Optimal Designs for Prediction in Random Coefficient Regression with One Observation per Individual

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Model-Oriented Data Analysis and Optimum Design

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Contents

Motivation

- RCR model with
  - n observational units (individuals)
  - ***One*** observation per unit
- OD for prediction of ***random effects***
- Earlier works
  - P. & Schwabe (2016), etc.:
    number of observations $\geq$ ***number of parameters***
  - Graßhoff et al. (2012):
    OD for ***fixed effects***

RCR model with one observation per individual

$$Y_i = \mathbf{f}(x_i)^\top \boldsymbol{\beta}_i + \varepsilon_i, \qquad i = 1, .., n, \qquad x_i \in \mathcal{X}$$

- $\mathbf{f} = (f_1, .., f_p)^\top$
- $\boldsymbol{\beta}_i = (\beta_{i1}, .., \beta_{ip})^\top$ *random*
  - $\mathrm{E}(\boldsymbol{\beta}_i) = \boldsymbol{\beta}_0$ *unknown*
  - $\mathrm{Cov}(\boldsymbol{\beta}_i) = \sigma^2\mathbf{D}$, $\mathbf{D}$ *known*, *non-singular*
- $\mathrm{E}(\varepsilon_i) = 0$, $\mathrm{Var}(\varepsilon_i) = \sigma^2$
- *All* $\boldsymbol{\beta}_i$ *and all* $\varepsilon_{i'}$ *uncorrelated*

Graßhoff et al. (2012): OD for estimation of $\boldsymbol{\beta}_0$

This work: *OD for prediction of* $\mathbf{b}_i = \boldsymbol{\beta}_i - \boldsymbol{\beta}_0$

MSE for prediction of individual effects

Main interest - k selected individuals, $k \in [p, n-p]$

$\rightarrow$ OD for prediction of $\mathbf{\Psi} = \frac{1}{k}\sum_{i=1}^{k} \mathbf{b}_i$

MSE of BLUP $\hat{\mathbf{\Psi}}$ for $\mathbf{\Psi}$:

$$\mathrm{Cov}(\hat{\mathbf{\Psi}} - \mathbf{\Psi}) = \sigma^2 \left(\frac{1}{k}\mathbf{D} - \frac{1}{k^2}\mathbf{D}\mathbf{M}_k\mathbf{D} + \frac{1}{k^2}\mathbf{D}\mathbf{M}_k\mathbf{M}^{-1}\mathbf{M}_k\mathbf{D} \right)$$

$$\mathbf{M} = \sum_{i=1}^{n} \mathbf{M}(x_i) \quad \& \quad \mathbf{M}_k = \sum_{i=1}^{k} \mathbf{M}(x_i)$$

$$\mathbf{M}(x_i) = \mathbf{g}(x_i)\mathbf{g}(x_i)^\top \quad \& \quad \mathbf{g}(x_i) = \frac{\mathbf{f}(x_i)}{\sqrt{\mathbf{f}(x_i)^\top \mathbf{D}\mathbf{f}(x_i) + 1}}$$

Two groups of individuals

Group 1 Group 2

k selected individuals & $n-k$ remaining ind.

Design regions

$\mathcal{X}_1$ & $\mathcal{X}_2$

$$\mathcal{X}_1 \cap \mathcal{X}_2 = \mathcal{X}$$

$\mathcal{X}_1 = \mathcal{X}_2 = \mathcal{X}$ - particular case

Group designs

Exact designs

Group 1   Group 2

$$\xi_{1,e} = \begin{pmatrix} x_{11}, \dots, x_{1N_1} \\ m_{11}, \dots, m_{1N_1} \end{pmatrix} \quad \& \quad \xi_{2,e} = \begin{pmatrix} x_{21}, \dots, x_{2N_2} \\ m_{21}, \dots, m_{2N_2} \end{pmatrix}$$

$x_{1j} \in \mathcal{X}_1$ support of $\xi_{1,e}$ & $x_{2j} \in \mathcal{X}_2$ support of $\xi_{2,e}$

$\sum_{j=1}^{N_1} m_{1j} = k$ & $\sum_{j=1}^{N_2} m_{2j} = n - k$

$N_1 = |\{x_{11}, \dots, x_{1N_1}\}|$ & $N_2 = |\{x_{21}, \dots, x_{2N_2}\}|$

Group designs

Approximate designs

Group 1 & **Group 2**

$$\xi_1 = \begin{pmatrix} x_{11}, \ldots, x_{1\tilde{N}_1} \\ w_{11}, \ldots, w_{1\tilde{N}_1} \end{pmatrix} \quad \& \quad \xi_2 = \begin{pmatrix} x_{21}, \ldots, x_{2\tilde{N}_2} \\ w_{21}, \ldots, w_{2\tilde{N}_2} \end{pmatrix}$$

$$\sum_{j=1}^{\tilde{N}_1} w_{1j} = 1,\ \tilde{N}_1 = |\{x_{11}, \ldots, x_{1\tilde{N}_1}\}| \quad \& \quad \sum_{j=1}^{\tilde{N}_2} w_{2j} = 1,\ \tilde{N}_2 = |\{x_{21}, \ldots, x_{2\tilde{N}_2}\}|$$

Information matrices

$$\mathbf{M}_{1,\xi} = \sum_{j=1}^{\tilde{N}_1} w_{1j}\mathbf{M}(x_{1j}) \quad \& \quad \mathbf{M}_{2,\xi} = \sum_{j=1}^{\tilde{N}_2} w_{2j}\mathbf{M}(x_{2j})$$

For exact designs: $\mathbf{M}_k = k\mathbf{M}_{1,\xi} \quad \& \quad \mathbf{M} = k\mathbf{M}_{1,\xi} + (n-k)\mathbf{M}_{2,\xi}$

$$w_{1j} = m_{1j}/k \quad \& \quad w_{2j} = m_{2j}/(n-k) \quad \& \quad \tilde{N}_\ell = N_\ell,\ \ell = 1, 2$$

Linear criterion

L-criterion for prediction of $\boldsymbol{\Psi}$:

$$\Phi_L = \mathrm{tr}\left(\mathrm{Cov}(\mathcal{L}\hat{\boldsymbol{\Psi}} - \mathcal{L}\boldsymbol{\Psi})\right)$$

For approximate designs

$$\Phi_L(\xi) = -\mathrm{tr}\left[\tilde{\mathbf{L}}\left(\frac{1}{k}\mathbf{M}_{1,\xi}^{-1} + \frac{1}{n-k}\mathbf{M}_{2,\xi}^{-1}\right)^{-1}\right]$$

$$\tilde{\mathbf{L}} = \mathbf{DLD} \quad \& \quad \mathbf{L} = \mathcal{L}^\top\mathcal{L}$$

The L-criterion is convex with respect to $(\mathbf{M}_{1,\xi}, \mathbf{M}_{2,\xi})$

Optimality condition

Design criterion

$\Downarrow$

Equivalence theorem for multiple-design problems [1]

$\Downarrow$

Optimality condition

[1] see P. (2022)

Linear criterion: The same design in both groups

If $\mathcal{X}_1 = \mathcal{X}_2 = \mathcal{X}$

Design with $\xi_1 = \xi_2$ ***may be*** *optimal*

L-criterion:

$$\Phi_L(\xi) = -\mathrm{tr}\left[\tilde{\mathbf{L}}\mathbf{M}_{1,\xi}\right]$$

Optimality condition:

$$\mathbf{g}(x)^\top \tilde{\mathbf{L}}\mathbf{g}(x) \leq \mathrm{tr}\left(\tilde{\mathbf{L}}\mathbf{M}_{1,\xi^*}\right), \quad \forall x \in \mathcal{X}$$

$\Rightarrow$

1) All designs with $\xi_1 = \xi_2$ optimal
2) Singular design optimal
3) No optimal designs with $\xi_1 = \xi_2$

Examples: Straight line regression

$$Y_i = \beta_{i1} + \beta_{i2} x_i + \varepsilon_i$$

- $\mathbf{f}(x) = (1, x)^\top$
- $\mathbf{D} = \mathrm{diag}(d_1, d_2)$
- *A*-criterion: $\mathbf{L} = \mathbb{I}_p$

Examples:

- Example 1: The same design region in both groups
- Example 2: Different design regions

Example 1: The same design region in both groups

$$Y_i = \beta_{i1} + \beta_{i2} x_i + \varepsilon_i$$

- $\mathcal{X}_1 = \mathcal{X}_2 = [-a, a], \ a > 0$
- $\xi_1 = \xi_2$
- All observations at endpoints: $-a$ & a

Designs:

$$\xi_1 = \begin{pmatrix} -a & a \\ 1 - w & w \end{pmatrix}$$

Example 1: The same design region in both groups

A-criterion:

$$\Phi_A(\xi) = -\frac{d_2 a^2 + d_1^2}{d_2 a^2 + d_1 + 1}$$

Ind. of designs

Optimality condition satisfied

$$\Updownarrow$$

$$\{d_2 \geq \frac{d_1^2}{d_1 + 1}\} \cup \{d_2 = 0\}$$

$$\Updownarrow$$

All $w \in [0, 1]$ optimal

Otherwise, no optimal endpoints designs with $\xi_1 = \xi_2$

Example 2: Different design regions

$$Y_i = \beta_{i1} + \beta_{i2} x_i + \varepsilon_i$$

- $\mathcal{X}_1 = [-1, 1] \quad \& \quad \mathcal{X}_2 = [-a, a], \; a > 0$
- All observations at endpoints: $\;-1 \;\; \& \;\; 1 \quad$ or $\quad -a \;\; \& \;\; a$
- In general $\xi_1 \neq \xi_2$

Designs:

$$\xi_1 = \begin{pmatrix} -1 & 1 \\ 1 - w_1 & w_1 \end{pmatrix} \qquad \& \qquad \xi_2 = \begin{pmatrix} -a & a \\ 1 - w_2 & w_2 \end{pmatrix}$$

Example 2: Different design regions

- Case 1: $d_1 = d$ & $d_2 = 0$ - *random intercept*

  Optimal designs:

  $$w_1^* = aw_2^* - \frac{a}{2} + \frac{1}{2}$$

  with $(w_1^*, w_2^*) \in [0, 1]^2$

- Case 2: $d_1 = 0$ & $d_2 = d$ - *random slope*

  Optimal designs:

  $$w_1^* = \frac{a + 2w_2^* - 1}{2a}$$

  with $(w_1^*, w_2^*) \in [0, 1]^2$

For $a = 1$: $w_1^* = w_2^*$ - same OD as in Example 1

Literature

- Graßhoff, U.; Doebler, A.; Holling, H.; Schwabe, R. (2012): Optimal design for linear regression models in the presence of heteroscedasticity caused by random coefficients. *Journal of Statistical Planning and Inference*, 142, 1108-1113.
- Prus, M.; Schwabe, R. (2016): Optimal designs for the prediction of individual parameters in hierarchical models. *Journal of the Royal Statistical Society, Series B*, 78, 175-191.
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Thank you for your attention!