Uncertain Resources and Designing for Additional Information

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ABSTRACT: In the present paper the concept of uncertain resources in experimental design is extended to situations in which the desire for additional information increases with the amount of experiments available. For a number of simple but relevant examples different strategies are compared and optimal designs are developed in the scope of the theory of generalized designs.

Key words: linear model, interactions, main effects, D-optimality, weighted optimality criteria, generalized design, marginal model.
AMS Subject Classification: 62K05

1. Introduction

Starting from the work of Mandal, Shah and Sinha (1991) the concept of uncertain resources has got increasing importance in the field of experimental design. The idea behind that concept can be described as follows: At the beginning of an experiment it is only sure that a comparatively small number of experiments can be performed and that there is a specified chance that additional experiments may be available on a second step. These additional experiments constitute the uncertain resources.

At the first glance there is no need for particular investigations on uncertain resources in the theory of *approximate* or *generalized* designs, because all experimental units can be subdivided in a suitable way, such that both the starting design as well as the design augmented with the additional resources can be chosen in an optimal way.

However, the quality of the inference based on any design is a direct function of the amount of experimental material available in it. Thus it is quite natural to start with a small amount of information desired in the starting design and increase the qualitative amount of information simultaneously with the amount of experiments available. This means that the underlying model can be investigated more precisely if the additional resources are present.

We will consider a general linear model

$$E(X(t)) = f(t)^T\theta$$

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for the outcome $X(t)$ of an experiment based on the setting $t = (t_1, ..., t_K)$ for the adjustable factors. This includes models with both qualitative and quantitative factors of influence (see Kurotschka (1984)). Based on the starting design of size (resource) R_1 we are interested only in a subset β_1 of the whole unknown parameter vector θ whereas additional experiments can be used to investigate a larger subset β_2 including β_1, e. g. $\beta_2 = \theta$. These additional uncertain resources of size $R_2 - R_1$ may become available with a prespecified probability α giving an augmented design of size R_2, while with probability $1 - \alpha$ only the experiments from the starting design are available.

In the setting of generalized designs we are looking for design pairs (δ_1, δ_2) under the side condition $R_1\delta_1 \leq R_2\delta_2$ - with the interpretation that $R_1\delta_1$ is the starting design, $R_2\delta_2$ is the augmented design, and $R_2\delta_2 - R_1\delta_1$ is the design for the supplementary experiments. Here, as usual, δ_1 and δ_2 are supposed to be discrete designs with finite support and weights summing up to 1.

There are two appealing strategies proposed by Mandal, Shah and Sinha (1991). Strategy I starts with an optimal starting design δ_1^* for β_1 and looks for an augmentation $\overline{\delta}_2$ optimal for β_2, whereas strategy II is oriented backwards and starts from an optimal design δ_2^* for β_2 in the augmented experiment and looks for a reduced design $\overline{\delta}_1$ which is optimal for β_1 (see Section 3). An early attempt to those strategies can be also found in Smith and Schmoyer (1982) and an iterative version of a strategy I type procedure has been considered e. g. by Chow (1992). An application to the setting of computer experiments has been given by Abt and Sinha (1993).

The present design problem leads to weighted optimality criteria such as those introduced by Läuter (1974) for the related situation of uncertain modelling (see also Bunke and Bunke (1986) and Bandemer et al. (1977) for a general treatment). The criteria are redefined in Section 2 to fit them to the present situation of uncertain resources and designing for additional information. Section 3 deals with the strategies I and II in relation to the optimality criteria. The implications are illustrated in the subsequent sections.

In particular, we will demonstrate these concepts in a simple one-dimensional regression model (Section 4) and in the setting of multi-factor models, i. e. models which depend on a number of different factors of influence (Section 5). There, in the starting design only main effects are considered to be of interest whereas in the presence of the additional resources also the interaction terms are to be investigated.

2. Criteria

Any reasonable criterion for judging a design pair (δ_1, δ_2) should be based on the information or covariance for the starting design $R_1\delta_1$ - weighted by the probability $1 - \alpha$ of no additional experiments - and on the information or covariance for the supplemented design $R_2\delta_2$ - weighted by the probability α of additional experiments. Apart from the approach by Mandal, Shah and Sinha (1991) which cannot be applied directly to the present situation of increasing interest in additional parameters there is a bulk of criteria which can be regarded as a generalization of the common D-criterion of minimizing the generalized variance (for the related generalization problem in a Bayesian approach see e. g. Atkinson and Donev (1992), p. 214).

Let $\mathbf{I}_1(\delta_1)$ be the information matrix of δ_1 associated with the parameters β_1 of interest in the starting experiment and let $\mathbf{I}_2(\delta_2)$ be the information matrix of δ_2 associated with the (larger) set of parameters β_2 which are to be investigated in the supplemented experiment. Particular examples will be given later on. Then, up to a constant factor σ^2, $\frac{1}{R_1}\mathbf{I}(\delta_1)^{-1}$ is the covariance matrix for the best linear unbiased estimator $\widehat{\beta}_1$ of β_1 based on the starting design of size R_1, and $\frac{1}{R_2}\mathbf{I}(\delta_2)^{-1}$ is the covariance matrix for the estimator $\widehat{\beta}_2$ of β_2 based on the supplemented experiment of size R_2.

The most reasonable design criterion is the expected generalized variance

$$EV(\delta_1, \delta_2) = \frac{\alpha}{R_2} \det \mathbf{I}_2(\delta_2)^{-1/p_2} + \frac{1-\alpha}{R_1} \det \mathbf{I}_1(\delta_1)^{-1/p_1}$$

which is to be minimized. Note that in order to make the information matrices $\mathbf{I}_1(\delta_1)$ and $\mathbf{I}_2(\delta_2)$ comparable their determinants have to be normalized by the power of one over the dimension p_1 and p_2 of the corresponding parameters β_1 and β_2 respectively. Note also that $\det\mathbf{I}_1(R_1\delta_1) = R_1^{p_1}\det\mathbf{I}_1(\delta_1)$ and $\det\mathbf{I}_2(R_2\delta_2) = R_2^{p_2}\det\mathbf{I}_2(\delta_2)$.

Alternatively one can consider the expected information

$$EI(\delta_1, \delta_2) = \alpha R_2 \det \mathbf{I}_2(\delta_2)^{1/p_2} + (1-\alpha)R_1 \det \mathbf{I}_1(\delta_1)^{1/p_1}$$

which is to be maximized. The latter is related to the C-criterion of Läuter (1974) who also proposed a criterion of the relative efficiency in the information which can be defined after renormalization according to

$$\mathrm{eff}(\delta_1, \delta_2) = \alpha \left(\frac{\det \mathbf{I}_2(\delta_2)}{\det \mathbf{I}_2(\delta_2^*)} \right)^{1/p_2} + (1-\alpha) \left(\frac{\det \mathbf{I}_1(\delta_1)}{\det \mathbf{I}_1(\delta_1^*)} \right)^{1/p_1}$$

which is to be maximized, where δ_1^* and δ_2^* are the D-optimal designs for β_1 and β_2 respectively. More reasonable again seems to be the minimization problem of the relative deficiency in the generalized variance

$$\mathrm{def}(\delta_1, \delta_2) = \alpha \left(\frac{\det \mathbf{I}_2(\delta_2)}{\det \mathbf{I}_2(\delta_2^*)} \right)^{-1/p_2} + (1-\alpha) \left(\frac{\det \mathbf{I}_1(\delta_1)}{\det \mathbf{I}_1(\delta_1^*)} \right)^{-1/p_1}$$

Also logarithmic versions of the criteria are of interest. For example, maximizing the expected logarithmic information

$$E_{\log}I(\delta_1, \delta_2) = \frac{\alpha}{p_2} \ln \det \mathbf{I}_2(\delta_2) + \frac{1-\alpha}{p_1} \ln \det \mathbf{I}_1(\delta_1),$$

which is related to Läuter's (1974) S-criterion, is equivalent to minimizing the expected logarithmic generalized variance $E_{\log}V = -E_{\log}I$. For a recent treatment of the last criterion in the related setting of uncertain modelling see e. g. Dette (1990).

All of the above criteria depend on the sizes of the resources through the proportion $\varrho = \frac{R_1}{R_2}$. In particular, for the efficiency, the deficiency and the logarithmic criterion this dependence comes in only by the constraint $\delta_2 \geq \varrho\delta_1$. In the subsequest examples the different influence on the optimality of design pairs (δ_1, δ_2) will be exhibited for each criterion. However, note that in case that the D-optimal designs δ_1^* and δ_2^* for the parameters β_1 and β_2 respectively satisfy the relation $\delta_2^* \geq \varrho\delta_1^*$ then the design pair (δ_1^*, δ_2^*) with the supplementary design $R_2\delta_2^* - R_1\delta_1^*$ is optimal with respect to each of the above criteria. Therefore the original problem of Mandal, Shah and Sinha (1991) in which $\beta_2 = \beta_1$ has a straightforward solution (δ_1^*, δ_1^*) in the setting of generalized designs.

3. Two Basic Strategies

Mandal, Shah and Sinha (1991) proposed to consider design pairs (δ_1, δ_2) in which either the starting design δ_1^* or the augmented design δ_2^* is optimal. In the first case the additional design $R_2\delta_2 - R_1\delta_1^*$ is chosen to obtain the best possible design $\overline{\delta}_2$ (strategy I), whereas in the second case a fraction $R_2\delta_2^* - R_1\delta_1$ is deleted from δ_2^* in such a way that the best possible desgin $\overline{\delta}_1$ remains (strategy II).

Let δ_1^* be D-optimal for β_1, i. e. δ_1^* maximizes $\det \mathbf{I}_1(\delta_1)$. The strategy I results in a design pair $(\delta_1^*, \overline{\delta}_2)$, where $\overline{\delta}_2$ maximizes $\det \mathbf{I}_2(\delta_2)$ under the constraint $\delta_2 \geq \varrho\delta_1^*$. Given δ_1^* the pair $(\delta_1^*, \overline{\delta}_2)$ is simultaneously optimal for each of the criteria introduced in the previous section and for each α. Analogoulsy, let δ_2^* be D-optimal for β_2, i. e. δ_2^* maximizes $\det \mathbf{I}_2(\delta_2)$. Then strategy II yields a design pair $(\overline{\delta}_1, \delta_2^*)$, where $\overline{\delta}_1$ maximizes $\det \mathbf{I}_1(\delta_1)$ under the constraint $\delta_1 \leq \varrho^{-1}\delta_2^*$. Given δ_2^* the pair $(\overline{\delta}_1, \delta_2^*)$ is simultaneously optimal for each criterion and each α. (For a recent survey on optimal desings under constraints see Cook and Fedorov (1994).)

Obviously, strategy I is preferable to strategy II if the probability α for the additional experiments is small, whereas strategy II dominates strategy I for large probabilities α. More precisely, in the general situations that neither δ_1^* nor δ_2^* is optimal for the alternative problem, there will be a critical value α_0 for each criterion such that strategy I produces a better design than strategy II for $\alpha < \alpha_0$, and vice versa for $\alpha > \alpha_0$.

4. An Example in Polynomial Regression

We start with a quite simple illustrating example. Assume that the underlying model equation is given by a one-dimensional quadratic regression

$$E(X(t)) = \theta_0 + \theta_1 t + \theta_2 t^2$$

on the standardized interval $-1 \leq t \leq 1$. In the starting experiment we are interested in the slope and the intercept, i. e. $\beta_1 = (\theta_0, \theta_1)$, whereas in case of additional experiments we are willing to investigate the whole parameter vector $\beta_2 = (\theta_0, \theta_1, \theta_2)$. Both the D-optimal designs δ_1^* and δ_2^* for β_1 and β_2 respectively are concentrated on $\{-1, 0, 1\}$. δ_1^* assigns weight $\frac{1}{2}$ to the midpoint 0 and weights $\frac{1}{4}$ to each of the endpoints -1 and 1, whereas δ_2^* assigns equal weights $\frac{1}{3}$ to each of them.

In case that the additional resource $R_2 - R_1$ exceeds $\frac{1}{2}R_1$ we observe that $R_1\delta_1^* \leq R_2\delta_2^*$ and the design pair (δ_1^*, δ_2^*) is optimal. So, we can start with a D-optimal design $R_1\delta_1^*$ for β_1 and augment it to a D-optimal design $R_2\delta_2^*$ for β_2 in case of availability of the additional resources.

		$R_1 = 24$			$R_1 = 28$		
		-1	0	1	-1	0	1
strategy I:	$R_1\delta_1^*$	6	12	6	7	14	7
	$R_2\overline{\delta}_2$	9	12	9	8	14	8
strategy II:	$R_2\delta_2^*$	10	10	10	10	10	10
	$R_1\overline{\delta}_1$	7	10	7	9	10	9

Table 1: design pairs $(\delta_1^*, \overline{\delta}_2)$ and $(\overline{\delta}_1, \delta_2^*)$, $R_1 = 24(28)$, $R_2 = 30$

criterion	$\varrho \to \frac{2}{3}$	$\varrho = \frac{24}{30}$	$\varrho = \frac{28}{30}$	$\varrho = 1$
EV	0.7605	0.6636	0.5695	0.5242
EI	0.5575	0.5288	0.5056	0.4953
eff	0.6667	0.5975	0.5370	0.5095
def	0.6667	0.5986	0.5385	0.5101
$E_{\log} I$	0.6667	0.5981	0.5377	0.5098

Table 2: critical values α_0

In the more interesting case $R_2 - R_1 < \frac{1}{2}R_1$, i. e. $\varrho = \frac{R_1}{R_2} > \frac{2}{3}$, such an augmentation is no longer possible. For strategy I only experiments at the endpoints -1 and 1 are to be added to $R_1\delta_1^*$ and the design $\overline{\delta}_2$, which assigns weights $\frac{1}{2}\varrho$ to 0 and $\frac{1}{4}(2-\varrho)$ to -1 and 1 each, is D-optimal for β_2 under the constraint $R_2\delta_2 \geq R_1\delta_1^*$. Alternatively , for strategy II, only experiments at the endpoints -1 and 1 are to be deleted to obtain the D-optimal design $\overline{\delta}_1$ under the constraint $R_1\delta_1 \leq R_2\delta_2^*$. Here, $\overline{\delta}_1$ assigns weights $\frac{1}{3}\varrho^{-1}$ to 0 and $\frac{1}{6}(3-\varrho^{-1})$ to -1 and 1 each. For the example $R_1 = 24(28)$ and $R_2 = 30$ the corresponding designs are presented in Table 1.

In Table 2 we exhibit critical values α_0 for each criterion for which the strategy I design $(\delta_1^*, \overline{\delta_2})$ is preferable in case $\alpha < \alpha_0$ and the strategy II design $(\overline{\delta}_1, \delta_2^*)$ performs better in case $\alpha > \alpha_0$. The second and third column present values of α_0 for the example $R_1 = 24(28)$ and $R_2 = 30$ of Table 1.

Despite their appealing simplicity both strategies do not produce an optimal design pair $(\delta_1, \delta_2)^*$ in general. In Table 3 optimal design pairs $(\delta_1, \delta_2)^*$ concentrated on $\{-1, 0, 1\}$ are given by their weights $\delta_1(0) = w^*$ and $\delta_2(0) = \varrho w^*$ for different values of α. The corresponding weights on ± 1 equal $\frac{1}{2}(1-w^*)$ and $\frac{1}{2}(1-\varrho w^*)$ respectively. Recall that $w^* = \frac{1}{2}$ for $\alpha = 0$ and $w^* = \varrho^{-1}\frac{1}{3}$ for $\alpha = 1$.

Table 4 exhibits integer approximations to the optimal design pairs $(\delta_1, \delta_2)^*$ in case of probabilities $\alpha = 0.25$, 0.5 and 0.75 for the availibility of additional experiments.

criterion	$\varrho = \frac{24}{30}$, $\alpha = 0.25$	$\alpha = 0.5$	$\alpha = 0.75$	$\varrho = \frac{28}{30}$, $\alpha = 0.25$	$\alpha = 0.5$	$\alpha = 0.75$
EV	0.4879	0.4717	0.4493	0.4701	0.4371	0.4001
EI	0.4810	0.4604	0.4388	0.4648	0.4283	0.3919
eff	0.4848	0.4663	0.4437	0.4681	0.4329	0.3954
def	0.4847	0.4662	0.4439	0.4670	0.4328	0.3965
$E_{\log} I$	0.4601	0.4385	0.4254	0.4216	0.3871	0.3685

Table 3: optimal weights w^* for different α and ϱ

		$R_1 = 24$								
		$\alpha = 0.25$			$\alpha = 0.5$			$\alpha = 0.75$		
criterion		-1	0	1	-1	0	1	-1	0	1
EV	$R_1\delta_1$	6	12	6	6	12	6	6	11	7
	$R_2\delta_2$	9	12	9	9	12	9	9	11	10
EI	$R_1\delta_1$	6	12	6	6	11	7	7	10	7
	$R_2\delta_2$	9	12	9	9	11	10	10	10	10
eff	$R_1\delta_1$	6	12	6	6	11	7	7	10	7
	$R_2\delta_2$	9	12	9	9	11	10	10	10	10
def	$R_1\delta_1$	6	12	6	6	12	6	6	11	7
	$R_2\delta_2$	9	12	9	9	12	9	9	11	10
$E_{\log} I$	$R_1\delta_1$	6	12	6	6	12	6	7	10	7
	$R_2\delta_2$	9	12	9	9	12	9	10	10	10
		$R_1 = 28$								
		$\alpha = 0.25$			$\alpha = 0.5$			$\alpha = 0.75$		
EV	$R_1\delta_1$	7	14	7	8	12	8	8	11	9
	$R_2\delta_2$	8	14	8	9	12	9	9	11	10
EI	$R_1\delta_1$	7	13	8	8	12	8	8	11	9
	$R_2\delta_2$	8	13	9	9	12	9	9	11	10
eff	$R_1\delta_1$	8	12	8	8	12	8	9	10	9
	$R_2\delta_2$	9	12	9	9	12	9	10	10	10
def	$R_1\delta_1$	7	14	7	8	12	8	8	12	8
	$R_2\delta_2$	8	14	8	9	12	9	9	12	9
$E_{\log} I$	$R_1\delta_1$	7	13	8	8	12	8	8	11	9
	$R_2\delta_2$	8	13	9	9	12	9	9	11	10

Table 4: "exact" optimal designs $(R_1\delta_1, R_2\delta_2)^*$

5. Two-factor Models

We consider models with complete product type interactions

$$E(X(t_1,t_2)) = (f_1(t_1) \otimes f_2(t_2))^T \theta$$

where $\otimes$ denotes the Kronecker product. Particular models possessing that structure are two-way layouts

$$E(X(i,j)) = \mu + \alpha_i^{(1)} + \alpha_j^{(2)} + \gamma_{ij}$$

linear regression

$$E(X(t_1,t_2)) = \theta_0 + \theta_1 t_1 + \theta_2 t_2 + \theta_{12} t_1 t_2$$

or, more complicated, intra-class models

$$E(X(i,t)) = \theta_{i0} + \theta_{i1} t$$

(see Kurotschka (1984)). In all those models product type designs $\delta_{(1)}^* \otimes \delta_{(2)}^*$ are known to be D-optimal for the whole parameter vector $\beta_2 = \theta$ if the components $\delta_{(k)}^*$ are D-optimal in the corresponding marginal models

$$E(X_{(k)}(t_k)) = f_k(t_k)^T \theta_{(k)}$$

(see Hoel (1965)). However, product type designs are not necessarily optimal for the subset of parameters β_1 associated with the main effects. (For exceptional situations see Schwabe (1995).) The construction of design pairs (δ_1, δ_2) for uncertain resources in two-factor models will be illustrated by means of the above mentioned examples.

Linear Regression.

Consider the unit square $0 \leq t_1, t_2 \leq 1$ as the underlying desing region. The product type design $\delta_2^* = \delta_{(1)}^* \otimes \delta_{(2)}^*$ which assigns equal weights $\frac{1}{4}$ to the four corners $(0,0)$, $(0,1)$, $(1,0)$ and $(1,1)$ of the square is D-optimal for the whole parameter vector $\beta_2 = \theta$. However, for the main effects $\beta_1 = (\theta_0, \theta_1, \theta_2)$ the observations at $(1,1)$ are of no use and the optimal design δ_1^* for β_1 assigns equal weights $\frac{1}{3}$ to the remaining relevant corners $(0,0)$, $(0,1)$ and $(1,0)$.

In case $\varrho = \frac{R_1}{R_2} > \frac{3}{4}$ the optimal design $R_1\delta_1^*$ for β_1 cannot be augmented to an optimal design $R_2\delta_2^*$ for β_2^*. Similarly to the example of quadratic regression in the previous section we can construct strategy I and strategy II designs (Table 5) for which the augmented design $\overline{\delta}_2$ assigns weight $1-\varrho$ to $(1,1)$ and the reduced design $\overline{\delta}_1$ assigns weight $\varrho - \frac{3}{4}$ to $(1,1)$ and equal weights to the remaining corners respectively. We determine their critical values (Table 6), derive optimal design pairs (Table 7) with $\delta_1(1,1) = w^*$, $\delta_2(1,1) = 1 - \varrho(1-w^*)$ and equal weights $\frac{1}{3}(1-w^*)$ resp. $\frac{1}{3}\varrho(1-w^*)$ on $(0,0)$, $(0,1)$, $(1,1)$, and give some integer approximations (Table 8) which coincide for all criteria in the present situation.

		$R_1 = 27$				$R_1 = 30$			
		$(0,0)$	$(0,1)$	$(1,0)$	$(1,1)$	$(0,0)$	$(0,1)$	$(1,0)$	$(1,1)$
strategy I:	$R_1\delta_1^*$	9	9	9	0	10	10	10	0
	$R_2\overline{\delta}_2$	9	9	9	5	10	10	10	2
strategy II:	$R_2\delta_2^*$	8	8	8	8	8	8	8	8
	$R_1\overline{\delta}_1$	8	8	8	3	8	8	8	6

Table 5: design pairs $(\delta_1^*, \overline{\delta}_2)$ and $(\overline{\delta}_1, \delta_2^*)$, $R_1 = 27(30)$, $R_2 = 32$

criterion	$\varrho \to \frac{3}{4}$	$\varrho = \frac{27}{32}$	$\varrho = \frac{30}{32}$	$\varrho \to 1$
EV	0.5323	0.3379	0.0983	0
EI	0.3763	0.2841	0.1190	0
eff	0.4605	0.3328	0.1326	0
def	0.4459	0.2888	0.0879	0
$E_{\log}I$	0.4536	0.3114	0.1093	0

Table 6: critical values α_0

	$\varrho = \frac{27}{32}$			$\varrho = \frac{30}{32}$		
criterion	$\alpha = 0.25$	$\alpha = 0.5$	$\alpha = 0.75$	$\alpha = 0.25$	$\alpha = 0.5$	$\alpha = 0.75$
EV	0	0	0.0417	0.0182	0.0790	0.1375
EI	0	0	0.0314	0	0.0501	0.1282
eff	0	0	0.0386	0	0.0675	0.1402
def	0	0	0.0357	0.0078	0.0660	0.1271
$E_{\log}I$	0	0	0.0370	0	0.0667	0.1333

Table 7: optimal weights w^* for different α and ϱ

		$R_1 = 27$				$R_1 = 30$			
criterion		$(0,0)$	$(0,1)$	$(1,0)$	$(1,1)$	$(0,0)$	$(0,1)$	$(1,0)$	$(1,1)$
$\alpha = 0.25$	$R_1\delta_1$	9	9	9	0	10	10	10	0
	$R_2\delta_2$	9	9	9	5	10	10	10	2
$\alpha = 0.5$	$R_1\delta_1$	9	9	9	0	10	9	9	2
	$R_2\delta_2$	9	9	9	5	10	9	9	4
$\alpha = 0.75$	$R_1\delta_1$	9	9	8	1	9	9	8	4
	$R_2\delta_2$	9	9	8	6	9	9	8	6

Table 8: "exact" optimal designs $(R_1\delta_1, R_2\delta_2)^*$

Note that for a different design region $-1 \le t_1, t_2 \le 1$ the product type design δ_2^* which assigns equal weights $\frac{1}{4}$ to each corner $(-1,-1)$, $(-1,1)$, $(1,-1)$ and $(1,1)$ is simultaneously D-optimal for β_1 and β_2 (see e. g. Schwabe (1995)) and (δ_2^*, δ_2^*) is an optimal design pair.

Two-way layout.

Assume that the settings $i = 0$ and $j = 0$ are control levels, which means that $\alpha_0^{(1)} = \alpha_0^{(2)} = 0$ and, additionally, for the corresponding interactions $\gamma_{0j} = \gamma_{i0} = 0$ for every setting i and j. The product type design $\delta_2 = \delta_{(1)}^* \otimes \delta_{(2)}^*$ which assigns equal weights $\frac{1}{(I+1)(J+1)}$ to each level combination (i,j) is D-optimal for the whole parameter vector $\beta_2 = (\mu, \alpha_1^{(1)}, \ldots, \alpha_I^{(1)}, \alpha_1^{(2)}, \ldots, \alpha_J^{(2)}, \gamma_{11}, \gamma_{12}, \ldots, \gamma_{IJ})$ where I and J are the numbers of non-control levels for the first and second factor respectively.

Again, for the main effects $\beta_1 = (\mu, \alpha_1^{(1)}, \ldots, \alpha_I^{(1)}, \alpha_1^{(2)}, \ldots, \alpha_J^{(2)})$ the D-optimal design δ_1^* is concentrated on those settings in which at least one control level is involved. More precisely, δ_1^* assigns equal weights $\frac{1}{I+J+1}$ to the settings $(0,0)$, $(0,1)$, ..., $(0,J)$, $(1,0)$, ..., $(I,0)$.

For $\frac{R_1}{R_2} > \frac{I+J+1}{(I+1)(J+1)}$ the design $R_1\delta_1^*$ cannot be augmented to $R_2\delta_2^*$ and designing for uncertain resources becomes important. This becomes relevant, for example, in case $I = J = 2$ if $R_2 < 1.8R_1$, and in case $I = 4$ and $J = 5$ if $R_2 < 3R_1$. In the simplest case $I = J = 1$ the results of Tables 5 to 8 carry over directly.

Intra-class model.

Consider the situation where the qualitative factor i acts on two levels 0 and 1 (the "0" denotes again a control level) and the quantitative factor t may vary on the standard interval $-1 \le t \le 1$.

The D-optimal design δ_2^* for the whole parameter vector $\beta_2 = \theta$ is given by the product type design $\delta_{(1)}^* \otimes \delta_{(2)}^*$ which assigns equal weights $\frac{1}{4}$ to $(0,1)$, $(0,-1)$, $(1,1)$ and $(1,-1)$. For the main effects $\beta_1 = (\theta_{00}, \theta_{01}, \theta_{10})$ the D-optimal design δ_1^* assigns weights $\frac{1}{3}$ to the control settings $(0,1)$ and $(0,-1)$ and reduced weights $\frac{1}{6}$ to the treatment settings $(1,1)$ and $(1,-1)$.

Again, for $\frac{R_1}{R_2} > \frac{3}{4}$ the design $R_1\delta_1^*$ cannot be augmented to $R_2\delta_2^*$ and designing for uncertain resources becomes relevant.

Remarks.

1. Note that in all examples the D-optimal design δ_1^* for the main effects can be written as $\delta_1^* = \frac{1}{p_{(1)}+p_{(2)}-1}(p_{(1)}\delta_{(1)}^* \otimes \delta_{(2)}^\circ + p_{(2)}\delta_{(1)}^\circ \otimes \delta_{(2)}^* - \delta_{(1)}^\circ \otimes \delta_{(2)}^\circ)$ where $p_{(k)}$ is the dimension of $\theta_{(k)}$ and $\delta_{(k)}^\circ$ is a suitable design which is optimal for the constant term in the kth marginal model, $k = 1, 2$.

2. In the presence of more than two factors of influence designing for uncertain resources becomes even more important as a substantially larger number of parameters is involved. Moreover, in a complete product type model β_2 may be a proper subset of the parameters, e. g. β_2 might collect all two-factor interactions besides the main effects β_1. Alternatively also models can be considered in which only interactions up to a certain order occur

(see Schwabe (1993) for optimal designs). Also block effects can be investigated more thorouhgly with the help of supplementary experiments.

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References

ABT, M. and B. K. SINHA (1993): Optimal strategies for computer experiments with uncertain resources. Universität Augsburg, *Anwendungsbezogene Optimierung und Steuerung, Report No. 450.*

ATKINSON, A. C. and A. N. DONEV (1992): *Optimum Experimental Designs.* Clarendon Press, Oxford.

BANDEMER, H. et al. (1977): *Theorie und Anwendung der optimalen Versuchsplanung I. Handbuch zur Theorie.* Akademie-Verlag, Berlin.

BUNKE, H. and O. BUNKE (Eds.) (1986): *Statistical Inference in Linear Models. Statistical Methods of Model Building, Vol. I.* Wiley, Chichester.

CHOW, K. L. (1992): A-optimal designs for supplementary experiments. *Theory Probab. Appl.* **37**, 126–129.

COOK, D. and V. FEDOROV (1995): Constraint optimization of experimental design. *Statistics* **26**, 129–178 (with discussion).

DETTE, H. (1990): A generalization of D- and D_1-optimal designs in polynomial regression. *Ann. Statist.* **18**, 1784–1804.

HOEL, P. G. (1965): Minimax designs in two dimensional regression. *Ann. Math. Statist.* **36**, 1097–1106.

KUROTSCHKA, V. G. (1984): A general approach to optimum design of experiments with qualitative and quantitative factors. In: J. K. GHOSH and J. ROY (Eds.): *Statistics: Applications and New Directions: Proceedings of the Indian Statistical Institute Golden Jubilee International Conference Calcutta 1981*, 353–368.

LÄUTER, E. (1974): Experimental design in a class of models. *Math. Operationsforsch. Statist.* **5**, 379–398.

MANDAL, N. K., K. R. SHAH and B. K. SINHA (1991): Uncertain resources and optimal designs: Problems and perspectives. *Calcutta Statist. Assoc. Bull.* **40**, 267–282.

SCHWABE, R. (1993): Experimental design for linear models with higher order interaction terms. In: H. SCHNEEWEISS and V. MAMMITZSCH (Eds.): *Proceedings of the 2nd Gauss Symposium, Conference B: Statistical Sciences, München 1993.* DeGruyter, Berlin (to appear).

SCHWABE, R. (1995): Model robust experimental design in the presence of interactions: The orthogonal case. In: A. PÁZMAN (Ed.): *PROBASTAT'94. Proceedings of the International Conference on Probability and Mathematical Statistics, Smolenice 1994. Tatra Mountains Math. Publ.* **7** (to appear).

SMITH, D. E. and D. D. SCHMOYER (1982): First-order "interruptible" designs. *Technometrics* **24**, 55–58.