Linear Aspects in Random Coefficient Regression Models: Optimal Designs for Different Design Criteria

Maryna Prus

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Contents

RCR model

$$Y_{ij} = \mathbf{f}(x_j)^\top \boldsymbol{\beta}_i + \varepsilon_{ij}, \quad i = 1, .., n, \quad j = 1, .., m, \quad x_j \in \mathcal{X}$$

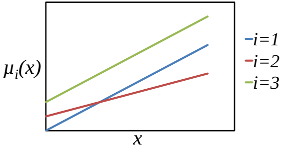
- $\mathbf{f} = (f_1, .., f_p)^\top$
- $\boldsymbol{\beta}_i = (\beta_{i1}, .., \beta_{ip})^\top$, $\mathrm{E}(\boldsymbol{\beta}_i) = \boldsymbol{\beta}$ *unknown*, $\mathrm{Cov}(\boldsymbol{\beta}_i) = \sigma^2 \mathbf{D}$

  Here: $\mathbf{D}$ *regular*
- $\mathrm{E}(\varepsilon_{ij}) = 0$, $\mathrm{Var}(\varepsilon_{ij}) = \sigma^2$
- *All* $\boldsymbol{\beta}_i$ *and all* $\varepsilon_{i'j}$ *uncorrelated*

Gladitz & Pilz (1982): $\boldsymbol{\beta}$ *known*

Individual response

$$\mu_i(x) = \mathbf{f}(x)^\top \boldsymbol{\beta}_i$$



RCR model

$$Y_{ij} = \mathbf{f}(x_j)^\top \boldsymbol{\beta}_i + \varepsilon_{ij} \qquad \equiv \qquad Y_{ij} = \mathbf{f}(x_j)^\top \boldsymbol{\beta} + \mathbf{f}(x_j)^\top \mathbf{b}_i + \varepsilon_{ij}$$

for $\mathbf{b}_i = \boldsymbol{\beta}_i - \boldsymbol{\beta}$

with $\mathrm{E}(\mathbf{b}_i) = 0$ & $\mathrm{Cov}(\mathbf{b}_i) = \sigma^2 \mathbf{D}$

i-th individual $\mathbf{Y}_i = (\mathbf{Y}_{i1}, \ldots, \mathbf{Y}_{im})^\top$:

$$\mathbf{Y}_i = \mathbf{F}\boldsymbol{\beta} + \mathbf{F}\mathbf{b}_i + \boldsymbol{\varepsilon}_i$$

$$\mathbf{F} = (\mathbf{f}(x_1), \ldots, \mathbf{f}(x_m))^\top \quad \& \quad \boldsymbol{\varepsilon}_i = (\varepsilon_{i1}, \ldots, \varepsilon_{im})^\top$$

All individuals $\mathbf{Y} = \left(\mathbf{Y}_1^\top, \ldots, \mathbf{Y}_n^\top\right)^\top$:

$$\mathbf{Y} = (\mathbf{1}_n \otimes \mathbf{F})\boldsymbol{\beta} + (\mathbf{I}_n \otimes \mathbf{F})\mathbf{b} + \boldsymbol{\varepsilon}$$

$$\mathbf{b} = \left(\mathbf{b}_1^\top, \ldots, \mathbf{b}_n^\top\right)^\top \quad \& \quad \boldsymbol{\varepsilon} = \left(\boldsymbol{\varepsilon}_1^\top, \ldots, \boldsymbol{\varepsilon}_n^\top\right)^\top$$

Aim: *Prediction of linear aspects* $\boldsymbol{\Psi} = \mathbf{K}\boldsymbol{\beta} + \mathbf{L}\mathbf{b}$

Estimable linear aspects

Definition

$\mathbf{\Psi} = \mathbf{K}\beta + \mathbf{L}\mathbf{b}$ *estimable(predictable)* $\Leftrightarrow$ $\exists\, \mathbf{U} :\ \mathrm{E}(\mathbf{U}\mathbf{Y}) = \mathrm{E}(\mathbf{\Psi})$

Lemma

$\mathbf{\Psi} = \mathbf{K}\beta + \mathbf{L}\mathbf{b}$ *estimable(predictable)* $\Leftrightarrow$ $\exists\, \mathbf{U} :\ \mathbf{K} = \mathbf{U}\,(\mathbf{1}_n \otimes \mathbf{F})$

Corollary

1. $\mathbf{\Psi} = \mathbf{L}\mathbf{b}$ *estimable(predictable)* $\forall\, \mathbf{L}$
2. $\mathbf{F}$ *full rank* $\Rightarrow$ $\mathbf{\Psi} = \mathbf{K}\beta + \mathbf{L}\mathbf{b}$ *estimable(predictable)* $\forall\, \mathbf{K}$ & $\forall\, \mathbf{L}$

Estimable linear aspects

Special cases:

- Population parameter $\Psi = \boldsymbol{\beta}$

  estimable if $\mathbf{F}$ *full rank* $\Leftrightarrow$ $\mathbf{F}^\top\mathbf{F}$ *regular*

- Individual deviations $\Psi = \mathbf{b}_i$

  always predictable

- Individual parameters $\Psi = \boldsymbol{\beta}_i = \boldsymbol{\beta} + \mathbf{b}_i$

  predictable if $\mathbf{F}$ *full rank* $\Leftrightarrow$ $\mathbf{F}^\top\mathbf{F}$ *regular*

Prediction of individual effects

- BLUP for individual parameters β_i:

$$\hat{\beta}_i = \mathbf{D}((\mathbf{F}^\top\mathbf{F})^{-1} + \mathbf{D})^{-1}\hat{\beta}_{i;\text{ind}} + (\mathbf{F}^\top\mathbf{F})^{-1}((\mathbf{F}^\top\mathbf{F})^{-1} + \mathbf{D})^{-1}\hat{\beta}$$

where $\hat{\beta} = (\mathbf{F}^\top\mathbf{F})^{-1}\mathbf{F}^\top\bar{\mathbf{Y}}$ & $\hat{\beta}_{i;\text{ind}} = (\mathbf{F}^\top\mathbf{F})^{-1}\mathbf{F}^\top\mathbf{Y}_i$, $\bar{\mathbf{Y}} = \frac{1}{n}\sum_{i=1}^{n}\mathbf{Y}_i$

- MSE matrix for $\hat{\mathbf{B}} = (\hat{\beta}_1^\top, ..., \hat{\beta}_n^\top)^\top$:

$$\sigma^2\left(\left(\mathbf{I}_n - \frac{1}{n}\mathbf{1}_n\mathbf{1}_n^\top\right) \otimes (\mathbf{F}^\top\mathbf{F} + \mathbf{D}^{-1})^{-1} + \frac{1}{n}\left(\mathbf{1}_n\mathbf{1}_n^\top\right) \otimes (\mathbf{F}^\top\mathbf{F})^{-1}\right)$$

Prediction of individual effects

- BLUP for individual deviations $\mathbf{b}_i$:

$$\hat{\mathbf{b}}_i = \mathbf{D}((\mathbf{F}^\top \mathbf{F})^{-1} + \mathbf{D})^{-1} \left(\hat{\beta}_{i;\mathrm{ind}} - \hat{\beta}\right)$$

where $\hat{\beta} = (\mathbf{F}^\top \mathbf{F})^{-1} \mathbf{F}^\top \bar{\mathbf{Y}}$ & $\hat{\beta}_{i;\mathrm{ind}} = (\mathbf{F}^\top \mathbf{F})^{-1} \mathbf{F}^\top \mathbf{Y}_i$, $\bar{\mathbf{Y}} = \frac{1}{n} \sum_{i=1}^n \mathbf{Y}_i$

- MSE matrix for $\hat{\mathbf{b}} = (\hat{\mathbf{b}}_1^\top, ..., \hat{\mathbf{b}}_n^\top)^\top$:

$$\sigma^2 \left(\left(\mathbf{I}_n - \frac{1}{n} \mathbf{1}_n \mathbf{1}_n^\top \right) \otimes (\mathbf{F}^\top \mathbf{F} + \mathbf{D}^{-1})^{-1} + \frac{1}{n} \left(\mathbf{1}_n \mathbf{1}_n^\top \right) \otimes \mathbf{D} \right)$$

Optimal designs

Experimental settings $x_1, \dots, x_m$ not necessarily all distinct

- *Distinct settings* $x_1, \dots, x_k$
- *Numbers of replications* $m_1, \dots, m_k$; $\sum_{j=1}^k m_j = m$

Individual design

$$\xi = \begin{pmatrix} x_1, \dots, x_k \\ w_1, \dots, w_k \end{pmatrix}$$

$$w_j = \frac{m_j}{m} \quad \& \quad \sum_{j=1}^{k} w_j = 1$$

Notation

$$\mathbf{M}(\xi) = \frac{1}{m}\mathbf{F}^\top\mathbf{F} \quad \& \quad \mathbf{\Delta} = m\mathbf{D}$$

IMSE-criterion

IMSE-criterion for prediction of individual parameters $\boldsymbol{\beta}_i$:

$$\Phi_{IMSE,\beta}(\xi) := \int_{\mathcal{X}} \mathrm{E}\left(\sum_{i=1}^{n}(\hat{\mu}_i(x;\xi)-\mu_i(x))^2\right)\nu(\mathrm{d}x)$$

$$\hat{\mu}_i(x;\xi) = \mathbf{f}(x)^\top \hat{\boldsymbol{\beta}}_i(\xi)$$

$$\Phi_{IMSE,\beta}(\xi) = \mathrm{tr}\left(\mathbf{M}(\xi)^{-1}\mathbf{V}\right) + (n-1)\,\mathrm{tr}\left((\mathbf{M}(\xi)+\boldsymbol{\Delta}^{-1})^{-1}\mathbf{V}\right)$$

$$\mathbf{V} = \int_{\mathcal{X}} \mathbf{f}(x)\mathbf{f}(x)^\top \nu(\mathrm{d}x)$$

weighted sum of IMSE-criterion in fixed effects model
and Bayesian IMSE-criterion

IMSE-criterion

IMSE-criterion for prediction of individual deviations $\mathbf{b}_i$:

$$\Phi_{IMSE,b}(\xi) := \int_{\mathcal{X}} \mathrm{E}\left(\sum_{i=1}^{n} \left(\hat{\mu}_i^b(x;\xi) - \mu_i^b(x)\right)^2\right) \nu(dx)$$

$$\mu_i^b(x) = \mathbf{f}(x)^\top \mathbf{b}_i \qquad \& \qquad \hat{\mu}_i^b(x;\xi) = \mathbf{f}(x)^\top \hat{\mathbf{b}}_i(\xi)$$

$$\Phi_{IMSE,b}(\xi) = \mathrm{tr}\left(\mathbf{\Delta V}\right) + (n-1)\mathrm{tr}\left(\left(\mathbf{M}(\xi) + \mathbf{\Delta}^{-1}\right)^{-1} \mathbf{V}\right)$$

$$\mathbf{V} = \int_{\mathcal{X}} \mathbf{f}(x)\mathbf{f}(x)^\top \nu(\mathrm{d}x)$$

Bayesian IMSE-criterion

D-criterion

D-criterion for prediction of individual parameters $\boldsymbol{\beta}_i$:

$$\Phi_{D,\beta}(\xi) := \ln\det\left(\mathrm{Cov}\left(\hat{\mathbf{B}}(\xi) - \mathbf{B}\right)\right)$$

$$\mathbf{B} = (\boldsymbol{\beta}_1^\top, \dots, \boldsymbol{\beta}_n^\top)^\top \quad \& \quad \hat{\mathbf{B}}(\xi) = (\hat{\boldsymbol{\beta}}_1(\xi)^\top, \dots, \hat{\boldsymbol{\beta}}_n(\xi)^\top)^\top$$

$$\Phi_{D,\beta}(\xi) = \ln\det\left(\mathbf{M}(\xi)^{-1}\right) + (n-1)\ln\det\left(\left(\mathbf{M}(\xi) + \boldsymbol{\Delta}^{-1}\right)^{-1}\right)$$

weighted sum of D-criterion in fixed effects model and Bayesian D-criterion

D singular: *modified D-criterion*

D-criterion

D-criterion for prediction of individual deviations **b**:

$$\Phi_{D,b}(\xi) := \ln\det\left(\mathrm{Cov}\left(\hat{\mathbf{b}}(\xi) - \mathbf{b}\right)\right)$$

$$\mathbf{b} = (\mathbf{b}_1^\top, \dots, \mathbf{b}_n^\top)^\top \quad \& \quad \hat{\mathbf{b}}(\xi) = (\hat{\mathbf{b}}_1(\xi)^\top, \dots, \hat{\mathbf{b}}_n(\xi)^\top)^\top$$

$$\Phi_{D,b}(\xi) = \ln\det(\mathbf{\Delta}) + (n-1)\ln\det\left((\mathbf{M}(\xi) + \mathbf{\Delta}^{-1})^{-1}\right)$$

Bayesian D-criterion

D singular: *modified D-criterion*

c-criterion

c-criterion for prediction of individual parameters β_i:

$$\Phi_{c,\beta}(\xi) := \sum_{i=1}^{n} \left(\mathrm{E} \left((\mathbf{c}^\top \hat{\beta}_i(\xi) - \mathbf{c}^\top \beta_i)^2 \right) \right)$$

$$\Phi_{c,\beta}(\xi) = \mathbf{c}^\top \mathbf{M}(\xi)^{-1} \mathbf{c} + (n-1)\, \mathbf{c}^\top (\mathbf{M}(\xi) + \mathbf{\Delta}^{-1})^{-1} \mathbf{c}$$

weighted sum of c-criterion in fixed effects model
and Bayesian c-criterion

Special case: $\mathbf{c} = \mathbf{f}(x_0)$

interpolation & extrapolation

c-criterion

c-criterion for prediction of individual deviations $\mathbf{b}_i$:

$$\Phi_{c,b}(\xi) := \sum_{i=1}^{n} \left(\mathrm{E}\left((\mathbf{c}^\top \hat{\mathbf{b}}_i(\xi) - \mathbf{c}^\top \mathbf{b}_i)^2 \right) \right)$$

$$\Phi_{c,b}(\xi) = \mathbf{c}^\top \boldsymbol{\Delta}\, \mathbf{c} + (n-1)\, \mathbf{c}^\top (\mathbf{M}(\xi) + \boldsymbol{\Delta}^{-1})^{-1} \mathbf{c}$$

Bayesian c-criterion

Special case: $\mathbf{c} = \mathbf{f}(x_0)$, $x_0 \in \mathcal{X}$ & $x_0 \notin \mathcal{X}$

interpolation & *extrapolation*

Optimality condition

Approximate design

$$\xi = \begin{pmatrix} x_1, \ldots, x_k \\ w_1, \ldots, w_k \end{pmatrix}$$

$$w_j \geq 0 \qquad \& \qquad \sum_{j=1}^{k} w_j = 1$$

General equivalence theorem

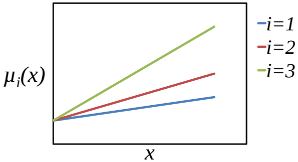
$\Downarrow$

Optimality condition for approximate designs

Example: straight line regression

$$Y_{ij} = \beta_{i1} + \beta_{i2} x_j + \varepsilon_{ij}, \qquad x_j \in [0, 1]$$

- $\mathbf{D} = \begin{pmatrix} d_1 & 0 \\ 0 & d_2 \end{pmatrix}$
- small intercept variance d_1



Individual optimal design:

$$\xi_w = \begin{pmatrix} 0 & 1 \\ 1-w & w \end{pmatrix}$$

IMSE- & *D*-optimal designs

Prediction of

individual parameters $\boldsymbol{\beta}_i$

- *IMSE-criterion*
- *D-criterion*

individual deviations $\mathbf{b}_i$

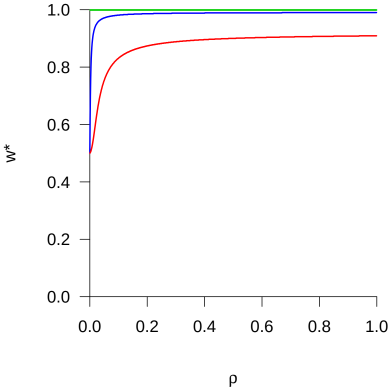
- *IMSE- & D-criterion*

$\rho = d_2/(1 + d_2)$

$d_1 = 0.001$

$n = 100$

$m = 10$



Efficiency of equi-replicated design $(w = 0.5)$

Prediction of

individual parameters $\boldsymbol{\beta}_i$

– *IMSE-criterion*

$$eff = \frac{\Phi_{IMSE,\beta}(\xi_{w^*})}{\Phi_{IMSE,\beta}(\xi_{0.5})}$$

– *D-criterion*

$$eff = \left(\frac{exp(\Phi_{D,\beta}(\xi_{w^*}))}{exp(\Phi_{D,\beta}(\xi_{0.5}))}\right)^{\frac{1}{2n}}$$

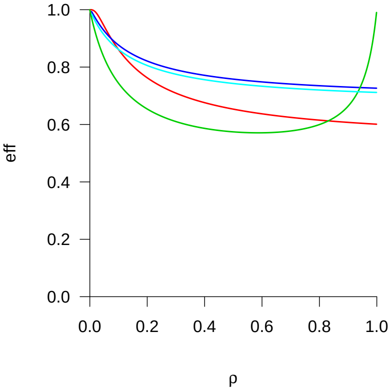
individual deviations $\mathbf{b}_i$

– *IMSE-criterion*

$$eff = \frac{\Phi_{IMSE,b}(\xi_{w^*})}{\Phi_{IMSE,b}(\xi_{0.5})}$$

– *D-criterion*

$$eff = \left(\frac{exp(\Phi_{D,b}(\xi_{w^*}))}{exp(\Phi_{D,b}(\xi_{0.5}))}\right)^{\frac{1}{2n}}$$



c-optimal designs: interpolation

Prediction of

individual parameters $\boldsymbol{\beta}_i$

- $x_0 = 0$
- $x_0 = 0.5$
- $x_0 = 1$

individual deviations $\mathbf{b}_i$

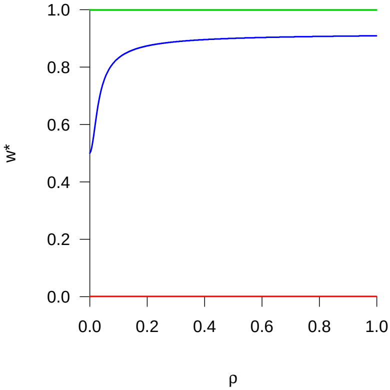
- *for all* $x_0 \in [0, 1]$

$\rho = d_2/(1 + d_2)$

$d_1 = 0.001$

$n = 100$

$m = 10$



Efficiency of optimal design in fixed effects model ($w = x_0$)

Prediction of

individual parameters $\boldsymbol{\beta}_i$

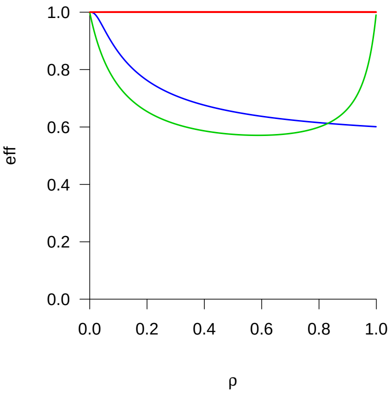
$$eff = \frac{\Phi_{c,\beta}(\xi_{w^*})}{\Phi_{c,\beta}(\xi_{x_0})}$$

- $x_0 = 0.5$
- $x_0 \in \{0, 1\}$

individual deviations $\mathbf{b}_i$

$$eff = \frac{\Phi_{c,b}(\xi_{w^*})}{\Phi_{c,b}(\xi_{x_0})}$$

- $x_0 = 0.5$
- $x_0 \in \{0, 1\}$



c-optimal designs: extrapolation

Prediction of

individual parameters $\boldsymbol{\beta}_i$

- $x_0 = 2$
- $x_0 = 10000$

individual deviations $\mathbf{b}_i$

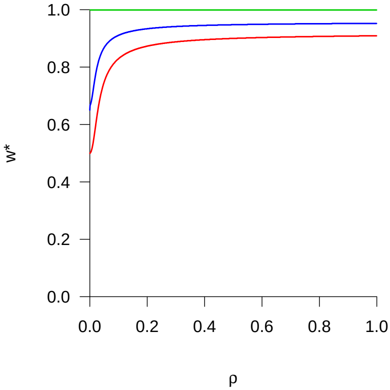
- *for all* $x_0 > 1$

$\rho = d_2/(1 + d_2)$

$d_1 = 0.001$

$n = 100$

$m = 10$



Efficiency of optimal design in fixed effects model ($\tilde{w} = \frac{x_0}{2x_0-1}$)

Prediction of

individual parameters β_i

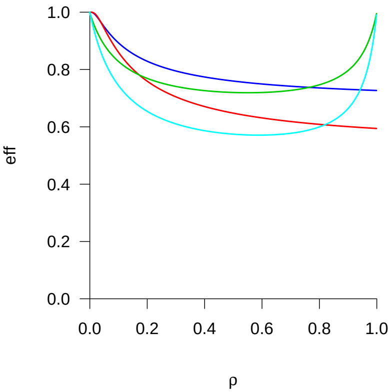
$$eff = \frac{\Phi_{c,\beta}(\xi_{w^*})}{\Phi_{c,\beta}(\xi_{\tilde{w}})}$$

- $x_0 = 2$
- $x_0 = 10000$

individual deviations $\mathbf{b}_i$

$$eff = \frac{\Phi_{c,b}(\xi_{w^*})}{\Phi_{c,b}(\xi_{\tilde{w}})}$$

- $x_0 = 2$
- $x_0 = 10000$



Outlook

- Different designs for different individuals
- Exact designs
- Unknown dispersion matrix of random effects
- ...

Thank you for your attention!

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