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Model-robust and model-sensitive designs

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Abstract

The main drawback of the optimal design approach is that it assumes the statistical model is known. To overcome this problem, a new approach to reduce the dependency on the assumed model is proposed. The approach takes into account the model uncertainty by incorporating the bias in the design criterion and the ability to test for lack-of-fit. Several new designs are derived and compared to the alternatives available from the literature.

Keywords: Precision; Bias; Lack-of-fit; Model-robustness; Model-sensitive; Model-discrimination; D-optimality; A-optimality

1. Introduction

The assumption that underlies most research work in optimal experimental design is that the proposed model adequately describes the response of interest. It is unlikely however that the experimenter is completely certain that the model will be correct and this should be reflected in the experimental design. Instead of searching for the optimal design to estimate the stated model several approaches have been proposed in the literature to account for model uncertainty. The resulting experimental designs are often referred to as model-robust

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designs. An overview of a considerable part of the work on model robust designs is given in Chang and Notz (1996). They point out that the practical value of the results they review is mainly in alerting the experimenter to the dangers of ignoring the approximate nature of any assumed model and in providing some insight concerning what features an experimental design should possess in order to be robust against departures from an assumed model while allowing a good fit of the assumed model. During the last 15 years, Dette (1990, 1991, 1992, 1993, 1994, 1995), Dette et al. (1995), Dette and Studden (1995), Fang and Wiens (2003), Heo et al. (2001), Liu and Wiens (1997), Wiens (1992, 1994, 1996, 1998, 2000) and Wiens and Zhou (1996, 1997) have done a considerable amount of work in this area, thereby extending the seminal work by Huber (1975), Pesotchinsky (1982), Sacks and Ylvisaker (1984) and Wiens (1990). A recurring theme is that uniform or equispaced designs perform well in terms of model-robustness when a Bayesian approach is adopted, when the maximum bias is to be minimized or when the minimum power of the lack-of-fit test is to be maximized. In the present paper, we will concentrate on practical design problems in which the number of observations available is small, just like DuMouchel and Jones (1994), who propose a Bayesian approach involving so-called primary and potential model terms. In contrast with some of the above-mentioned work, we also assume that the estimated model and the true but unknown model are linear regression models, that the experimental errors are homogeneous and uncorrelated, and that the model is estimated using ordinary least squares. This is the problem industrial statisticians most often consider.

2. Model-robust versus model-sensitive designs

In a model-robust approach, one looks for designs that yield reasonable results for the true model even if the postulated model is different. The pioneering work in this area is from Box and Draper (1959). They assume that the true model is composed of a primary model—the one that will eventually be estimated—plus some potential terms. The design strategy they propose minimizes the integrated mean squared error over the region of interest. This criterion can be decomposed into the sum of a bias component and a variance component. The problem with this and similar criteria is that the optimal design will depend on the parameters of the potential terms. Several authors who have worked on the problem of balancing precision and bias have proposed solutions to overcome this dependency on the parameters. Welch (1983) for instance minimized the average variance and the average bias in the extreme points of the design region for maximal parameter values, whereas Montepiedra and Fedorov (1997) develop a method to find designs that strike a balance between the variance and the bias. DuMouchel and Jones (1994) used a Bayesian approach to obtain designs that are less sensitive to the model assumption. The authors claim that their criterion leads to designs that are more resistant to the bias caused by the potential terms, and at the same time yields precise estimates of the primary terms. Inspired by the papers of Box and Draper (1959) and DuMouchel and Jones (1994), Kobilinsky (1998) developed a design criterion combining bias and variance properties in a more explicit way.

In contrast with the model-robust approach, model-sensitive design approaches lead to designs that facilitate the improvement of the model by detecting lack-of-fit. Examples of such approaches can be found in Atkinson (1972), Atkinson and Cox (1974) and Atkinson

and Fedorov (1975a, b). These authors searched for designs that were good in detecting lack-of-fit by maximizing the dispersion matrix somehow. Jones and Mitchell (1978) elaborated on this idea by maximizing the minimal or average noncentrality parameter over a region of possible values for the potential parameters. Studden (1982) combined the detection of lack-of-fit with a precise estimation of the primary terms. This combined approach was also used in Atkinson and Donev (1992).

According to Chang and Notz (1996), a good model-robust design should (i) allow the experimenter to fit the assumed model, (ii) allow the detection of model inadequacy, and (iii) allow reasonable efficient inferences concerning the assumed model when it is adequate. The purpose of this paper is to construct experimental designs that meet these requirements and that lead to a small bias between the estimated model and the true model. A first attempt to combine bias and lack-of fit aspects is given by DeFeo and Myers (1992) who minimize bias and at the same time maximize the power of the lack-of-fit test of the potential terms. They show that a rotated design has the same bias properties as the initial design and use this result to maximize the power of the lack-of-fit test. In this paper we develop two new design criteria that take into account both model-robust and model-sensitive aspects, combining efficiency in estimating the primary terms, protection against bias caused by the potential terms and ability to test for lack-of-fit and thereby increasing the knowledge on the true model. In Section 3 we will introduce the notation and describe some existing approaches. In Section 4 we develop our generalized criteria and in Section 5 we illustrate their use with some theoretical examples. Section 6 contains our conclusion.

3. The model

We assume there exists a relationship between the expected response and the experimental factors $x_1, x_2, \ldots, x_k$. The model that will be fitted is

$$Y = \mathbf{x}_1'\boldsymbol{\beta}_1 + \varepsilon \tag{1}$$

with $\mathbf{x}_1$ a p-dimensional vector of powers and products of the factors and $\boldsymbol{\beta}_1$ the p-dimensional vector of unknown parameters. We further assume that the expected response was possibly misspecified and that the true model is given by

$$Y = \mathbf{x}'\boldsymbol{\beta} + \varepsilon = \mathbf{x}_1'\boldsymbol{\beta}_1 + \mathbf{x}_2'\boldsymbol{\beta}_2 + \varepsilon = \eta(\mathbf{x}) + \varepsilon, \tag{2}$$

with $\mathbf{x}_2$ the q-dimensional vector containing powers and products of the factors not included in the fitted model, $\mathbf{x}' = [\mathbf{x}_1' \ \mathbf{x}_2']$ and $\boldsymbol{\beta}' = [\boldsymbol{\beta}_1' \ \boldsymbol{\beta}_2']$. We will refer to $\mathbf{x}_1'\boldsymbol{\beta}_1$ as the primary terms and to $\mathbf{x}_2'\boldsymbol{\beta}_2$ as the potential terms. Note that it is implicitly assumed that there are 2^q possible models ranging from the model with only the primary terms to the full model containing all primary and potential terms. Also, it is interesting to point out that simply estimating the more complicated model (2) is in practice often impossible because a large number of possibly important regressors would require an experiment involving a large number of observations. This makes that researchers often stick to the simpler primary model (1). To simplify the notation in the sequel of the paper, we will assume that the model has been reparametrized in terms of the orthonormal polynomials with respect to a measure μ on the design region. In the examples of Sections 5 and 6, we will use the uniform

measure on the design region because we assume that all the points in the design region are equally important. The orthonormalization ensures that the effects are well separable and independent so that a simple prior distribution on the potential terms can be used.

3.1. Model-robust design strategies

Box and Draper (1959) were the first to investigate the effect of model misspecification. They introduced the integrated mean squared error (IMSE) with respect to a measure μ on the design region. If we denote the fitted response value for factor settings $\mathbf{x}_1$ under the primary model (1) by $\hat{y}(\mathbf{x}_1)$, the IMSE can be defined as

$$\begin{aligned}\text{IMSE}&=\mathbf{E}_\mu\mathbf{E}_\varepsilon[\eta(\mathbf{x})-\hat{y}(\mathbf{x}_1)]^2\\&=\mathbf{E}_\mu\mathbf{E}_\varepsilon[\eta(\mathbf{x})-\mathbf{E}_\varepsilon[\hat{y}(\mathbf{x}_1)]]^2+\mathbf{E}_\mu\mathbf{E}_\varepsilon[\mathbf{E}_\varepsilon[\hat{y}(\mathbf{x}_1)]-\hat{y}(\mathbf{x}_1)]^2\end{aligned}$$

which consists of the expected squared bias and the expected prediction variance. If we denote by $\mathbf{X}_1$ the $n\times p$ model matrix for the primary terms and by $\mathbf{X}_2$ the $n\times q$ model matrix for the potential terms, we have that $\hat{y}(\mathbf{x}_1)=\mathbf{x}_1'(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{Y}$ and $\mathbf{E}_\varepsilon[\mathbf{Y}]=\mathbf{X}_1\boldsymbol{\beta}_1+\mathbf{X}_2\boldsymbol{\beta}_2$. As a result,

$$\begin{aligned}\text{IMSE}&=\mathbf{E}_\mu[\mathbf{x}_1'\boldsymbol{\beta}_1+\mathbf{x}_2'\boldsymbol{\beta}_2-\mathbf{x}_1'(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'(\mathbf{X}_1\boldsymbol{\beta}_1+\mathbf{X}_2\boldsymbol{\beta}_2)]^2\\&\quad+\mathbf{E}_\mu[\mathbf{x}_1'(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{x}_1\sigma^2]\\&=\mathbf{E}_\mu[\mathbf{x}_2'\boldsymbol{\beta}_2-\mathbf{x}_1'(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{X}_2\boldsymbol{\beta}_2]^2+\mathbf{E}_\mu[\mathbf{x}_1'(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{x}_1\sigma^2].\end{aligned}$$

In this expression, $(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{X}_2$ is the so-called alias matrix. We will denote it by $\mathbf{A}$ in the sequel of the paper. Now, denoting $\mu_{ij}=\mathbf{E}_\mu(\mathbf{x}_i\mathbf{x}_j')$ and using the well-known result that

$$\begin{aligned}\mathbf{E}_\mu[\mathbf{x}_1'(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{x}_1]&=\mathbf{E}_\mu[\text{trace}\{\mathbf{x}_1'(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{x}_1\}]=\mathbf{E}_\mu[\text{trace}\{\mathbf{x}_1\mathbf{x}_1'(\mathbf{X}_1'\mathbf{X}_1)^{-1}\}]\\&=\text{trace}[\mu_{11}(\mathbf{X}_1'\mathbf{X}_1)^{-1}],\end{aligned}$$

we obtain

$$\begin{aligned}\text{IMSE}&=\mathbf{E}_\mu[\mathbf{x}_2'\boldsymbol{\beta}_2-\mathbf{x}_1'\mathbf{A}\boldsymbol{\beta}_2]^2+\sigma^2\,\text{trace}[\mu_{11}(\mathbf{X}_1'\mathbf{X}_1)^{-1}]\\&=\boldsymbol{\beta}_2'\mathbf{E}_\mu[(\mathbf{x}_2'-\mathbf{x}_1'\mathbf{A})'(\mathbf{x}_2'-\mathbf{x}_1'\mathbf{A})]\boldsymbol{\beta}_2+\sigma^2\,\text{trace}[\mu_{11}(\mathbf{X}_1'\mathbf{X}_1)^{-1}]\\&=\boldsymbol{\beta}_2'[\mathbf{A}'\mu_{11}\mathbf{A}-\mathbf{A}'\mu_{12}-\mu_{21}\mathbf{A}+\mu_{22}]\boldsymbol{\beta}_2+\sigma^2\,\text{trace}[\mu_{11}(\mathbf{X}_1'\mathbf{X}_1)^{-1}].\end{aligned}$$

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,

$$\text{IMSE}=\boldsymbol{\beta}_2'[\mathbf{A}'\mathbf{A}+\mathbf{I}_q]\boldsymbol{\beta}_2+\sigma^2\,\text{trace}(\mathbf{X}_1'\mathbf{X}_1)^{-1}.$$

From this result, Box and Draper (1959) concluded that bias can be minimized by looking for designs for which that $\mathbf{A}=\mathbf{0}_{p\times q}$. In general however the design that minimizes IMSE will depend on the values of $\boldsymbol{\beta}_2$. To cope with this dependence, Kobilinsky (1998) suggested to put a prior distribution on the potential parameters. As it is unlikely that these terms are large, the following distribution was considered to be appropriate:

$$\boldsymbol{\beta}_2\sim\mathcal{N}(0,\tau^2\sigma^2\mathbf{I}_q).$$

Because $\mathbf{x}_2$ is orthonormalized, it is reasonable to assume that all elements in $\boldsymbol{\beta}_2$ have equal variances and that they are uncorrelated with each other. Under this assumption, we obtain that

$$\begin{aligned}\mathbf{E}_{\boldsymbol{\beta}}[\text{IMSE}] &= \mathbf{E}_{\boldsymbol{\beta}}[\boldsymbol{\beta}_2'[\mathbf{A}'\mathbf{A}+\mathbf{I}_q]\boldsymbol{\beta}_2 + \sigma^2 \operatorname{trace}(\mathbf{X}_1'\mathbf{X}_1)^{-1}] \\ &= \operatorname{trace}(\mathbf{A}'\mathbf{A}\tau^2\sigma^2\mathbf{I}_q + \tau^2\sigma^2\mathbf{I}_q) + \sigma^2 \operatorname{trace}(\mathbf{X}_1'\mathbf{X}_1)^{-1} \\ &= \tau^2\sigma^2 \operatorname{trace}(\mathbf{A}'\mathbf{A}+\mathbf{I}_q) + \sigma^2 \operatorname{trace}(\mathbf{X}_1'\mathbf{X}_1)^{-1}.\end{aligned}$$

It is clear that $\tau^2 = 0$ indicates that the primary model is the true model. In that case, minimization of the expected IMSE will lead to the minimization of $\operatorname{trace}(\mathbf{X}_1'\mathbf{X}_1)^{-1}$ and thus to an A-optimal design for the primary model (1).

Based on a similar prior distribution of the potential terms, DuMouchel and Jones (1994) proposed a Bayesian D-optimality criterion to find designs that yield precise estimates for the primary terms and give some protection against the existence of the potential terms. As the posterior covariance matrix of $\hat{\boldsymbol{\beta}}$ is

$$\operatorname{cov}(\hat{\boldsymbol{\beta}}) = \sigma^2\left(\mathbf{X}'\mathbf{X} + \frac{\mathbf{K}}{\tau^2}\right)^{-1}$$

with $\mathbf{X}' = [\mathbf{X}_1' \ \mathbf{X}_2']$ and

$$\mathbf{K} = \begin{pmatrix} \mathbf{0}_{p\times p} & \mathbf{0}_{p\times q} \\ \mathbf{0}_{q\times p} & \mathbf{I}_q \end{pmatrix}$$

they proposed to maximize the following determinant:

$$\frac{1}{\sigma^2}\left|\mathbf{X}'\mathbf{X} + \frac{\mathbf{K}}{\tau^2}\right|.$$

This criterion has the clear advantage that the information matrix for the full model (2), i.e. $\mathbf{X}'\mathbf{X}$, can be singular without causing problems. Therefore it is possible to use this criterion for design problems in which $p \leqslant n < p+q$, that is in cases where the number of observations n available is insufficient to estimate the full model. Such small experiments are common in industry.

The choice of τ^2 is of course an arbitrary one. Kobilinsky (1998) suggests $\tau^2 = 1/q$ so that the global effect of the q potential terms is of the same order of magnitude as the residual error. DuMouchel and Jones (1994) suggest to take $\tau^2 = 1$ so that the effect of any of the potential terms is not larger than the residual standard error. They use a less stringent orthogonalization procedure which only orthogonalizes the potential terms with respect to the primary terms. The primary terms are not orthogonalized relative to each other, nor are the potential terms. The orthonormalization used in this paper leads to simpler mathematical derivations.

The approaches of Box and Draper (1959), DuMouchel and Jones (1994) and Kobilinsky (1998) aim at finding designs that yield precise estimates of the primary terms and ensure that predictions are close to the expected response. They do not explicitly consider the possibility of performing a lack-of-fit test and therefore do not provide information on the appropriateness of the primary model. In the next section we consider some existing approaches to deal with this discrimination problem.

3.2. Model-sensitive design strategies

An approach which takes into account both the experimental effort for determining which model is true and the effort for precise estimation of the parameters is given by Atkinson and Donev (1992). They proposed to combine the D-optimality criterion for the primary model and the D_s-optimality criterion for the potential terms. The resulting criterion is given by

$$\max\left\{\frac{\alpha}{p}\log|\mathbf{X}_1'\mathbf{X}_1| + \frac{1-\alpha}{q}\log|\mathbf{X}_2'\mathbf{X}_2 - \mathbf{X}_2'\mathbf{X}_1(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{X}_2|\right\},$$

where $\alpha \in [0, 1]$ represents the belief in the primary model (1). When $\alpha = 1$, this criterion reduces to the D-optimality criterion for the primary model, whereas for $\alpha = 0$ it becomes the D_s-optimality criterion for the potential model parameters $\boldsymbol{\beta}_2$. When $\alpha = p/(p+q)$, the combined criterion leads to D-optimal designs for the full model (2).

Note that the D_s-optimality criterion for the potential terms is related to the noncentrality parameter

$$\delta = \frac{\boldsymbol{\beta}_2'[\mathbf{X}_2'\mathbf{X}_2 - \mathbf{X}_2'\mathbf{X}_1(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{X}_2]\boldsymbol{\beta}_2}{\sigma^2} \tag{3}$$

to test for lack-of-fit in the direction of the potential terms. Therefore, it is likely that the power of the lack-of-fit test will increase with decreasing α. The matrix $\mathbf{X}_2'\mathbf{X}_2 - \mathbf{X}_2'\mathbf{X}_1(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{X}_2$ is well known in the literature on model-sensitive designs. It is usually referred to as the dispersion matrix. In the sequel of this paper, we will denote it by $\mathbf{L}$.

4. A combined approach

The advantages of the approaches described in the previous section will be combined in a flexible criterion that includes three important aspects: precise estimation of the primary model, minimization of the bias caused by the potential terms and possibility to test for lack-of-fit.

The criterion of Kobilinsky (1998) that was derived in the previous section

$$\min\{\tau^2\sigma^2\,\mathrm{trace}(\mathbf{A}'\mathbf{A} + \mathbf{I}_q) + \sigma^2\,\mathrm{trace}(\mathbf{X}_1'\mathbf{X}_1)^{-1}\}$$

takes into account precision and bias but not lack-of-fit. As this criterion was derived by computing the expected IMSE over the prior distribution of potential terms, it is natural to apply the same idea to the lack-of-fit term. As the noncentrality parameter also depends on the values of $\boldsymbol{\beta}_2$, we will maximize the expected noncentrality parameter over the prior distribution. The expected noncentrality parameter can be computed as

$$\begin{aligned}\mathbf{E}_{\boldsymbol{\beta}}[\delta] &= \mathbf{E}_{\boldsymbol{\beta}}\left[\frac{\boldsymbol{\beta}_2'[\mathbf{X}_2'\mathbf{X}_2 - \mathbf{X}_2'\mathbf{X}_1(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{X}_2]\boldsymbol{\beta}_2}{\sigma^2}\right]\\ &= \tau^2\,\mathrm{trace}[\mathbf{X}_2'\mathbf{X}_2 - \mathbf{X}_2'\mathbf{X}_1(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{X}_2]\\ &= \tau^2\,\mathrm{trace}[\mathbf{L}].\end{aligned}$$

To combine the three aspects in one criterion we specify weights α_2 and α_3 to attach more or less importance on the different properties. A possible criterion is then given by

$$\min\left\{\frac{1}{p}\operatorname{trace}(\mathbf{X}_1'\mathbf{X}_1)^{-1}-\frac{\alpha_2}{q}\operatorname{trace}(\mathbf{L})+\frac{\alpha_3}{q}\operatorname{trace}(\mathbf{A}'\mathbf{A}+\mathbf{I}_q)\right\}.$$

Similarly, the criterion

$$\max\left\{\frac{\alpha}{p}\log|\mathbf{X}_1'\mathbf{X}_1|+\frac{1-\alpha}{q}\log|\mathbf{X}_2'\mathbf{X}_2-\mathbf{X}_2'\mathbf{X}_1(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{X}_2|\right\}$$

of Atkinson and Donev (1992), which takes into account precision and lack-of-fit, can be augmented with a term that represents the bias. As this criterion deals with determinants, a natural extension is given by

$$\min\left\{\frac{1}{p}\log|(\mathbf{X}_1'\mathbf{X}_1)^{-1}|+\frac{\alpha_2}{q}\log|\mathbf{L}^{-1}|+\frac{\alpha_3}{q}\log|\mathbf{A}'\mathbf{A}+\mathbf{I}_q|\right\}.$$

Because these criteria do not allow for singular design matrices for the full model, we can use the idea of DuMouchel and Jones (1994) to allow for smaller designs and generalize the previous criteria to the following generalized A- and D-optimality criteria:

$$\text{GA}:\min\left\{\frac{1}{p}\operatorname{trace}(\mathbf{X}_1'\mathbf{X}_1)^{-1}-\frac{\alpha_2}{q}\operatorname{trace}\left(\mathbf{L}+\frac{\mathbf{I}_q}{\tau^2}\right)+\frac{\alpha_3}{q}\operatorname{trace}(\mathbf{A}'\mathbf{A}+\mathbf{I}_q)\right\}$$

and

$$\text{GD}:\min\left\{\frac{1}{p}\log|(\mathbf{X}_1'\mathbf{X}_1)^{-1}|+\frac{\alpha_2}{q}\log\left|\left(\mathbf{L}+\frac{\mathbf{I}_q}{\tau^2}\right)^{-1}\right|+\frac{\alpha_3}{q}\log|\mathbf{A}'\mathbf{A}+\mathbf{I}_q|\right\}.$$

It is easy to see that these criteria generalize those proposed by Atkinson and Donev (1992), DuMouchel and Jones (1994) and Kobilinsky (1998) as well as the ordinary D- and A-optimality criteria. For $\alpha_2=\alpha_3=0$ the GD-optimality criterion produces the D-optimal design for the primary model. We will refer to this design as D_1-optimal in the sequel. For $\alpha_3=0,_2\alpha\ =q/p$ and $\tau^2=\infty$, we obtain the D-optimal design for the full model, denoted by D_{full}. For $\alpha_3=0,\alpha_2=q/p$ and finite values for τ^2, we find the Bayesian D-optimal designs introduced by DuMouchel and Jones (1994). This is because

$$\left|\mathbf{X}'\mathbf{X}+\frac{\mathbf{K}}{\tau^2}\right|=|\mathbf{X}_1'\mathbf{X}_1|\left|\mathbf{X}_2'\mathbf{X}_2+\frac{\mathbf{I}_q}{\tau^2}-\mathbf{X}_2'\mathbf{X}_1(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{X}_2\right|.$$

5. Illustrations

In this section, we illustrate the use of the GD-optimality criterion in a number of simple experimental situations. For an application to the five component mixture experiment described in Snee (1981) and revisited in DuMouchel and Jones (1994), we refer the interested reader to Goos et al. (2002). The GA-optimality criterion in general leads to different designs but to similar results. The designs here were obtained with a point exchange algorithm.

A list of candidate design points has to be provided as an input to the algorithm, the first part of which is devoted to their orthonormalization. The starting design was partly generated in a random fashion and completed by adding those points from the list of candidates that had the largest prediction variance for the fitted model. Including the nonrandom part in the generation of the starting design led to experimental designs that were consistently better than those obtained using a full random starting design. As in the algorithm of Fedorov (1972), the starting design was improved by considering exchanges of design points with candidate points and carrying out the best exchange each time. The KL-exchange idea of Atkinson and Donev (1989) was implemented to speed up the algorithm. Finally, in order to avoid getting stuck in a local optimum, this procedure was repeated 100 times for each design problem considered. For the first design problem, the GD-designs are compared to an equidistant design because, in the case of one explanatory variable, this design option is an easy and an effective way to reduce the bias. It should also be mentioned that the GD-optimal designs discussed below are not just optimal for the α_2- and α_3-values reported but also in their neighborhood. To avoid the GD-criterion breaking down when the number of observations n is smaller than the number of parameters in the full model, $p+q$, we used $\tau^2 = 1$ as was recommended by DuMouchel and Jones (1994). When $n \geqslant p+q$, we used $\tau^2 = \infty$.

5.1. *One explanatory variable*

5.1.1. *GD-optimal designs*

Firstly, assume that the primary model consists of $p=3$ terms, $\beta_0+\beta_1 x+\beta_2 x^2$, and that there is $q=1$ potential term, $\beta_3 x^3$. As a result, $\boldsymbol{\beta}_1=[\beta_0\ \beta_1\ \beta_2]'$ and $\boldsymbol{\beta}_2=[\beta_3]$. Also, assume that $n=8$ and, because $n \geqslant p+q$, $\tau^2=\infty$. By varying the values of α_2 and α_3 we obtain several designs. The extreme ones are displayed in Fig. 1. The designs were computed using a grid of 21 equidistant points on $[-1,+1]$. The values of the different determinants in the GD-optimality criterion are given in Fig. 1 as well. DX1 represents $|\mathbf{X}_1'\mathbf{X}_1|^{-1/p}$, the measure used for the precision of the primary terms, $\text{Dlof}=|\mathbf{L}|^{-1/q}$ provides an idea of the ability to detect lack-of-fit and $\text{Dbias}=|\mathbf{A}'\mathbf{A}+\mathbf{I}_q|^{1/q}$ represents the degree of bias. These measures were defined such that the smaller the value obtained, the better the design performs with respect to this criterion. Notice also that the minimum value of Dbias is one. It is also useful to mention that, in cases where alternative GD-optimal designs were found, we have displayed the most symmetric one.

For $\alpha_2=\alpha_3=0$, the D-optimal design for the primary model was obtained. This design is displayed in Panel 1 of Fig. 1. When either α_2 or α_3 is increased, different designs are obtained. For example, choosing a large value for α_3, e.g. $\alpha_3=10$, produces the design in Panel 2. This design leads to a small bias, as indicated by the Dbias-value that is close to one. Choosing $\alpha_2=q/p=\frac{1}{3}$ and $\alpha_3=0$ leads to the D-optimal design for the full model (see Panel 3). The Dlof-value shows that this design allows a good detection of lack-of-fit at the expense of the precision. Compared to the D-optimal design for the primary model, the design in Panel 3 will lead to a much smaller bias. This implies that an increased power for detecting lack-of-fit is to some extent related to a smaller bias. Further increasing α_2 to one allows an even better detection of the lack-of-fit and also leads to a slightly smaller bias (see Panel 4). Choosing $\alpha_2=\alpha_3=1$ or larger values for α_2 and α_3 produces a design

1. $\alpha_2 = 0, \alpha_3 = 0$
$\Rightarrow$ D_1-optimal

DX1	0.0816
Dlof	-
Dbias	2.44570

2. $\alpha_2 = 0$, $\alpha_3 = 10$
$\Rightarrow$ minimal bias

DX1	0.1211
Dlof	0.2452
Dbias	1.0004

3. $\alpha_2 = \frac{q}{p} = \frac{1}{3}, \alpha_3 = 0$
$\Rightarrow$ D_{full}-optimal

DX1	0.0928
Dlof	0.0705
Dbias	1.5370

4. $\alpha_2 = 1$, $\alpha_3 = 0$
$\Rightarrow$ good LOF

DX1	0.0955
Dlof	0.0659
Dbias	1.4556

5. $\alpha_2 = 1$, $\alpha_3 = 1$
$\Rightarrow$ good bias & LOF

DX1	0.1184
Dlof	0.0615
Dbias	1.0052

Fig. 1. GD-optimal designs for several values of α_2 and α_3, and for $\tau^2 = \infty$.

that is good for detecting lack-of-fit and that leads to a limited amount of bias (see Panel 5). Introducing finite values for τ^2 creates no new designs for this example. Probably, this is due to the fact that $n > p + q$.

The average squared prediction variance and average squared bias for an arbitrary value of β_3 are given in Table 1 . The value chosen is $\beta_3 = 1$. The table also contains the noncentrality parameter δ for the lack-of-fit test. The table shows that the loss of precision in the estimation of the primary model is compensated by substantial reductions in the bias and by the ability to test for lack-of-fit. Table 1 also shows that choosing positive values for both α_2 and α_3 (design option 5) leads to a design that performs excellently with respect to both bias (1.0052) and detection of lack-of-fit (large δ). Using a positive α_2 and setting $\alpha_3 = 0$ (design options 3 and 4) provides a design that allows a good detection of the lack-of-fit (large δ) but it also leads to a substantial reduction in the bias (considerably smaller than the value of 2.4457 for design option 1). Using a positive α_3 and setting $\alpha_2 = 0$ (design option 2) leads to a small bias (1.0004), but the resulting design does not perform that well as to the

Table 1
Bias, variance and lack-of-fit measures

Design	Bias^2	Avg var	δ	p-value for lof
1	2.4457	0.1345	—	—
2	1.0004	0.1652	4.0774	0.0740
3	1.5370	0.1130	14.1928	0.0114
4	1.4556	0.1313	15.1686	0.0101
5	1.0052	0.1562	16.2521	0.0089

detection of the lack-of-fit (small δ). As a result, designs that perform well with respect to lack-of-fit detection also perform reasonably well with respect to the bias, but the opposite is not necessarily true. DuMouchel and Jones (1994) point out that an idea of the significance of the lack-of-fit test can be obtained by assuming that the expectation of the F-statistic

$$F = \frac{(\text{SSE(primary model)} - \text{SSE(full)})/d_1}{\text{SSE(full)}/(n-d_2)},$$

with SSE(M) the sum of squared errors of model M and d_1 and d_2 the degrees of freedom for the test, is equal to

$$F_s \approx \frac{\mathbf{E}((\text{SSE(primary model)} - \text{SSE(full)})/d_1)}{\mathbf{E}(\text{SSE(full)}/d_2)} = \frac{\sigma^2 + \delta\sigma^2/d_1}{\sigma^2} = 1 + \frac{\delta}{d_1},$$

where δ is the noncentrality parameter introduced in (3). The number d_1 is equal to q if it is possible to test the full model, whereas $d_2 = n$—total number of independent parameters in the full model. The p-values obtained using the F_s-statistic are displayed in the last column of Table 1. It is clear than choosing a positive value for α_2, as in design options 3, 4 and 5, leads to small p-values, indicating that a powerful lack-of-fit test can be carried out if any of these designs is used.

5.1.2. Comparison to equidistant design

A recurring theme in the literature on model-robust designs is that equidistant or uniform designs perform well in terms of bias reduction and protection against lack-of-fit. For the present design region and $n = 8$, such a design would have observations at ± 1, ± 0.7143, ± 0.4286 and ± 0.1429. In Table 2, the performance with respect to precision (DX1), lack-of-fit (Dlof) and bias (Dbias) of the equidistant design is compared to that of the five designs in Fig. 1. The performances of the six design options displayed in the table are relative with respect to design options 1, 5 and 2 because these are the best designs with respect to precision, lack-of-fit and bias, respectively. The equidistant design performs quite well with respect to bias, but it does not allow a very good detection of lack-of-fit. Overall, the design displayed in Panel 5 of Fig. 1 seems to be a better choice, as this design performs better with respect to bias and lack-of-fit, while it is only slightly worse in terms of precision.

The equidistant design is easy to construct in the case of a single experimental variable. When more than one variable is involved in an experiment and the number of observations available is small, it becomes much more difficult to construct these type of designs. This of

Table 2
Performance of the equidistant design compared to the five designs in Fig. 1.

Design	DX1	Dlof	Dbias
1	100.00%	—	36.49%
2	67.37%	25.07%	100.00%
3	87.92%	87.25%	58.17%
4	85.46%	93.19%	61.59%
5	68.95%	100.00%	98.16%
Equidist.	75.20%	66.95%	83.28%

course limits their attractiveness. For the next examples, some of which have a constrained design region, we will not discuss the equidistant design explicitly anymore. It can however be seen that some of the designs produced by the approach presented in this paper provide a good coverage of the entire design region.

5.2. *Two dimensions*

As another illustration, consider the two-dimensional problem where the primary model consists of $p=4$ terms, that is $\beta_0+\beta_1x_1+\beta_2x_2+\beta_{12}x_1x_2$, and the full model has $q=2$ extra potential terms: $\beta_{11}x_1^2+\beta_{22}x_2^2$. The design region considered is a 5×5 grid on $[-1,+1]^2$.

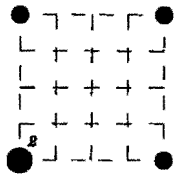
For $n=5$, we found the three designs displayed in Fig. 2. The first design is a D-optimal design for the primary model. The second design is obtained as soon as the values of α_2 and/or α_3 become noticeably larger than zero. The design in Panel 3 is obtained for larger values of α_2 and α_3. The design in Panel 2 of Fig. 2 was also found by DuMouchel and Jones (1994) and supports the common practice of adding center points to a design in order to carry out a lack-of-fit test.

As $n<p+q$ in this example, a finite τ-value had to be used to obtain a nonsingular dispersion matrix $\mathbf{L}$. For the same reason, Dlof will not exist for the designs shown. Therefore, Dlof_τ-values that are defined as $|\mathbf{L}+\mathbf{I}_q/\tau^2|^{-1/q}$ will be reported instead of the Dlof-values defined earlier. The results reported were obtained for $\tau=1$. The same designs can also be found for other values of τ.

For $n=8$ and $\tau^2=\infty$, we obtain a larger number of different designs. The most important ones are represented in Fig. 3. Panel 1 shows a duplicated 2^2 factorial design, which is the D_1-optimal 8-point design for the primary model. When α_3 is increased, this design gradually changes into a 2^2 factorial design with four center points (see Panel 3). The design obtained for $\alpha_3=2$ covers the entire design region very well and is displayed in Panel 2 of Fig. 3. When α_2 is increased, most design points move away from the cornerpoints. This allows the lack-of-fit to be tested and the bias to be reduced to some extent. For a good performance on both criteria, it is necessary to choose positive values for both α_2 and α_3. This is illustrated in the Panels 6 and 7 of Fig. 3. Introducing finite values for τ^2 does not lead to new designs in this example.

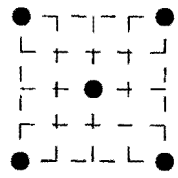
1. $\alpha_2 = \alpha_3 = 0 \Rightarrow D_1$-optimal

DX1	0.1051
$Dlof_\tau$	-
Dbias	1.9640



2. $\alpha_2 = \alpha_3 = 0.1$

DX1	0.1182
$Dlof_\tau$	0.3140
Dbias	1.4243



3. $\alpha_2 = \alpha_3 = 5$

DX1	0.2585
$Dlof_\tau$	0.2825
Dbias	1.0424

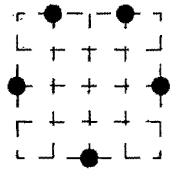


Fig. 2. GD-optimal 5-point designs for several values of α_2 and α_3, and for $\tau^2 = 1$.

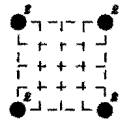
5.3. *A constrained design region*

We reconsider the second example of DuMouchel and Jones (1994) with two constrained variables. In the example, $x_1 + x_2 \leqslant 1$ so that the set of candidate points only contains 15 points on a triangle. The primary model is the full quadratic model in the two variables, so that $p = 6$. The full model includes $q = 4$ potential cubic terms: $x_1^3, x_1^2x_2, x_1x_2^2, x_2^3$. The number of observations n equals nine. As $n < p + q$, a finite τ-value had to be used. The results for $\tau = 1$ are displayed in Fig. 4.

From Panel 1 in Fig. 4, it can be seen that the D_1-optimal design has minimum support, i.e. the number of distinct design points of the design is equal to the number of parameters in the primary model. When α_2 and/or α_3 are increased, the number of distinct design points is increased so that the bias is substantially decreased and the ability to test for lack-of-fit is substantially increased. As in the previous example, it is important to select positive values for α_2 and α_3 for a good performance on both criteria. Note that, when α_2 and/or α_3 are large, then the GD-optimal designs contain nine distinct design points, as can be seen in the Panels 2, 3 and 4 of Fig. 4.

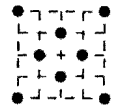
1. $\alpha_2 = \alpha_3 = 0$
$\Rightarrow$ D_1-optimal

DX1	0.0625
Dlof	-
Dbias	1.9639



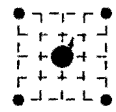
2. $\alpha_2 = 0, \alpha_3 = 2$
$\Rightarrow$ small bias

DX1	0.0991
Dlof	0.2828
Dbias	1.0221



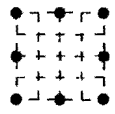
3. $\alpha_2 = 0, \alpha_3 = 5$
$\Rightarrow$ minimal bias

DX1	0.1051
Dlof	-
Dbias	1.0000



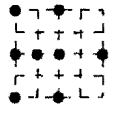
4. $\alpha_2 = \frac{q}{p}, \alpha_3 = 0$
$\Rightarrow$ D_{full}-optimal

DX1	0.0857
Dlof	0.1237
Dbias	1.3093



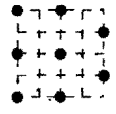
5. $\alpha_2 = 10, \alpha_3 = 0$
$\Rightarrow$ good w.r.t. LOF

DX1	0.1540
Dlof	0.1029
Dbias	1.1492



6. $\alpha_2 = \alpha_3 = 5$
$\Rightarrow$ good w.r.t. bias & LOF

DX1	0.1155
Dlof	0.1115
Dbias	1.1014



7. $\alpha_2 = 5, \alpha_3 = 10$
$\Rightarrow$ good w.r.t. bias & LOF

DX1	0.1216
Dlof	0.1265
Dbias	1.0164

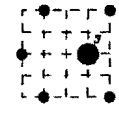


Fig. 3. GD-optimal 8-point designs for several values of α_2 and α_3, and $\tau^2 = \infty$.

6. Conclusions

In this paper, we have derived a generalization of several existing design criteria in order to take into account possible misspecification of the model when designing an experiment. Traditionally, the optimal design approach assumes that the specified model is known. In most applications however, the model is unknown. The design criteria presented are the first to take into account the potential bias from the unknown true model as well as the power of a lack-of-fit test. Several simple examples are used to illustrate the properties of the designs produced by the new criteria. The examples show that the new design criteria lead to designs that perform well with respect to bias and with respect to the detection of lack-of-fit, while maintaining a reasonable estimation precision for the assumed model. Based on

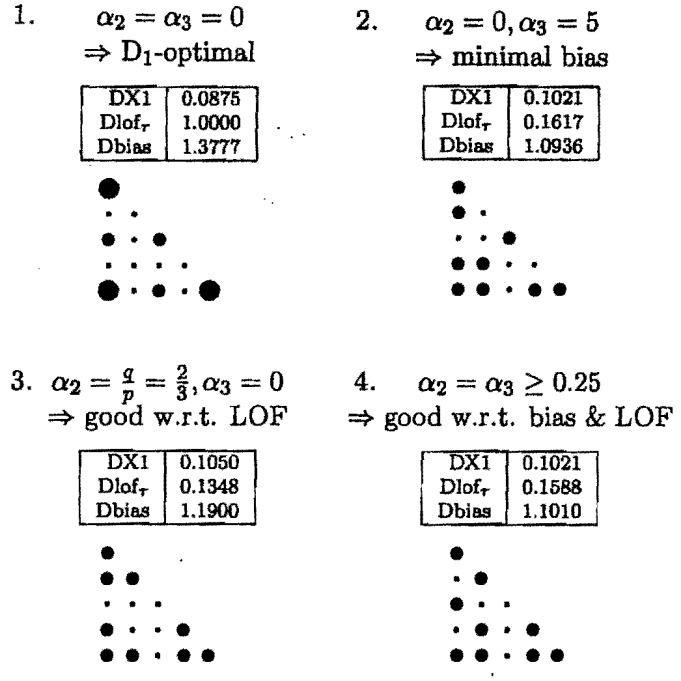


Fig. 4. GD-optimal designs for several values of α_2 and α_3, $\tau = 1$.

our experience with the design criteria, we would recommend trying several values for α_2 and α_3 and evaluating the resulting designs with respect to precision, detection of lack-of-fit and bias. For the instances discussed in this paper and for the practical application in Goos et al. (2002), α_2- and α_3-values of 5 to 10 led to a reasonable trade-off between these three objectives. In general, the choice of α_2 and α_3 is however fairly subjective.

The GD-optimality criterion presented here was successfully embedded in a two-stage approach in Ruggoo and Vandebroek (2003). They use a positive α_2-value and $\alpha_3 = 0$ for computing a first stage design. In doing so, they neglect bias in the first stage and concentrate a substantial amount of experimental effort on the detection of deviations from the assumed model. In the second stage, α_2 is set to zero and a positive α_3 is used to minimize the bias from the unknown true model after all the data have been collected.

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