Optimal design of experiments

Session 3: Basics of optimal design

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Optimal design

- plan experiments so that they contain as much information as possible
- several approaches are possible to maximize amount of information
- we start with "intuitive" approach
- several small examples
- Microsoft Excel, as in Goos & Leemans (2004) (see outprint)

Strengths of optimal design

- can be done for any number of observations n
- can be done for any number of experimental variables m
- can be done for any degree of the model: first-order, second-order, ...
- can cope with constraints on the design region (see freeze-drying experiment in Session 4)

Strengths of optimal design

- can cope with quantitative *and* qualitative variables at same time
- flexibility: it allows the researcher to create a tailor-made design
- can be used when
  - heterogeneous variance
  - correlated observations
  - blocked experiments
  - split-plot experiments
  - nonlinear models

Selling point of optimal design

Optimal design of experiments helps you to construct the design that best fits your problem.

Weaknesses of optimal design

- depend on assumed model
- no replication
- not always nice and symmetric
- sometimes strange, exotic factor levels
- several criteria can be used for computing optimal designs
- optimal design requires computational effort

Computation of optimal designs

→ difficult

→ specialized software

- SAS `proc optex`
- JMP
- Design Expert
- Minitab
- ...

→ for nonstandard problems, you have to program your own software (correlated observations, nonlinear models)

Requirements of good design

(Box & Draper, 1971)

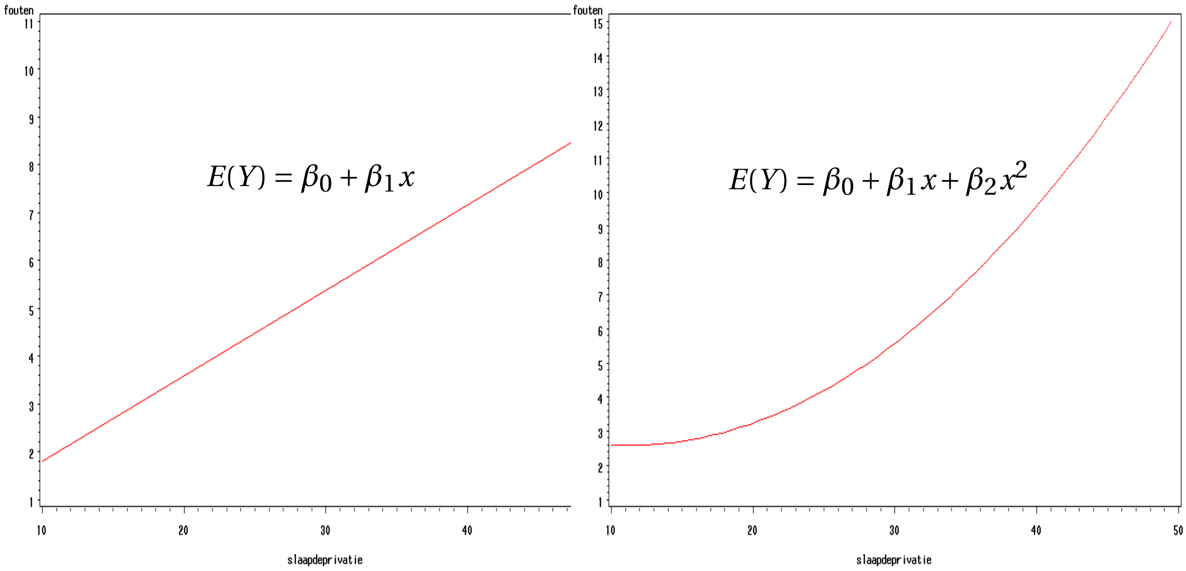
1. Generate a satisfactory distribution of information throughout the region of interest.
2. Ensure that the fitted values are as close as possible to the true values of the response.
3. Allow detection of lack-of-fit.
4. Allow estimation of transformations of both the response and the quantitative experimental factors.
5. Allow blocked experiments.
6. Allow designs to be built up sequentially.

7. Provide an estimate of error from replication.
8. Be insensitive to wild observations and to violation of normality assumptions.
9. Require a minimum of experimental runs.
10. Provide simple data patterns and allow visual appreciation.
11. Ensure simplicity of calculation.
12. Behave well when errors occur in the settings of the explanatory variables.

Example

- relationship between the amount of sleep deprivation and the number of mistakes made in a test
- 6 test persons
- between 12 and 48 hours of sleep deprivation
- how many hours of sleep deprivation for each test person?
  - 12, 19.2, 26.4, 33.6, 40.8, 48 hours?
  - 12, 12, 30, 30, 48, 48 hours?
  - ...

Expected effect?



Linear model

$$Y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \epsilon \text{ with } \mathbf{X} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_6 \end{bmatrix} \text{ and } \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}$$

assumptions:

- $\epsilon_i \sim N(0, \sigma^2)$
- independence of ϵ_i and ϵ_j

Ordinary least squares

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

$$\begin{aligned}\text{var}(\hat{\beta}) &= \sigma^2(\mathbf{X}^T\mathbf{X})^{-1} \\ &= \begin{bmatrix} \text{var}(\hat{\beta}_0) & \text{cov}(\hat{\beta}_0,\hat{\beta}_1) \\ \text{cov}(\hat{\beta}_0,\hat{\beta}_1) & \text{var}(\hat{\beta}_1) \end{bmatrix}\end{aligned}$$

- see `psycho.xls` (linear model)

Quadratic model

$Y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \epsilon_i$

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \epsilon \text{ with } \mathbf{X} = \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ \vdots & \vdots & \vdots \\ 1 & x_6 & x_6^2 \end{bmatrix} \text{ and } \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}$$

assumptions:

- $\epsilon_i \sim N(0, \sigma^2)$
- independence of ϵ_i and ϵ_j

Ordinary least squares

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- see `psycho.xls` (quadratic model)