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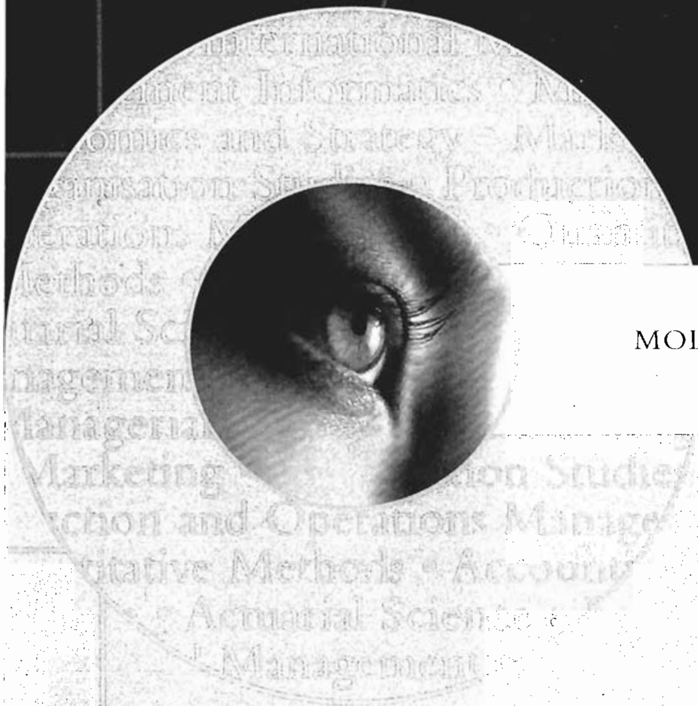

RESEARCH REPORT

EFFICIENCY OF BLOCKING TWO-STAGE MODEL-ROBUST AND MODEL-SENSITIVE DESIGNS

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Efficiency of blocking two-stage model-robust and model-sensitive designs

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Abstract

In two-stage experimentation, it is recommended that a block effect is included in the model to capture a possible shift in the mean response between the stages. In this paper, it is investigated how the inclusion of a block effect in the model affects the design and analysis of the experiment.

Keywords: MGD-MGD two-stage designs, posterior probabilities, blocking, bias, lack of fit, weighted mean efficiency factor (WMEF)

1 Introduction

In a two-stage design strategy, the first stage design is obtained using some optimality criterion and then conditional on information provided by the first stage data, the second stage design is chosen to create certain desirable conditions in the combined design. In the literature, the two-stage design procedures have been developed within the non-linear framework as the classical alphabetic optimality criteria require prior knowledge of the model parameters due to the non-linearity of the problem. For example Myers, Myers, Carter and White (1996) propose a two-stage design procedure for the logistic regression that uses D-optimality in the first stage followed by Q-optimality in the second. The development of two-stage designs for linear models has been limited in the literature. Neff (1996) developed Bayesian two-stage designs under model uncertainty for mean estimation models. Montepiedra and Yeh (1998) also developed a two-stage strategy for the construction of D-optimal approximate designs for the linear model. Lin, Myers and

Ye (2000) obtained Bayesian two-stage *D*-*D* optimal designs for mixture models. Ruggoo and Vandebroek (2003a) reviewed and extended work by Neff (1996). Essentially, in a two-stage design approach, it is possible to efficiently design experiments when initial knowledge of the regressors is poor.

Two-stage model-robust and model-sensitive designs have recently been developed by Ruggoo and Vandebroek (2003b) (henceforth referred to as RUVA) for linear models. They assume that the model that shall be fitted comprises p primary or important terms. In addition to these primary terms there are q potential terms that are possibly important but not in the assumed model. In the first stage they use a criterion that facilitates the improvement of the proposed primary model by detecting lack of fit in the direction of the potential terms. The design in the second stage is then based on model information from the first stage and minimizes bias with respect to the potential terms. Briefly the two-stage approach of RUVA is as follows: the linear model that will be fitted by the experimenter is of the form

$$y = \mathbf{x}'_{pri}\boldsymbol{\beta}_{pri} + \varepsilon,$$

with $\mathbf{x}_{pri}$ being a p-dimensional vector of powers and products of the experimental factors and $\boldsymbol{\beta}_{pri}$ the p-dimensional vector of unknown parameters attached to the primary terms. The product $\mathbf{x}'_{pot}\boldsymbol{\beta}_{pot}$ contains the terms that one wishes to protect against in designing the experiment, where $\mathbf{x}_{pot}$ is the q-dimensional vector containing powers and products of the factors and $\boldsymbol{\beta}_{pot}$ is the q-dimensional vector associated with the potential terms. The model is reparametrized in terms of the orthonormal polynomials with respect to a measure μ on the design region. Also, the prior distribution of $\boldsymbol{\beta}_{pot}$ is assumed to be $N(\mathbf{0}, \tau^2\sigma^2\mathbf{I}_q)$ where τ^2 is the common prior variance of the potential terms' coefficients, measured in units of the random error variance σ^2 of the error terms.

Assume that $\mathbf{y}_i|\boldsymbol{\beta} \sim N(\mathbf{X}_i\boldsymbol{\beta}, \sigma^2\mathbf{I}_{n_i})$ for each stage i $(i = 1, 2)$ and that the first and second stage comprise n_1 and n_2 runs respectively so that the total number of design points in the combined design is $n = n_1 + n_2$. $\mathbf{X}$ is the extended design matrix of dimension $n \times (p + q)$ for the combined stages, so that $\mathbf{X}' = [\ \mathbf{X}'_1\ \mathbf{X}'_2\ ]$. $\mathbf{X}_1 = [\ \mathbf{X}_{pri(1)}\ \mathbf{X}_{pot(1)}\ ]$ is of dimension $n_1 \times (p + q)$ and $\mathbf{X}_2 = [\ \mathbf{X}_{pri(2)}\ \mathbf{X}_{pot(2)}\ ]$ is of dimension $n_2 \times (p + q)$. These matrices represent respectively the first and second stage designs expanded to full model space. $\mathbf{X}_{pri(i)}$ and $\mathbf{X}_{pot(i)}$ correspond to the primary and potential terms respectively for each stage i ($i = 1, 2$). Finally $\mathbf{X}'_{pri} = [\ \mathbf{X}'_{pri(1)}\ \mathbf{X}'_{pri(2)}\ ]$ is of dimension $n \times p$ and $\mathbf{X}'_{pot} = [\ \mathbf{X}'_{pot(1)}\ \mathbf{X}'_{pot(2)}\ ]$ is of dimension $n \times q$. These matrices are respectively the combined first and second stage design matrices for the primary and potential terms models only.

Before observing the first stage data, the experimenter has specified a set of $(p + q)$ regressors defining the full model. The true relationship between the response and the input variables is believed to contain all primary terms and a subset q_i $(0 \leq q_i \leq q)$ of the potential terms. Consequently the total number of possible models is $m = 2^q$. The first stage design is obtained by minimizing

$$\sum_{k=1}^{m} p(M_k)\ \mathrm{GD}_1^{(k)},$$

where

$$\mathrm{GD}_1^{(k)} = \left[\frac{1}{p} \log \left| \mathbf{X}_{pri(1)}^{(k)\prime}\ \mathbf{X}_{pri(1)}^{(k)} \right|^{-1} + \frac{\alpha_L}{q_k} \log \left| \mathbf{L}^{(k)} + \frac{\mathbf{I}_q^{(k)}}{\tau^2} \right|^{-1} \right] \tag{1}$$

and $p(M_k)$'s are prior probabilities for each of the competing 2^q models computed using the effect inheritance assumptions in screening experiments (See RUVA and Bingham and Chipman (2002)). $\mathbf{X}_{pri(1)}^{(k)}$, $\mathbf{L}^{(k)}$ and $\mathbf{I}_q^{(k)}$ are the matrices corresponding to $\mathbf{X}_{pri(1)}$, $\mathbf{L}$ and $\mathbf{I}_q$ expanded to model space M_k and

$$\mathbf{L} = \mathbf{X}'_{pot(1)}\mathbf{X}_{pot(1)} - \mathbf{X}'_{pot(1)}\mathbf{X}_{pri(1)} \left(\mathbf{X}'_{pri(1)}\mathbf{X}_{pri(1)}\right)^{-1} \mathbf{X}'_{pri(1)}\mathbf{X}_{pot(1)},$$

is the dispersion matrix encountered in the literature on model-sensitive designs and which gives us an idea of the lack of fit in the direction of the potential terms (see, e.g., Atkinson and Donev (1992) for further details).

The objective of the second stage is to use model information from the first stage to minimize bias with respect to potential terms. The second stage design points are then obtained by minimizing

$$\sum_{k=1}^{m} p(M_k|\mathbf{y}_1)\ \mathrm{GD}_2^{(k)},$$

where

$$\mathrm{GD}_2^{(k)} = \left[\frac{1}{p} \log \left| \mathbf{X}_{pri}^{(k)\prime} \, \mathbf{X}_{pri}^{(k)} \right|^{-1} + \frac{\alpha_B}{q_k} \log \left| \mathbf{A}^{(k)\prime} \mathbf{A}^{(k)} + \mathbf{I}_q^{(k)} \right| \right]. \tag{2}$$

$\mathbf{X}_{pri}^{(k)}$, $\mathbf{A}^{(k)}$ and $\mathbf{I}_q^{(k)}$ are the matrices corresponding to $\mathbf{X}_{pri}$, $\mathbf{A}$ and $\mathbf{I}_q$ expanded to model space M_k where

$$\mathbf{A} = \left(\mathbf{X}_{pri}' \mathbf{X}_{pri} \right)^{-1} \mathbf{X}_{pri}' \mathbf{X}_{pot}$$

is the alias matrix in the combined stage. The posterior probabilities $p(M_k|\mathbf{y}_1)$, reflect model importance and are computed from first stage data using the approach proposed by Box and Meyer (1993) and also used by Neff (1996). Finally α_L and α_B are weights that attach more or less importance on the different properties. The expression on the right hand side of (2) essentially comprises of two components: a variance and the squared bias and is akin to the integrated mean squared error criterion of Box and Draper (1959), except for the weight, α_B attached to the squared bias component (See RUVA for further details). RUVA refers to their approach as the MGD-MGD two-stage procedure (MGD - Model Generalized D-optimality) and the approach produces designs with significantly smaller bias errors compared to standard unique stage designs used in the literature. They also improve coverage over the factor space and possess good variance properties for the assumed primary model.

As can be seen in the development above, RUVA do not assume any block effect in the design and analysis of their experiments. However we note that each stage is randomized separately which, from the point of view of randomization analysis, implies that the experiment consists of separate blocks of sizes n_1 and n_2 respectively. Further justification for blocking the experiment with respect to the two stages is the fact that the second stage will be conducted at a later time period so that there may have been a shift in the mean response between the two stages. The first stage design is not affected by the block structure but we can expect the second stage design to be different if the blocked nature of the experiment is taken into account.

The overall objective of this paper is to investigate whether a more efficient combined design is obtained if the experiment is designed and analyzed assuming the first and second stages to be respectively the first and second blocks of the experiment. It is also investigated whether a block effect in the model leads to more efficient estimates of the parameters of the primary terms.

The two-stage procedure incorporating a block effect in the model is developed in Sections 2 and 3. We then illustrate the new procedure in Section 4 followed by an evaluation and comparison of the blocked experiment with RUVA's unblocked two-stage designs in Section 5. Section 6 contains a short discussion.

2 Blocking the two-stage designs

There are several situations in which it may not be possible to perform all the runs of an experiment under homogeneous conditions. In such cases, experiments are often blocked such that experimental units within the blocks are more homogeneous than those from different blocks. In essence, the primary gain with blocking is that the effects of the experimental variables can be estimated more precisely. Atkinson and Donev (1989), Goos and Vandebroek (2001) and more recently Goos (2002) and references therein give excellent discussions on designs for blocked response surface experiments in general.

In practice the first and second stage of the two-stage designs would be randomized separately and say, performed over different time periods, by different operators or with different batches of materials, and consequently can be thought of as in two separate blocks. Recall that the experimenter will fit the primary model using the combined design at the end of the experiment so that an extension of the model to include a fixed block effect would be

$$\mathbf{y} = \mathbf{X}_{pri}\boldsymbol{\beta}_{pri} + \mathbf{i}\delta + \boldsymbol{\varepsilon}, \tag{3}$$

where

$$\mathbf{X}_{pri} = \begin{bmatrix} \mathbf{X}_{pri(1)} \\ \mathbf{X}_{pri(2)} \end{bmatrix} \quad \text{and} \quad \mathbf{i} = \begin{bmatrix} \mathbf{0}_{n_1} \\ \mathbf{1}_{n_2} \end{bmatrix},$$

and δ is an additive block effect corresponding to the second stage of the experiment. $\mathbf{0}_{n_1}$ and $\mathbf{1}_{n_2}$ are respectively $n_2 \times 1$ vectors of zeroes and ones (See, e.g., Goos (2002) for details on fixed block effects analysis). If a block effect is included in the model, we shall need to find new expressions for the variance of the primary terms and also for the squared bias component in (2) to be able to develop our second stage design criterion.

From (3), the parameter estimates under the usual ordinary least squares can be obtained by solving

$$\begin{pmatrix} \widehat{\boldsymbol{\beta}}_{pri} \\ \widehat{\delta} \end{pmatrix} = \begin{pmatrix} \mathbf{X}_{pri}^{'}\mathbf{X}_{pri} & \mathbf{X}_{pri}^{'}\mathbf{i} \\ \mathbf{i}'\mathbf{X}_{pri} & \mathbf{i}'\mathbf{i} \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{X}_{pri}^{'} \\ \mathbf{i}' \end{pmatrix} \mathbf{y}.$$

Using Harville's (1997) Theorem 8.5.11 on the inverse of a partitioned matrix, we obtain

$$\begin{aligned} \widehat{\boldsymbol{\beta}}_{pri} &= \left(\mathbf{X}_{pri}^{'}\mathbf{X}_{pri} - \mathbf{X}_{pri}^{'}\mathbf{i}(\mathbf{i}'\mathbf{i})^{-1}\mathbf{i}'\mathbf{X}_{pri}\right)^{-1}\mathbf{X}_{pri}^{'}\mathbf{y} \\ &\qquad -\left(\mathbf{X}_{pri}^{'}\mathbf{X}_{pri} - \mathbf{X}_{pri}^{'}\mathbf{i}(\mathbf{i}'\mathbf{i})^{-1}\mathbf{i}'\mathbf{X}_{pri}\right)^{-1}\mathbf{X}_{pri}^{'}\mathbf{i}(\mathbf{i}'\mathbf{i})^{-1}\mathbf{i}'\mathbf{y} \\ &= \left(\mathbf{X}_{pri}^{'}\mathbf{X}_{pri} - \mathbf{X}_{pri(2)}^{'}\mathbf{1}_{n_2}(n_2)^{-1}\mathbf{1}_{n_2}^{'}\mathbf{X}_{pri(2)}\right)^{-1}\mathbf{X}_{pri}^{'}\mathbf{y} \\ &\qquad -\left(\mathbf{X}_{pri}^{'}\mathbf{X}_{pri} - \mathbf{X}_{pri(2)}^{'}\mathbf{1}_{n_2}(n_2)^{-1}\mathbf{1}_{n_2}^{'}\mathbf{X}_{pri(2)}\right)^{-1}\mathbf{X}_{pri}^{'}\mathbf{i}\,(n_2)^{-1}\,\mathbf{i}'\mathbf{y} \\ &= \left(\mathbf{X}_{pri}^{'}\mathbf{X}_{pri} - n_2^{-1}\mathbf{X}_{pri(2)}^{'}\mathbf{1}_{n_2}\mathbf{1}_{n_2}^{'}\mathbf{X}_{pri(2)}\right)^{-1}\mathbf{X}_{pri}^{'}\left(\mathbf{I}_n - n_2^{-1}\mathbf{i}\mathbf{i}^{'}\right)\mathbf{y}. \end{aligned} \qquad (4)$$

Also the variance-covariance of the least squares estimators $\widehat{\boldsymbol{\beta}}_{pri}$ and $\widehat{\delta}$ is

$$\text{var}(\widehat{\boldsymbol{\beta}}_{pri}, \widehat{\delta}) = \sigma^2 \begin{bmatrix} \mathbf{X}_{pri}^{'}\mathbf{X}_{pri} & \mathbf{X}_{pri}^{'}\mathbf{i} \\ \mathbf{i}'\mathbf{X}_{pri} & \mathbf{i}'\mathbf{i} \end{bmatrix}^{-1}. \qquad (5)$$

The variance-covariance matrix of $\widehat{\boldsymbol{\beta}}_{pri}$ will thus be given by the upper left hand submatrix of (5). Again using Harville's (1997) Theorem 8.5.11 on the inverse of a partitioned matrix, we find that

$$\begin{aligned} \text{var}(\widehat{\boldsymbol{\beta}}_{pri}) &= \sigma^2\{\mathbf{X}_{pri}^{'}\mathbf{X}_{pri} - \mathbf{X}_{pri}^{'}\mathbf{i}(\mathbf{i}'\mathbf{i})^{-1}\mathbf{i}'\mathbf{X}_{pri}\}^{-1} \\ &= \sigma^2\{\mathbf{X}_{pri}^{'}\mathbf{X}_{pri} - \mathbf{X}_{pri(2)}^{'}\mathbf{1}_{n_2}(n_2)^{-1}\mathbf{1}_{n_2}^{'}\mathbf{X}_{pri(2)}\}^{-1} \\ &= \sigma^2\{\mathbf{X}_{pri}^{'}\mathbf{X}_{pri} - n_2^{-1}\mathbf{X}_{pri(2)}^{'}\mathbf{1}_{n_2}\mathbf{1}_{n_2}^{'}\mathbf{X}_{pri(2)}\}^{-1}. \end{aligned} \qquad (6)$$

Considering the first term on the right hand side of (2) implies that, on inclusion of a block effect in our model, the measure of efficiency of the coefficients of the primary terms will become

$$\frac{1}{p}\log\left|\mathbf{X}_{pri}^{'}\mathbf{X}_{pri} - n_2^{-1}\mathbf{X}_{pri(2)}^{'}\mathbf{1}_{n_2}\mathbf{1}_{n_2}^{'}\mathbf{X}_{pri(2)}\right|^{-1}.$$

To obtain the new alias matrix $\mathbf{A}_B$, with the block structure we now derive the new expression for the bias. Since the experimenter will eventually fit the primary terms, the squared bias component (SBC) with respect to the measure μ on the design region becomes

$$\text{SBC} = \text{E}_\mu\{\mathbf{x}'_{pri}\boldsymbol{\beta}_{pri} + \mathbf{x}'_{pot}\boldsymbol{\beta}_{pot} - \mathbf{x}'_{pri}\widehat{\boldsymbol{\beta}}_{pri}\}^2. \tag{7}$$

Now from (4)

$$\widehat{\boldsymbol{\beta}}_{pri} = \mathbf{B}\mathbf{X}'_{pri}(\mathbf{I}_n - n_2^{-1}\mathbf{i}\mathbf{i}')\mathbf{y},$$

where

$$\begin{aligned}\mathbf{B} &= \left(\mathbf{X}'_{pri}\mathbf{X}_{pri} - n_2^{-1}\mathbf{X}'_{pri(2)}\mathbf{1}_{n_2}\mathbf{1}'_{n_2}\mathbf{X}_{pri(2)}\right)^{-1} \\ &= \{\mathbf{X}'_{pri}\mathbf{X}_{pri} - n_2^{-1}\mathbf{X}'_{pri}\mathbf{i}\mathbf{i}'\mathbf{X}_{pri}\}^{-1}.\end{aligned}$$

Therefore (7) becomes

$$\begin{aligned}&\text{E}_\mu\{\mathbf{x}'_{pri}\boldsymbol{\beta}_{pri} + \mathbf{x}'_{pot}\boldsymbol{\beta}_{pot} - \mathbf{x}'_{pri}\mathbf{B}\mathbf{X}'_{pri}(\mathbf{I}_n - n_2^{-1}\mathbf{i}\mathbf{i}')\mathbf{y}\}^2 \\ &= \text{E}_\mu\{\mathbf{x}'_{pri}\boldsymbol{\beta}_{pri} + \mathbf{x}'_{pot}\boldsymbol{\beta}_{pot} - \mathbf{x}'_{pri}\mathbf{B}\mathbf{X}'_{pri}(\mathbf{I}_n - n_2^{-1}\mathbf{i}\mathbf{i}')(\mathbf{X}_{pri}\boldsymbol{\beta}_{pri} + \mathbf{X}_{pot}\boldsymbol{\beta}_{pot})\}^2 \\ &= \text{E}_\mu\{\mathbf{x}'_{pri}\boldsymbol{\beta}_{pri} + \mathbf{x}'_{pot}\boldsymbol{\beta}_{pot} - \mathbf{x}'_{pri}\mathbf{B}\mathbf{B}^{-1}\boldsymbol{\beta}_{pri} - \mathbf{x}'_{pri}\mathbf{B}\mathbf{X}'_{pri}(\mathbf{I}_n - n_2^{-1}\mathbf{i}\mathbf{i}')\mathbf{X}_{pot}\boldsymbol{\beta}_{pot}\}^2 \\ &= \text{E}_\mu\{\mathbf{x}'_{pot}\boldsymbol{\beta}_{pot} - \mathbf{x}'_{pri}\mathbf{B}\mathbf{X}'_{pri}(\mathbf{I}_n - n_2^{-1}\mathbf{i}\mathbf{i}')\mathbf{X}_{pot}\boldsymbol{\beta}_{pot}\}^2 \\ &= \boldsymbol{\beta}'_{pot}\text{E}_\mu\{(\mathbf{x}'_{pot} - \mathbf{x}'_{pri}\mathbf{A}_B)'(\mathbf{x}'_{pot} - \mathbf{x}'_{pri}\mathbf{A}_B)\}\boldsymbol{\beta}_{pot} \\ &= \boldsymbol{\beta}'_{pot}\{\mathbf{A}'_B\mu_{11}\mathbf{A}_B - \mathbf{A}'_B\mu_{12} - \mu_{21}\mathbf{A}_B + \mu_{22}\}\boldsymbol{\beta}_{pot},\end{aligned}$$

where

$$\begin{aligned}\mathbf{A}_B &= \mathbf{B}\mathbf{X}'_{pri}(\mathbf{I}_n - n_2^{-1}\mathbf{i}\mathbf{i}')\mathbf{X}_{pot} \\ &= \left(\mathbf{X}'_{pri}\mathbf{X}_{pri} - n_2^{-1}\mathbf{X}'_{pri(2)}\mathbf{1}_{n_2}\mathbf{1}'_{n_2}\mathbf{X}_{pri(2)}\right)^{-1} \\ &\qquad \left(\mathbf{X}'_{pri}\mathbf{X}_{pot} - n_2^{-1}\mathbf{X}'_{pri(2)}\mathbf{1}_{n_2}\mathbf{1}'_{n_2}\mathbf{X}_{pot(2)}\right),\end{aligned} \tag{8}$$

is the alias matrix which essentially transcribes bias errors to parameter estimates, $\widehat{\boldsymbol{\beta}}_{pri}$. As we have assumed orthonormal polynomials, we have that $\mu_{11} = \mathbf{I}_p$, $\mu_{12} = \mathbf{0}_{p\times q}$, $\mu_{21} = \mathbf{0}_{q\times p}$ and $\mu_{22} = \mathbf{I}_q$. As a consequence,

$$\text{SBC} = \boldsymbol{\beta}'_{pot}\{\mathbf{A}'_B\mathbf{A}_B + \mathbf{I}_q\}\boldsymbol{\beta}_{pot}. \tag{9}$$

RUVA uses the expected value of the SBC over the potential parameters for use in their second stage criterion.

3 Development of the two-stage procedure with block effect

The first stage design is not affected by the block structure and can be obtained in a fashion similar to that of RUVA described in Section 1. To obtain the second stage design, we consider a generalization of the second stage design criterion of RUVA in (2) and incorporate our variance term and SBC obtained respectively in (6) and (9). Consequently, the second stage design incorporating the blocked nature of the experiment is obtained by minimizing

$$\sum_{k=1}^{m} p(M_k|\mathbf{y}_1)\ \mathrm{GD}_{2B}^{(k)},$$

where

$$\mathrm{GD}_{2B}^{(k)} = \left[\frac{1}{p}\log \left| \mathbf{X}_{pri}^{(k)\prime}\mathbf{X}_{pri}^{(k)} - n_2^{-1}\mathbf{X}_{pri(2)}^{(k)\prime}\mathbf{1}_{n_2}\mathbf{1}_{n_2}^{\prime}\mathbf{X}_{pri(2)}^{(k)} \right|^{-1} + \frac{\alpha_B}{q_k}\log \left| \mathbf{A}_B^{(k)\prime}\mathbf{A}_B^{(k)} + \mathbf{I}_q^{(k)} \right| \right] \tag{10}$$

and $\mathbf{A}_B^{(k)}$ is obtained for model space M_k from (8) above.

4 Illustration of the procedure

Consider the three-dimensional problem where the primary model consists of $p = 5$ terms, $\mathbf{x}^{(\mathrm{pri})} = \{1,\ x_1,\ x_2,\ x_3,\ x_1^2\}$ and $q = 3$ potential terms, $\mathbf{x}^{(\mathrm{pot})} = \{x_1x_2,\ x_2^2,\ x_3^2\}$. The design region is the $5 \times 5 \times 5$ grid on $[-1, +1]^3$. Since the second stage design is dependent on the first stage data, response data from the first stage experiment are needed for the computation of the posterior probabilities used as weights in the second stage criterion. Suppose we have resources for 20 runs and the true model from which data will be simulated is

$$y = 42.0 + 11.5\ x_1 + 12.8\ x_2 + 10.5\ x_3 + 14.6\ x_1^2 - 7.4\ x_2^2 + \varepsilon. \tag{11}$$

The true model comprises all the primary terms and one potential term, namely the quadratic term in x_2. We assume $\varepsilon \sim N(0, 1)$ and the illustration will be for one simulation only. We assume an equal partition in the two stages so that $n_1 = 10$ and $n_2 = 10$

and also the following default values: $\alpha_L = 20$ in the first stage, $\alpha_B = 10$ in the second stage, and $\tau = 5$ in both stages.

The first stage design, being independent of the block effect, can be obtained in a fashion similar to that of RUVA and is shown in Table 1.

Table 1: First stage design with 10 runs

run	First stage design		
	X_1	X_2	X_3
1	-1	-1	-1
2	-1	-1	1
3	-1	0	0
4	-1	1	0
5	-1	1	1
6	0	-1	-1
7	0.5	0	0
8	1	-1	0
9	1	-1	1
10	1	1	-1

Using this design, response data can be simulated from the true model (11) to compute the posterior model probabilities and also in the numerical construction of the second stage design. The corresponding prior and posterior probabilities are in shown Table 2. It can be seen that the primary terms model has the highest prior probability as this is the model which the experimenter had belief on before conducting the experiment. But once first stage data is obtained, the true model (11) has the highest posterior probability indicating that it will be given the largest weight in the second stage criterion.

The second stage design (SSD) of RUVA and the one we developed including the block effect can then be obtained following Section 3. The resulting designs are shown in Table 3. The SSD's are different when the block effect is taken into account. It would be interesting to see whether blocking the two-stage experiment affects the orthogonality structure of the experiment. As argued by Trinca and Gilmour (1998), the efficiency in estimating

Table 2: Prior and posterior model probabilities of different competing models

Terms in M_i	$p(M_i)$	$p(M_i\|\mathbf{y}_1)$
$1\ x_1\ x_2\ x_3\ x_1^2$ (Primary model)	0.5787037	0
$1\ x_1\ x_2\ x_3\ x_1^2\ x_1x_2$	0.1157407	0
$1\ x_1\ x_2\ x_3\ x_1^2\ x_2^2$ (True model)	0.1157407	0.9584726
$1\ x_1\ x_2\ x_3\ x_1^2\ x_3^2$	0.1157407	0
$1\ x_1\ x_2\ x_3\ x_1^2\ x_1x_2\ x_2^2$	0.0231481	0.025106
$1\ x_1\ x_2\ x_3\ x_1^2\ x_1x_2\ x_3^2$	0.0231481	0
$1\ x_1\ x_2\ x_3\ x_1^2\ x_2^2\ x_3^2$	0.0231481	0.0138377
$1\ x_1\ x_2\ x_3\ x_1^2\ x_1x_2\ x_2^2\ x_3^2$	0.0046296	0.0025825

Table 3: Second stage designs (SSD's) with and without the block effect

run	SSD - No blocks			SSD - With blocks		
	X_1	X_2	X_3	X_1	X_2	X_3
1	-1	-0.5	0.5	-1	-1	1
2	-1	-0.5	0.5	-1	0	0
3	-1	0	0	-1	0	0
4	-1	0	0	-1	0.5	-1
5	-0.5	-0.5	-1	0	-0.5	1
6	1	-0.5	-1	0	0	-1
7	1	-0.5	0	0	0	1
8	1	-0.5	0	1	-0.5	-1
9	1	-0.5	0.5	1	0	-0.5
10	1	0	-0.5	1	0	0

parameters is preserved completely in designs that block orthogonally. To investigate this property we use the idea of the weighted mean efficiency factor (WMEF) suggested by John and Williams (1995) but adapted by Trinca and Gilmour (2000) for the parameters of a response surface model. We shall compare the WMEF for our combined first and second stage designs with and without a block effect.

We first define the efficiency factor (EF) for the estimate of a parameter, β_i,

$$\mathrm{EF}(\hat{\beta}_i) = \frac{V_*(\hat{\beta}_i)/\sigma_*^2}{V(\hat{\beta}_i)/\sigma^2} \times 100\%.$$

$V_*(\hat{\beta}_i)$ and σ_*^2 are the variance of $\hat{\beta}_i$ and the error variance respectively obtained from an unblocked analysis. $V(\hat{\beta}_i)$ and σ^2 are the variance of $\hat{\beta}_i$ and the error variance respectively obtained from an analysis with block effect. If any parameter is estimated orthogonally to block differences then it has 100% efficiency. The WMEF is then given by

$$\mathrm{WMEF} = \frac{1}{\sum_{i=2}^{p} w_i} \sum_{i=2}^{p} w_i \, \mathrm{EF}(\hat{\beta}_i)$$

where we are considering our p primary terms and w_i represents the weights given to the parameter $\hat{\beta}_i$. The intercept is usually given weight zero. For further details on the WMEF and weight structures, see Trinca and Gilmour (2000).

We shall be using unit weights, except for the intercept which is given weight zero, in our calculations for the WMEF and consider regressors present in the primary model only. All computations are carried out using the orthonormalized values of the design points. If we assume that the combined experiment designed without taking blocking into account will be analyzed with a block effect then the WMEF is 97.3%. If the experiment was designed taking into account the block effect, the WMEF increases to 99.3%. Recalling that an orthogonally blocked response surface design will have a WMEF of 100%, suggests that blocking the two-stage design, attempts to construct an orthogonally blocked experiment in the primary terms.

5 Some further evaluation and comparison of designs

The values of the different determinants in (10) will now be used as measures of efficiency of the precision and bias components when a block effect is included in the design and analysis of the experiment. A measure of precision of the primary terms is given by

$$\mathrm{D}^*_{\mathrm{X_{pri}}} = \left|\mathbf{X}'_{pri}\mathbf{X}_{pri} - n_2^{-1}\mathbf{X}'_{pri(2)}\mathbf{1}_{n_2}\mathbf{1}'_{n_2}\mathbf{X}_{pri(2)}\right|^{-1/p}, \tag{12}$$

and

$$\mathrm{D}^*_{\mathrm{bias}} = \left|\mathbf{A}^{*'}_B\mathbf{A}^*_B + \mathbf{I}_q\right|^{1/q} \tag{13}$$

represents the degree of bias. Note that $\mathbf{A}^*_B$ comprise the design points for the primary and potential terms expanded to contain regressors in the true model only. Also these quantities have been defined such that the smaller the value obtained, the better the design performs with respect to that criterion. Since we have a simulation procedure, the performance of the two-stage procedures is measured by the average of $\mathrm{D}^*_{\mathrm{X_{pri}}}$ and $\mathrm{D}^*_{\mathrm{bias}}$ over 200 simulations, i.e.

$$\mathrm{AD}^*_{\mathrm{X_{pri}}} = \frac{\sum_{j=1}^{200}\mathrm{D}^*_{\mathrm{X_{pri(j)}}}}{200}, \qquad \mathrm{AD}^*_{\mathrm{bias}} = \frac{\sum_{j=1}^{200}\mathrm{D}^*_{\mathrm{bias(j)}}}{200}.$$

To have an idea of the effect of including a block component in the two-stage procedure, we shall evaluate and compare our blocked combined experiment with the combined unblocked design of RUVA under different models using (12) and (13), i.e. assuming as if RUVA's designs would be analyzed with a block effect.

We consider two cases discussed in RUVA for our evaluation purposes. The design region is the $5 \times 5 \times 5$ grid on $[-1, +1]^3$, ε is simulated from a $\sim N(0, 1)$ distribution, $\alpha_L = 20$ in the first stage and $\alpha_B = 10$ in the second stage and $\tau = 5$ in both stages.

Case I :

We again consider the example used in the illustration, i.e. we have $p = 5$ terms, $\mathbf{x}^{(\mathrm{pri})} = \{1,\ x_1,\ x_2,\ x_3,\ x_1^2\}$ and $q = 3$ potential terms, $\mathbf{x}^{(\mathrm{pot})} = \{x_1x_2,\ x_2^2,\ x_3^2\}$. First stage data is simulated as before from (11).

Case II :

We examine data simulated from

$$y = 40.0 + 11.5\ x_1 + 12.8\ x_2 + 10.5\ x_3 + 14.6\ x_1^2 + 9.8\ x_1x_2 - 7.4\ x_1x_3 - 8.7\ x_2^2 + \varepsilon,$$

a model comprising five primary terms, namely $\{1,\ x_1,\ x_2,\ x_3,\ x_1^2\}$ and an additional five potential terms, $\{x_1x_2,\ x_1x_3,\ x_2x_3,\ x_2^2,\ x_3^2\}$.

Tables 4 and 5 show the results of the different evaluations. Values in brackets in columns two and three, are the standard deviations over the 200 simulated data sets. In general incorporating a block effect in the design and analysis of the two-stage procedures leads to an improvement in the design properties. In Case I, inclusion of the block effect leads to a good reduction in variance as opposed to the bias which does not change much. Including the block effect in Case II, leads to a good reduction in bias but with a slight increase in variance compared to the unblocked experiment. These results corroborate with the fact that there will always be a trade-off between bias and variance when searching for designs incorporating a composite design criterion. However, by varying the weights α_B in the second stage criterion, it is possible to obtain a reduction in both the variance and bias component for the blocked experiment. In Case I, by increasing α_B to 20, we have a reduction in the bias at the expense of the variance component that increases, but it is still smaller than the variance of the unblocked experiment. In Case II, by decreasing α_B to 5, we note an improvement in both properties for the blocked experiment. The experimenter is thus free to vary the weights according to the importance he/she wants to place on the different components.

6 Discussion

It is well known that any design strategy that involves minimum variance will work counter to a strategy involving protection against bias. These two aspects of a design, namely variance and bias can be thought of as the two arms of a weighing scale: a reduction in bias will lead to an increase in variance and vice-versa. The experimenter has a difficult choice to make: he/she may be willing to have a minimum variance design but it may turn out to be for the wrong assumed model. Therefore it is imperative for a design criterion

Table 4: Comparison of the two-stage MGD-MGD procedure without and with a block effect.

Case I $y = 42.0 + 11.5\ x_1 + 12.8\ x_2 + 10.5\ x_3 + 14.6\ x_1^2 - 7.4\ x_2^2 + \varepsilon.$

Two-Stage Approach ($n_1 = n_2 = 10$)	$\mathrm{AD}^*_{\mathrm{X_{pri}}}$	$\mathrm{AD}^*_{\mathrm{bias}}$
MGD-MGD (Without block effect)	0.065394	1.333055
($\alpha_B = 10$)	(0.0028702)	(0.022730)
MGD-MGD (With block effect)	0.054926	1.334051
($\alpha_B = 10$)	(0.0013657)	(0.0058856)
MGD-MGD (With block effect)	0.060231	1.322489
($\alpha_B = 20$)	(0.0022352)	(0.0054652)

Table 5: Comparison of the two-stage MGD-MGD procedure without and with a block effect.

Case II $y = 40.0 + 11.5\ x_1 + 12.8\ x_2 + 10.5\ x_3 + 14.6\ x_1^2 + 9.8\ x_1x_2 - 7.4\ x_1x_3 - 8.7\ x_2^2 + \varepsilon.$

Two-Stage Approach ($n_1 = n_2 = 12$)	$\mathrm{AD}^*_{\mathrm{X_{pri}}}$	$\mathrm{AD}^*_{\mathrm{bias}}$
MGD-MGD (Without block effect)	0.0431736	1.114668
($\alpha_B = 10$)	(0.0005729)	(0.0094607)
MGD-MGD (With block effect)	0.044730	1.050213
($\alpha_B = 10$)	(0.0010592)	(0.0006742)
MGD-MGD (With block effect)	0.042937	1.054506
($\alpha_B = 5$)	(0.0005833)	(0.0029673)

to make explicit provision for departures from the assumed model. It is exactly in this direction that RUVA developed their two-stage procedure. Their design strategy takes into account several design criteria simultaneously, and with the flexibility about a model in mind too.

In this paper, we have extended the approach of RUVA by including a block effect in their two-stage procedure. It can be seen that blocking generally leads to an improvement in the design properties. Other simulations carried out with different models indicate that the size of the improvements are in general case dependent. The general recommendation is that the experimenter should always account for the block effect both in the design and analysis of the two-stage experiments. This will ensure more precise estimation of parameters of the primary model and also to less bias in the direction of the potential terms. Furthermore the parameter estimates will not be affected by any possible shift in the mean response between the two stages of the experiment.

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