On Optimal Design in Random Coefficient Regression Models and Alike

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Outline

Prologue: Examples

1. RCR Model

2. Design Issues

3. Random Intercept

4. Random Slope

5. Several Treatments

Epilogue: Messages

Prologue: Why Population Parameters?

- Example 1: neural science

social

"education" on

ical spines / μm)

ed measures

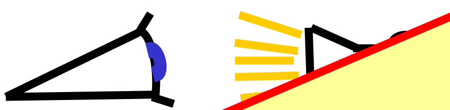
But:

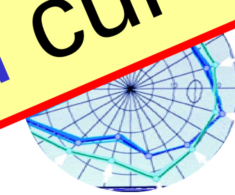
Each individual has its own mean!

octodon degus

Why Population Parameters?

- Example 2: perimetry

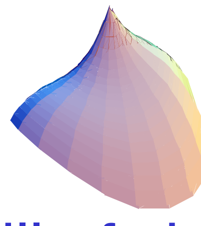




retina

…ues for the visual
…y in decibel luminescence)

- …al diagnostics



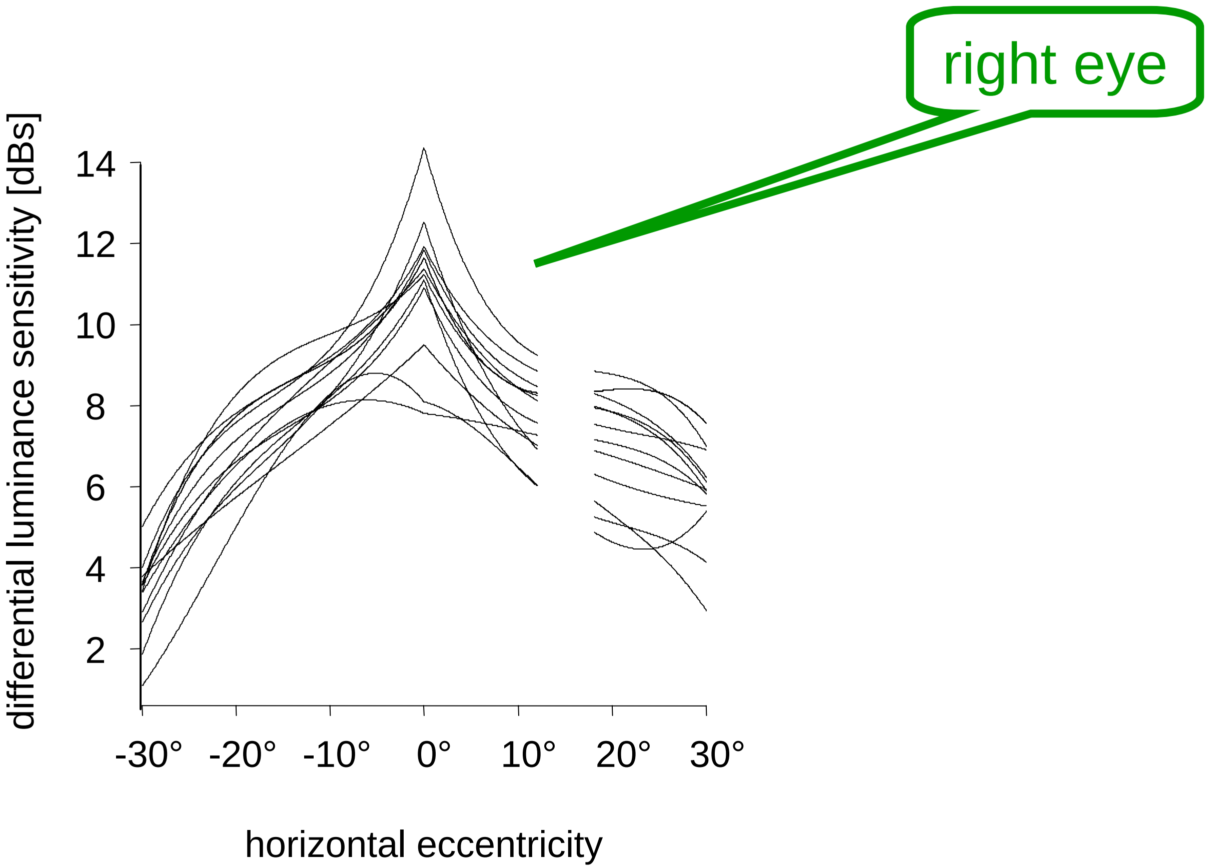
hill of vision

But:
Each individual has its own curve!

Example 2: perimetry

individual hills of vision:

age: 30 - 40



1. RCR Model

- Example: individual regression lines

$$Y_{ij} = a_i + b_i x_{ij} + \varepsilon_{ij}$$

individual $i=1,\ldots,n$

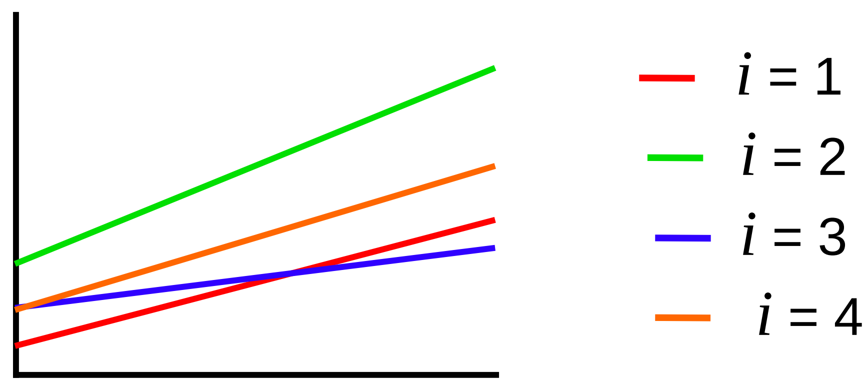
replication $j=1,\ldots,m_i$

explanatory variable

error

$$\varepsilon_{ij} \sim N(0,\sigma^2)$$

- individual curves:



1. RCR Model

- Example: individual regression lines

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individual $i=1,\dots,n$

replication $j=1,\dots,m_i$

explanatory variable

error

$$\varepsilon_{ij} \sim N(0, \sigma^2)$$

- individual parameters:

population parameters

$$\begin{pmatrix} a_i \\ b_i \end{pmatrix} \sim N\left(\begin{pmatrix} \mu \\ \beta \end{pmatrix}, \sigma^2 \begin{pmatrix} d_\mu & d_{\mu\beta} \\ d_{\mu\beta} & d_\beta \end{pmatrix} \right)$$

Random Coefficient Model

- individual curves are given by a common linear model

$$Y_{ij} = a_i + f(x_{ij})^\top b_i + \varepsilon_{ij}$$

$$\varepsilon_{ij} \sim N(0, \sigma^2)$$

independent

- individual parameters: $(a_i, b_i) \sim N((\mu, \beta), \sigma^2 D)$

population parameters

Individual Observation Vector

$$Y_i = \begin{pmatrix} Y_{i1} \\ \vdots \\ Y_{im_i} \end{pmatrix} = F_i \begin{pmatrix} \mu \\ \beta \end{pmatrix} + F_i \begin{pmatrix} a_i - \mu \\ b_i - \beta \end{pmatrix} + \varepsilon_i$$

θ

- individual design matrix

$$F_i = \begin{pmatrix} 1 & f(x_{i1})^\top \\ \vdots & \vdots \\ 1 & f(x_{im_i})^\top \end{pmatrix}$$

Individual Covariance Matrix

$$\mathrm{Cov}(Y_i) = \sigma^2 V_i$$

where

$$V_i = I_{m_i} + F_i D F_i^{\top}$$

example:
random intercept

$$D = \begin{pmatrix} d_\mu & 0 \\ 0 & 0 \end{pmatrix}$$

$$V_i = I_{m_i} + d_\mu \mathbf{1}_{m_i} \mathbf{1}_{m_i}^{\top}$$

Estimation of Population Parameters

general least squares

$$\hat{\theta} = \left(\sum_{i=1}^{n} F_i^{\top} V_i^{-1} F_i\right)^{-1} \sum_{i=1}^{n} F_i^{\top} V_i^{-1} F_i \hat{\theta}_i$$

- individual “estimates”

independent of D

$$\hat{\theta}_i = \left(F_i^{\top} V_i^{-1} F_i\right)^{-1} F_i^{\top} V_i^{-1} Y_i = \left(F_i^{\top} F_i\right)^{-1} F_i^{\top} Y_i$$

- covariance matrix

depends on D, in general

$$\mathrm{Cov}(\hat{\theta}) = \sigma^2 \left(\sum_{i=1}^{n} F_i^{\top} V_i^{-1} F_i\right)^{-1}$$

2. Design Issues

- all individuals under the same regime:

$$m_i \equiv m$$
$$x_{ij} \equiv x_j$$

uniform design

$$F_i \equiv F_1,\ V_i \equiv V_1$$

- estimation: mean of individual estimates

$$\hat{\theta} = \frac{1}{n}\sum_{i=1}^{n} \hat{\theta}_i$$

- does not require the knowledge of D (WLS=OLS)

Covariance in Uniform Designs

$$\mathrm{Cov}(\hat{\theta}) = \frac{\sigma^2}{n}\left(F_1^{\top} V_1^{-1} F_1\right)^{-1}$$

$$= \frac{\sigma^2}{n}\left(\left(F_1^{\top} F_1\right)^{-1} + D\right)$$

covariance in the model without random effects:

$$Y_{ij} = \mu + f(x_{ij})^{\top}\beta + \varepsilon_{ij} \qquad (D = 0)$$

Optimal Uniform Designs

- How to choose $x_1, \ldots, x_m$?

- quality measured in terms of the standardised covariance:

$$\left(F_1^\top F_1\right)^{-1} + D$$

Uniform designs are optimal !

weighted generalised designs

Schmelter (2004)

Linear Criteria

- minimize

A, IMSE, c

$$\operatorname{trace}\left(L \left(\left(F_1^\top F_1 \right)^{-1} + D \right) L^\top \right)$$

$$= \operatorname{trace}\left(L \left(F_1^\top F_1 \right)^{-1} L^\top \right) + \underbrace{\operatorname{trace}\left(L D L^\top \right)}_{\text{constant !}}$$

- result

Luoma (2000), Liski et al. (2002)

$(x_1, \ldots, x_m)$ optimal in reduced model

$\Rightarrow$

$(x_1, \ldots, x_m)$ optimal in mixed model

D- and G-criteria

- minimize

$$\det\left(\left(F_1^\top F_1\right)^{-1} + D\right)$$

D-criterion

$$\neq \det\left(\left(F_1^\top F_1\right)^{-1}\right) + \det(D)$$

- resp.

$$\sup_x\left(f(x)^\top\left(\left(F_1^\top F_1\right)^{-1} + D\right)f(x)\right)$$

G-criterion

$$\leq \sup_x\left(f(x)^\top\left(F_1^\top F_1\right)^{-1} f(x)\right) + \sup_x\left(f(x)^\top D f(x)\right)$$

- optimal designs may differ !

3. Random Intercept

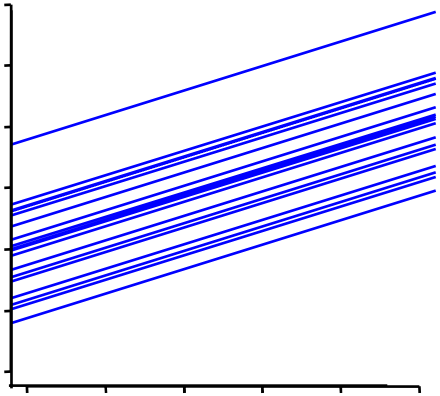
- parallel individual curves

$$Y_{ij} = a_i + f(x_{ij})^\top \beta + \varepsilon_{ij}$$

$$D = \begin{pmatrix} d & 0 \\ 0 & 0 \end{pmatrix}$$

- example: parallel lines

$$Y_{ij} = a_i + \beta x_{ij} + \varepsilon_{ij}$$



Three Models

- no individual effect

$$Y_{ij} = \mu + f(x_{ij})^\top \beta + \ldots$$

no block ...

- random intercept ...

$$Y_{ij} = a_i + \ldots + \varepsilon_{ij}$$

... block effects

- fix... ...al intercept

$$\ldots a_i + f(x_{ij})^\top \beta + \varepsilon_{ij}$$

fixed block effects

$$\mathrm{Info}_d(\beta) = \frac{1}{1+md}\,\mathrm{Info}_0(\beta) + \frac{md}{1+md}\,\mathrm{Info}_\infty(\beta)$$

$\mathrm{Info}_0(\beta)$

↑ $d \to 0$

$\mathrm{Info}_d(\beta)$

↓ $d \to \infty$

$\mathrm{Info}_\infty(\beta)$

Uniform Design

$$\mathrm{Info}_\infty(\beta) = \mathrm{Info}_0(\beta) = \mathrm{Info}_d(\beta)$$

- G- and D-optimal designs

  do not depend on $d = d_\mu$

  resp. on the intra individual correlation $\gamma = \frac{d}{1+d}$

4. Random Slope

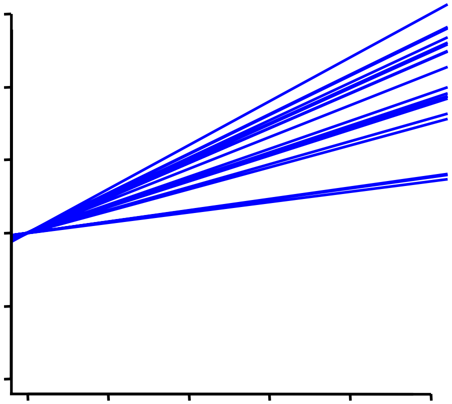
- common intercept

$$Y_{ij} = \mu + b_i x_{ij} + \varepsilon_{ij}$$

$$D = \begin{pmatrix} 0 & 0 \\ 0 & d \end{pmatrix}$$

- standard interval

$$0 \le x_{ij} \le 1$$



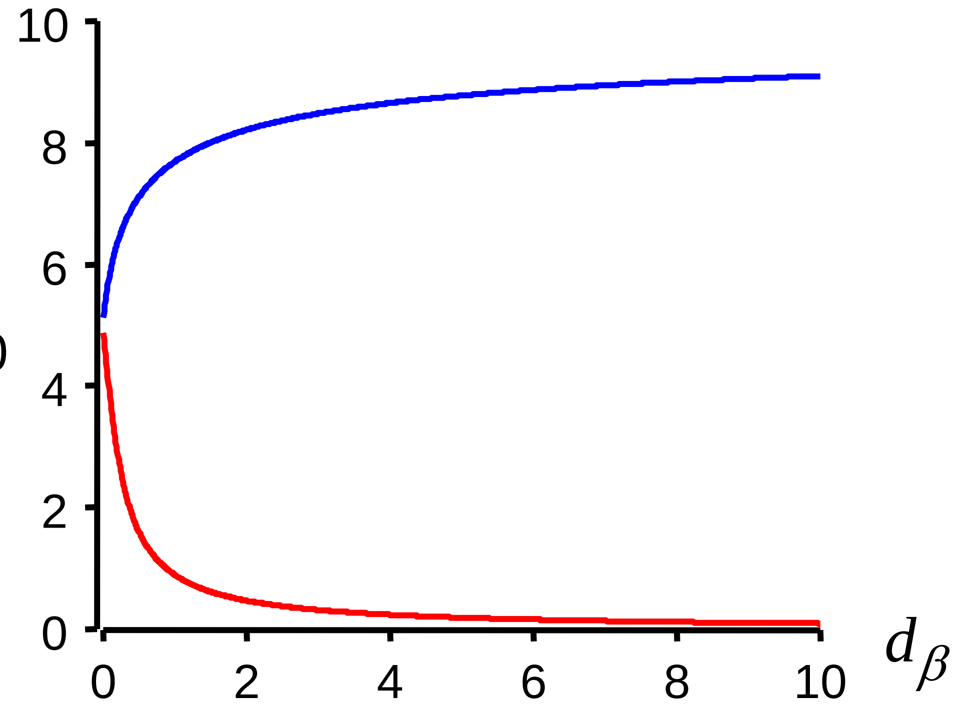
Uniform Design

- G- and D-optimal designs
  depend on the variance ratio $d = d_\beta$

$m = 10$

optimal frequency
m_0 in design point 0

$m_1 = m - m_0$



Uniform Design

- G- and D-optimal designs

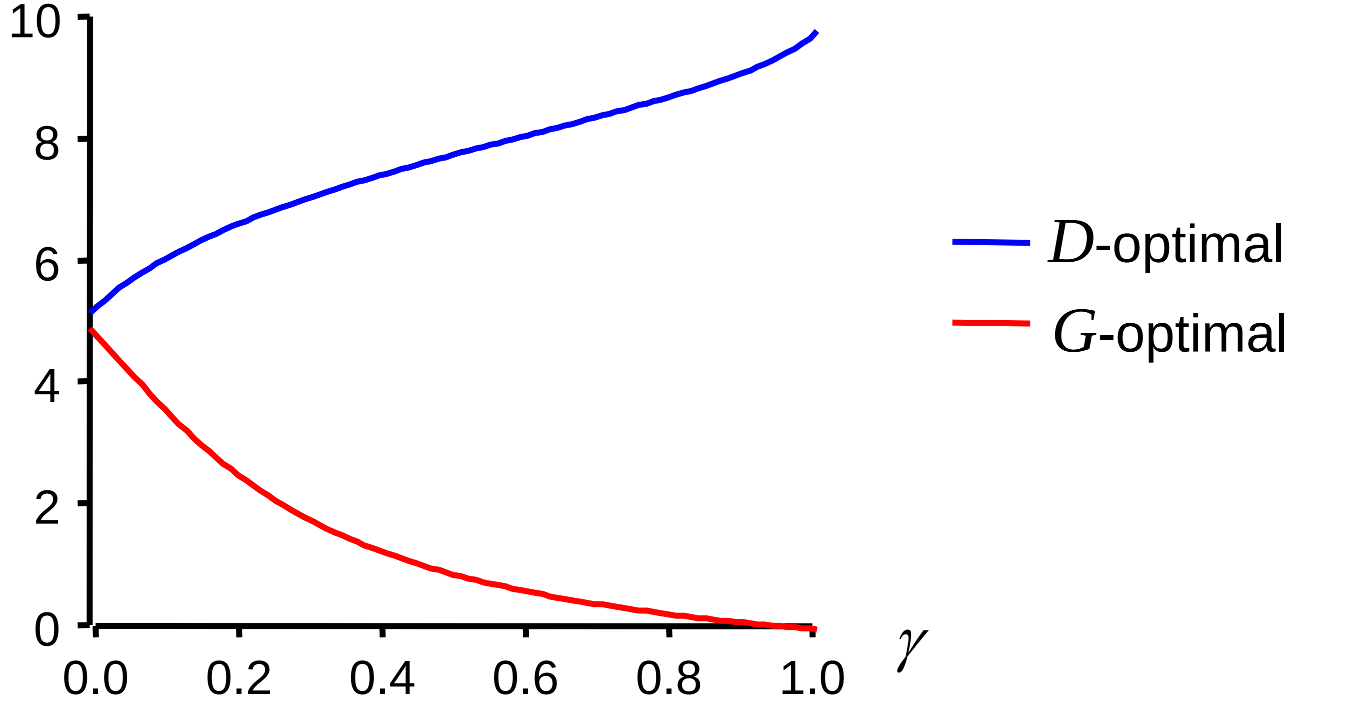
depend on the “intra individual correlation” $\gamma = \frac{d}{1+d}$

$m = 10$

optimal frequency

m_0 in design point 0

$m_1 = m - m_0$

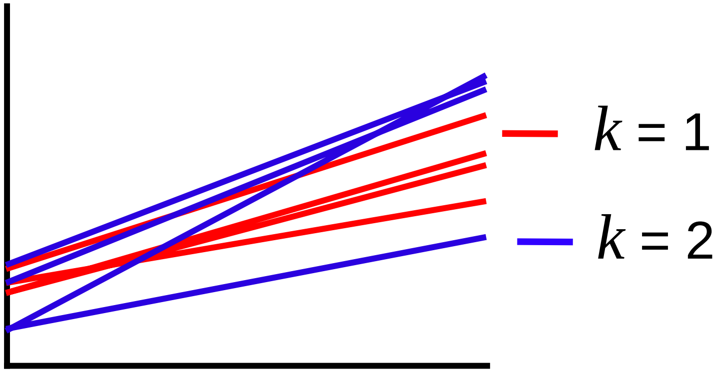


5. Several Treatments

- individuals nested in 2 groups $k = 1,2$

$$Y_{kij} = a_{ki} + b_{ki} x_{kij} + \varepsilon_{kij} \qquad i = 1, \ldots, n_k$$

- linear regression, common intercept



$$\begin{pmatrix} a_{ki} \\ b_{ki} \end{pmatrix} \sim N\left(\begin{pmatrix} \mu \\ \beta_k \end{pmatrix}, \sigma^2 \begin{pmatrix} d_\mu & d_{\mu\beta} \\ d_{\mu\beta} & d_\beta \end{pmatrix} \right)$$

Random Intercept

- linear regression, 2 groups, common intercept

$$Y_{kij} = a_{ki} + \beta_k x_{kij} + \varepsilon_{kij}$$

D-opt $= D_\beta$-opt

$d \to 0$:

$$Y_{kij} = \mu + \beta_k x_{kij} + \varepsilon_{kij}$$

D-opt $= D_\beta$-opt

$d \to \infty$:

$$Y_{kij} = \mu_{ki} + \beta_i x_{kij} + \varepsilon_{kij}$$

D-opt $\neq D_\beta$-opt

Uniform Designs are Optimal

(in the setting of generalised designs)

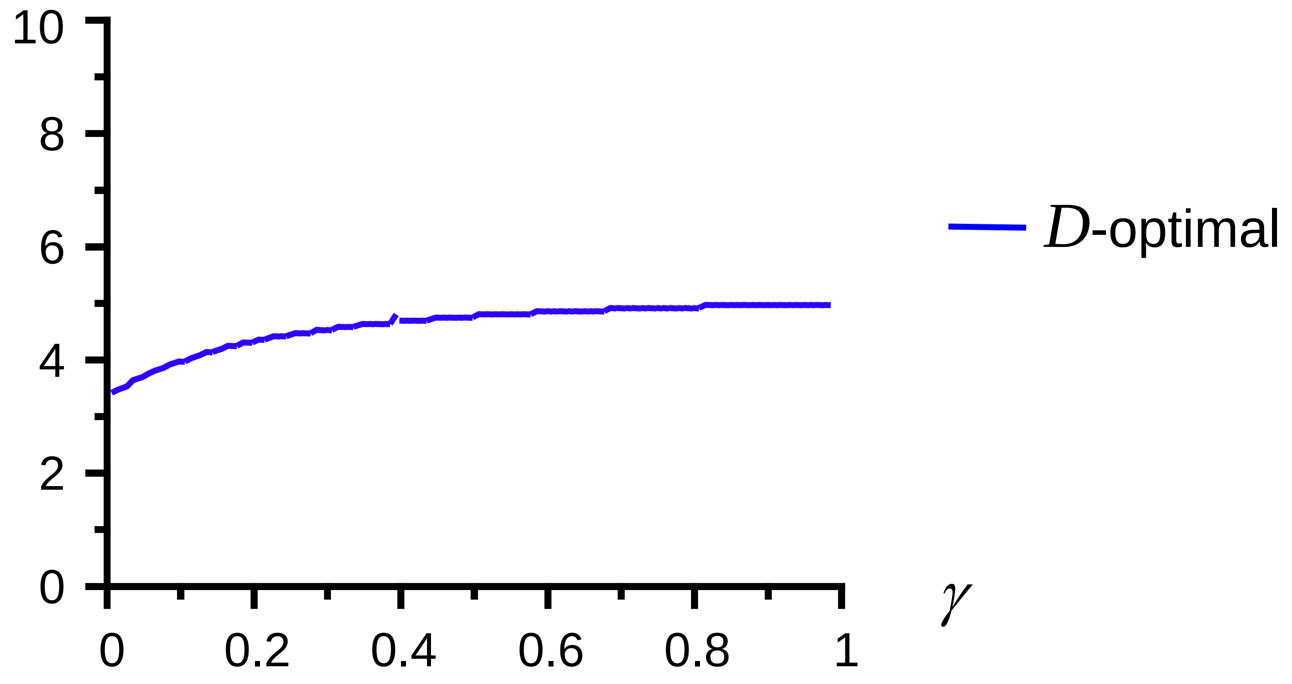
Schmelter (2005)

- D-optimal designs depend on $d = d_\mu$ resp. γ

m = 10

optimal frequency

m_0 in design point 0



$m_1 = m - m_0$

Epilogue: Messages

- random intercept

Standard designs are suitable !

- random slope

Don‘t do D- or G-optimality !