Canonical Analysis of Multi-stratum Designs and Standard Errors for Eigenvalues

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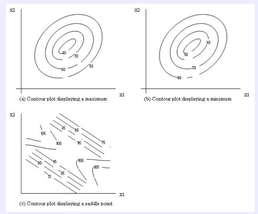
1 Introduction

1.1 Second Order Response Surface Model

Fitted Model:

$$\hat{y} = \hat{b_0} + \mathbf{x}'\hat{\mathbf{b}} + \mathbf{x}'\hat{\mathbf{B}}\mathbf{x}$$



where $\mathbf{x} = (x_1, x_2, ..., x_k)'$, $\hat{\mathbf{b}} = (\hat{b}_1, \hat{b}_2, ..., \hat{b}_k)'$ and $\hat{\mathbf{B}} = \begin{pmatrix} \hat{b}_{11} & \hat{b}_{12}/2 \cdots \hat{b}_{1k}/2 \\ \hat{b}_{12}/2 & \hat{b}_{22} \cdots \hat{b}_{2k}/2 \\ \vdots & \vdots \ddots \vdots \\ \hat{b}_{1k}/2 & \hat{b}_{2k}/2 \cdots \hat{b}_{kk} \end{pmatrix}$

1.2 Exploring Second Order Model (Canonical Analysis)

A Canonical Form (rotation of axes)

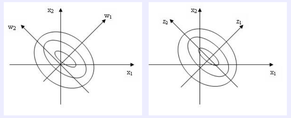
$$\hat{y} = \hat{b_0} + \sum_i^k \theta_i w_i + \sum_i^k \lambda_i w_i^2$$

where w's are new design points obtained by rotation of axes, & $lambda$'s are eigenvalues of $\hat{B}$

B Canonical Form (rotation of axes & shift of origin)

$$\hat{y} = \hat{y}_s + \mathbf{z}'\mathbf{\Lambda}\mathbf{z}$$

where z's are new design points obtained by shifting the origin to stationary point, & $\hat{y}_s = \hat{b}_0 + \frac{1}{2}\mathbf{w}'\hat{\boldsymbol{\theta}}$



A canonical form B canonical form

1.3 Multi-stratum Design

When one or more factors are 'hard to change' (in terms of time, cost etc.)

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \sum_i^S \mathbf{Z_i}\boldsymbol{\alpha}_i + \boldsymbol{\epsilon}$$

2 Research Problem

Bisgaard & Ankenman (1996) described the double linear regression (DLR) method to estimate the standard errors for eigenvalues.But they discussed this method only for completely randomized error control structure. Our objective was to check can we modify DLR method to estimate the standard errors for eigenvalues for multi-stratum error control structure?

3 Methodology

3.1 Modified DLR Method

- Fit the full second order linear mixed model

$$E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta} + \sum_i^s \mathbf{Z_i}\boldsymbol{\alpha_i}$$

Using the fixed effects of fitted model, construct matrix $\hat{\mathbf{B}}$, Where $\hat{\mathbf{B}}$ is same as before, and calculate its eigenvalues and corresponding eigenvectors.

- Using the eigenvectors of $\hat{\mathbf{B}}$ rotate the axes, such that new axes are the principal axes of ellipsoidal contours of response, and redefine the design points $(\mathbf{w})$
- Using these new design points, again fit the full second order linear mixed model as in step 1
- The coefficients of interaction terms, for the fixed effects, would now be very close to zero and coefficients of quadratic terms would be equal to eigenvalues of $\hat{\mathbf{B}}$ up to numerical rounding.
- The standard errors of the quadratic terms of the fixed effects now can be used as approximated standard errors for the eigenvalues of $\hat{\mathbf{B}}$.

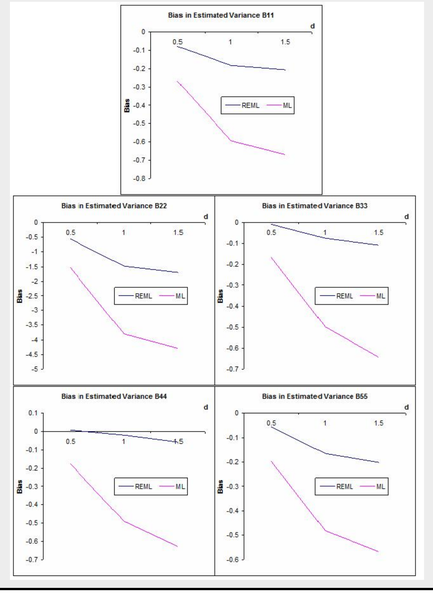
4 Results

Data: Letsinget et al (1996)

REML		
Eigenvalues of $\hat{\mathbf{B}}$	Estimates	SE
294.029219	294.029219	42.97248
84.222153	84.222152	36.38129
8.165963	8.165963	42.32715
-56.399507	-56.399507	40.71135
-114.651618	-114.651618	45.03625

ML		
Eigenvalues of $\hat{\mathbf{B}}$	Estimates	SE
280.921893	280.921893	21.75851
77.550423	77.550423	18.18189
6.299696	6.299696	15.10634
-55.975931	-55.975931	15.58601
-111.094489	-111.094489	21.62687

Simulation Study



5 Conclusions

- With a slight modification double regression method can be used to estimate the standard errors for eigenvalues for multi-stratum Response Surface designs
- For a particular data set ML estimates may give smaller standard errors for eigenvalues than REML estimates, but ML estimates have more bias in standard errors than REML estimates.

6 Future Plans

- develop a formal test of hypothesis to test $\lambda = 0$
- what if we have some prior knowledge? (Bayesian approach)

7 References

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