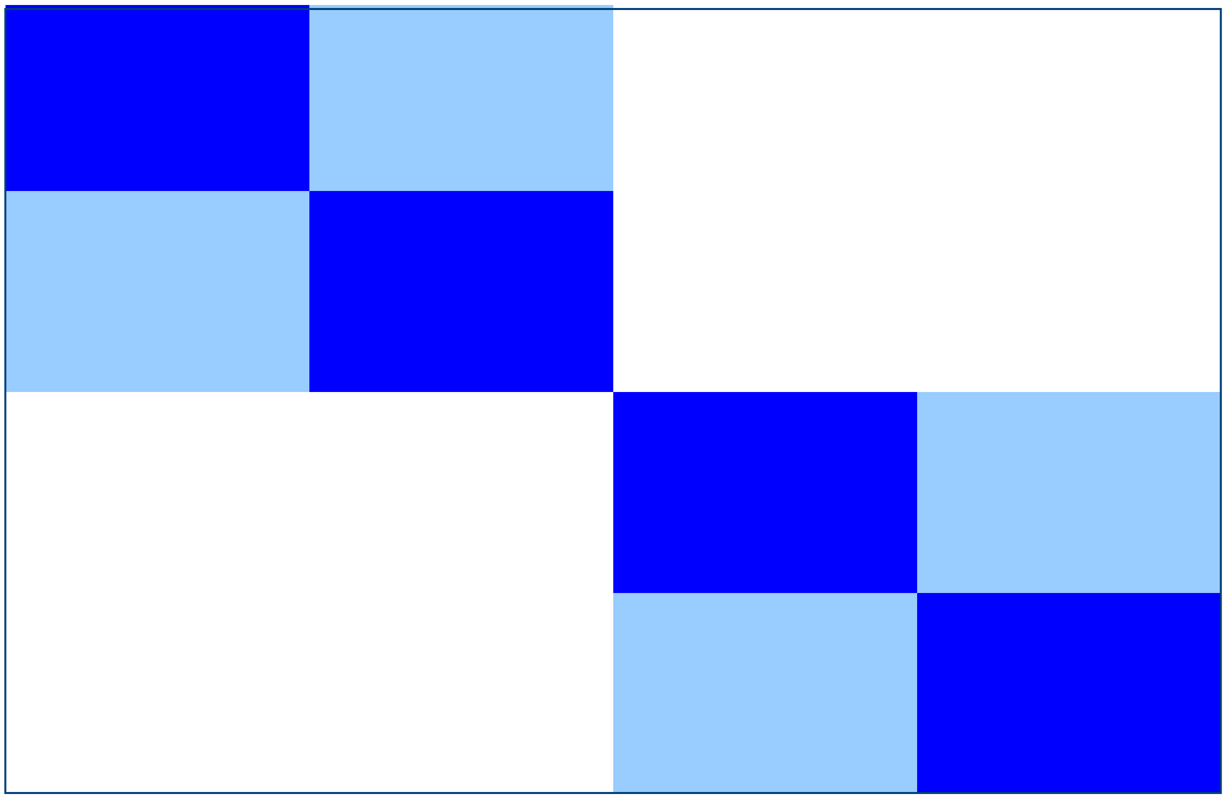
# Illustration for a split-split-plot design

- Three quantitative factors
    - One very-hard-to-change/whole-plot factor
    - One hard-to-change/sub-plot factor
    - One easy-to-change/sub-sub-plot factor
- Interest in main-effects model
- Budget allows for 8 tests/runs provided there are only
    - 2 independent settings of the very-hard-to-change factor (i.e. two whole plots)
    - 4 independent settings of the hard-to-change factor (i.e. four sub-plots)
- The easy-to-change factor is reset for each test/run

# Variance-Covariance Matrix





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# Starting Design

Determinant = 0.026

| WP | SP | X1 | X2 | X3 |
|---|---|---|---|---|
| 1 | 1 | 0.25 | 0.37 | -0.66 |
| 1 | 1 | 0.25 | 0.37 | 0.05 |
| 1 | 2 | 0.25 | -0.69 | -0.87 |
| 1 | 2 | 0.25 | -0.69 | -0.72 |
| 2 | 3 | 0.57 | 0.44 | -0.59 |
| 2 | 3 | 0.57 | 0.44 | 0.49 |
| 2 | 4 | 0.57 | -0.87 | -0.74 |
| 2 | 4 | 0.57 | -0.87 | -0.74 |

# Design after optimizing row 1

Determinant = 1.456

| WP | SP | X1 | X2 | X3 |
|---|---|---|---|---|
| 1 | 1 | -1.00 | 1.00 | -1.00 |
| 1 | 1 | -1.00 | 1.00 | 0.05 |
| 1 | 2 | -1.00 | -0.69 | -0.87 |
| 1 | 2 | -1.00 | -0.69 | -0.72 |
| 2 | 3 | 0.57 | 0.44 | -0.59 |
| 2 | 3 | 0.57 | 0.44 | 0.49 |
| 2 | 4 | 0.57 | -0.87 | -0.74 |
| 2 | 4 | 0.57 | -0.87 | -0.74 |

# Design after optimizing row 2

Determinant = 3.182

| WP | SP | X1 | X2 | X3 |
|---|---|---|---|---|
| 1 | 1 | -1.00 | 1.00 | -1.00 |
| 1 | 1 | -1.00 | 1.00 | 1.00 |
| 1 | 2 | -1.00 | -0.69 | -0.87 |
| 1 | 2 | -1.00 | -0.69 | -0.72 |
| 2 | 3 | 0.57 | 0.44 | -0.59 |
| 2 | 3 | 0.57 | 0.44 | 0.49 |
| 2 | 4 | 0.57 | -0.87 | -0.74 |
| 2 | 4 | 0.57 | -0.87 | -0.74 |

# Design after optimizing row 3

Determinant = 6.46

| WP | SP | X1 | X2 | X3 |
|---|---|---|---|---|
| 1 | 1 | -1.00 | 1.00 | -1.00 |
| 1 | 1 | -1.00 | 1.00 | 1.00 |
| 1 | 2 | -1.00 | -1.00 | 1.00 |
| 1 | 2 | -1.00 | -1.00 | -0.72 |
| 2 | 3 | 0.57 | 0.44 | -0.59 |
| 2 | 3 | 0.57 | 0.44 | 0.49 |
| 2 | 4 | 0.57 | -0.87 | -0.74 |
| 2 | 4 | 0.57 | -0.87 | -0.74 |

# Design after optimizing row 4

Determinant = 7.20

| WP | SP | X1 | X2 | X3 |
|---|---|---|---|---|
| 1 | 1 | -1.00 | 1.00 | -1.00 |
| 1 | 1 | -1.00 | 1.00 | 1.00 |
| 1 | 2 | -1.00 | -1.00 | 1.00 |
| 1 | 2 | -1.00 | -1.00 | -1.00 |
| 2 | 3 | 0.57 | 0.44 | -0.59 |
| 2 | 3 | 0.57 | 0.44 | 0.49 |
| 2 | 4 | 0.57 | -0.87 | -0.74 |
| 2 | 4 | 0.57 | -0.87 | -0.74 |

# Design after optimizing row 5

Determinant = 16.777

| WP | SP | X1 | X2 | X3 |
|---|---|---|---|---|
| 1 | 1 | -1.00 | 1.00 | -1.00 |
| 1 | 1 | -1.00 | 1.00 | 1.00 |
| 1 | 2 | -1.00 | -1.00 | 1.00 |
| 1 | 2 | -1.00 | -1.00 | -1.00 |
| 2 | 3 | 1.00 | 1.00 | -1.00 |
| 2 | 3 | 1.00 | 1.00 | 0.49 |
| 2 | 4 | 1.00 | -0.87 | -0.74 |
| 2 | 4 | 1.00 | -0.87 | -0.74 |

# Design after optimizing row 6

Determinant = 19.86

| WP | SP | X1 | X2 | X3 |
|---|---|---|---|---|
| 1 | 1 | -1.00 | 1.00 | -1.00 |
| 1 | 1 | -1.00 | 1.00 | 1.00 |
| 1 | 2 | -1.00 | -1.00 | 1.00 |
| 1 | 2 | -1.00 | -1.00 | -1.00 |
| 2 | 3 | 1.00 | 1.00 | -1.00 |
| 2 | 3 | 1.00 | 1.00 | 1.00 |
| 2 | 4 | 1.00 | -0.87 | -0.74 |
| 2 | 4 | 1.00 | -0.87 | -0.74 |

# Design after optimizing row 7

Determinant = 26.19

| WP | SP | X1 | X2 | X3 |
|---|---|---|---|---|
| 1 | 1 | -1 | 1 | -1 |
| 1 | 1 | -1 | 1 | 1 |
| 1 | 2 | -1 | -1 | 1 |
| 1 | 2 | -1 | -1 | -1 |
| 2 | 3 | 1 | 1 | -1 |
| 2 | 3 | 1 | 1 | 1 |
| 2 | 4 | 1 | -1 | 1 |
| 2 | 4 | 1 | -1 | -0.74 |

# Final Design

Determinant = 27.86

| WP | SP | X1 | X2 | X3 |
|---|---|---|---|---|
| 1 | 1 | -1 | 1 | -1 |
| 1 | 1 | -1 | 1 | 1 |
| 1 | 2 | -1 | -1 | 1 |
| 1 | 2 | -1 | -1 | -1 |
| 2 | 3 | 1 | 1 | -1 |
| 2 | 3 | 1 | 1 | 1 |
| 2 | 4 | 1 | -1 | 1 |
| 2 | 4 | 1 | -1 | -1 |

# Proof-of-concept example

- 2 hard-to-change or whole-plot factors $w_1$ and $w_2$
- 5 easy-to-change or sub-plot factors $s_1$-$s_5$

| Whole plot | $w_1$ | $w_2$ | $s_1$ | $s_2$ | $s_3$ | $s_4$ | $s_5$ |
|---|---|---|---|---|---|---|---|
| 1 | 1 | 1 | 1 | −1 | 1 | 1 | 1 |
| 1 | 1 | 1 | −1 | −1 | −1 | −1 | −1 |
| 1 | 1 | 1 | −1 | 1 | 1 | −1 | 1 |
| 2 | −1 | 1 | 1 | −1 | 1 | −1 | −1 |
| 2 | −1 | 1 | −1 | 1 | 1 | −1 | 1 |
| 2 | −1 | 1 | 1 | 1 | −1 | 1 | −1 |
| 3 | 1 | −1 | 1 | −1 | −1 | 1 | 1 |
| 3 | 1 | −1 | 1 | 1 | −1 | −1 | −1 |
| 3 | 1 | −1 | −1 | −1 | 1 | −1 | −1 |
| 4 | −1 | −1 | −1 | −1 | 1 | 1 | −1 |
| 4 | −1 | −1 | −1 | −1 | −1 | 1 | −1 |
| 4 | −1 | −1 | 1 | 1 | 1 | −1 | 1 |
| 5 | 1 | 1 | −1 | 1 | −1 | −1 | −1 |
| 5 | 1 | 1 | −1 | 1 | −1 | 1 | 1 |
| 5 | 1 | 1 | 1 | −1 | 1 | 1 | −1 |
| 6 | −1 | 1 | 1 | 1 | 1 | 1 | −1 |
| 6 | −1 | 1 | 1 | −1 | −1 | −1 | 1 |
| 6 | −1 | 1 | −1 | −1 | −1 | 1 | 1 |
| 7 | 1 | −1 | 1 | 1 | 1 | 1 | 1 |
| 7 | 1 | −1 | 1 | −1 | −1 | −1 | 1 |
| 7 | 1 | −1 | −1 | 1 | 1 | 1 | −1 |
| 8 | −1 | −1 | −1 | −1 | 1 | −1 | 1 |
| 8 | −1 | −1 | 1 | 1 | −1 | −1 | −1 |
| 8 | −1 | −1 | −1 | 1 | −1 | 1 | 1 |

# Diagonal information matrix

| $I$ | $w_1$ | $w_2$ | $s_1$ | $s_2$ | $s_3$ | $s_4$ | $s_5$ |
|---|---|---|---|---|---|---|---|
| 6 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 6 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 6 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 22 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 22 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 22 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 22 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 22 |

# D-Optimal Design Stage 1

| *Whole plot* | $w_1$ | $w_2$ | $w_3$ | $w_4$ | $w_5$ | $w_6$ | $w_7$ |
|---|---|---|---|---|---|---|---|
| 1 | 1 | −1 | −1 | −1 | 1 | 1 | −1 |
| 2 | 1 | −1 | 1 | −1 | 1 | −1 | 1 |
| 3 | −1 | 1 | −1 | −1 | 1 | 1 | −1 |
| 4 | −1 | −1 | −1 | 1 | 1 | 1 | 1 |
| 5 | −1 | 1 | 1 | −1 | −1 | −1 | 1 |
| 6 | −1 | −1 | −1 | 1 | −1 | 1 | −1 |
| 7 | −1 | −1 | 1 | −1 | 1 | −1 | −1 |
| 8 | 1 | 1 | −1 | 1 | 1 | −1 | −1 |
| 9 | 1 | 1 | 1 | −1 | 1 | 1 | 1 |
| 10 | −1 | 1 | −1 | 1 | 1 | −1 | −1 |
| 11 | 1 | −1 | −1 | −1 | 1 | −1 | 1 |
| 12 | −1 | −1 | 1 | −1 | −1 | 1 | −1 |
| 13 | 1 | −1 | 1 | −1 | −1 | −1 | −1 |
| 14 | 1 | 1 | −1 | −1 | −1 | 1 | 1 |
| 15 | −1 | 1 | −1 | 1 | −1 | −1 | 1 |
| 16 | 1 | 1 | 1 | −1 | −1 | 1 | −1 |
| 17 | 1 | −1 | −1 | 1 | −1 | 1 | 1 |
| 18 | −1 | −1 | −1 | −1 | −1 | −1 | 1 |
| 19 | 1 | 1 | −1 | −1 | −1 | −1 | −1 |
| 20 | −1 | 1 | 1 | −1 | 1 | 1 | 1 |

# D-optimal Design Stage 2

| Whole plot | $s_1$ | $s_2$ | $s_3$ | $s_4$ | Whole plot | $s_1$ | $s_2$ | $s_3$ | $s_4$ |
|---|---|---|---|---|---|---|---|---|---|
| 1 | −1 | 1 | −1 | C | 11 | 1 | 1 | 1 | B |
| 1 | 1 | −1 | 1 | C | 11 | 1 | 1 | −1 | A |
| 1 | −1 | −1 | −1 | A | 11 | −1 | −1 | −0.1 | B |
| 1 | 0.1 | 1 | 1 | A | 11 | −1 | 1 | 1 | C |
| 1 | 1 | −1 | −1 | B | 11 | 1 | −1 | −1 | C |
| 2 | 1 | 1 | 0.2 | C | 12 | 1 | 1 | 1 | B |
| 2 | −1 | 1 | 1 | B | 12 | 1 | 1 | −1 | A |
| 2 | 1 | −1 | −1 | B | 12 | 1 | −1 | 1 | C |
| 2 | −1 | −1 | 1 | A | 12 | −0.1 | −1 | −1 | B |
| 2 | −1 | 1 | −1 | A | 12 | −1 | −0.3 | 1 | A |
| 3 | −1 | −1 | 1 | A | 13 | 1 | −0.2 | 1 | B |
| 3 | −1 | −1 | −1 | C | 13 | −1 | 1 | 1 | C |
| 3 | −1 | 1 | 1 | B | 13 | −1 | 1 | −1 | B |
| 3 | 1 | 1 | −1 | A | 13 | 0.1 | −1 | 0 | A |
| 3 | 1 | 1 | 1 | C | 13 | 1 | 1 | −1 | C |
| 4 | 1 | 0 | 0.3 | B | 14 | −1 | 1 | 0.2 | A |
| 4 | −1 | −1 | 1 | C | 14 | 1 | 1 | 1 | C |
| 4 | −0.1 | −1 | −1 | A | 14 | 0.1 | −1 | 1 | B |
| 4 | −1 | 1 | 1 | A | 14 | 1 | −1 | −1 | C |
| 4 | 1 | 1 | −1 | C | 14 | −1 | 0 | −1 | B |
| 5 | −1 | 1 | −1 | C | 15 | −1 | 1 | 1 | B |

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# Algorithms

- Simultaneous optimization of whole-plot, sub-plot and sub-sub-plot factors' levels
  - The candidate-set-free or coordinate-exchange algorithm's computing time does not increase exponentially with the number of factors
  - This is unlike the point-exchange algorithm which requires a candidate set
- Trinca & Gilmour (Technometrics, 2001) sequentially optimize the whole-plot, sub-plot and sub-sub-plot factors' levels
- Trinca & Gilmour (Technometrics, 2015) present an improved version and beat the design of Jones & Goos (2007) by 1%

# Discussion and recent developments

# Discussion

- Using the principles of optimal experimental design, it is possible to conduct experiments to study many factors
- Optimal experimental design also works for split-plot and split-split-plot experiments
  - Useful whenever there are hard- or very-hard-to-change factors
  - Useful whenever experiments span multiple steps of a production process
- Which algorithm you use for seeking optimal experimental designs is of secondary importance
- Do not be afraid to leave the well-paved path of orthogonal 2-level designs if necessary

# Recent developments

- Increasingly, Bayesian approaches are used to cope with the uncertainty about the variance components
- A composite criterion has been proposed to account for the fact that a proper analysis of split-plot and split-split-plot data requires estimating the variance components too
- A lack-of-fit test has been proposed for split-plot and split-split-plot data based on pure error estimates of the variance components
- A local search algorithm has been presented to simultaneously search for D- and I-optimal designs

# References


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Thank you for your attention !

# Optimal design: getting more out of experiments with hard-to-change factors

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