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Partially orthogonal blocked three-level response surface designs

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1. Introduction

Designs for fitting second-order polynomial response surfaces to model the relationship between one or more response variables and several quantitative treatment factors have been studied since the pioneering work of [7]. The original emphasis was on sequences of small designs being used to sequentially explore promising regions of the factor space, fitting first-order polynomial models and then augmenting them to be able to fit the second-order model. The sequential nature of the design led to the introduction of the central composite design, which adds axial points and center points to a two-level factorial or fractional factorial design. This is particularly appropriate in experiments in which, to quote the first line of that paper, "experimentation is sequential and the error fairly small".

Response surface methods have also been adapted for use in many fields in which the error (run-to-run variation) is considerably larger and sequential experimentation is either impossible or most naturally carried out in larger stages than originally suggested by [7]. In such applications, the first experiment is usually considerably larger than envisaged by Box and Wilson and is therefore designed to fit the second-order polynomial in one stage. The large run-to-run variation also pushes the compromise between bias and variance more towards ensuring low variances for parameter estimators and this means that three-level designs are used much more often. Also, it is often necessary or economical to use only three levels of each factor for practical reasons. Because of the use of larger experiments and large background variation, blocking is very often desirable, so that larger sources of variation, e.g. between days, can be separated in the analysis to improve the precision of parameter estimates. Work on the blocking of response surface designs focuses on orthogonal blocking of central composite designs, or other classes of designs, such as Box-Behnken designs, both of which are available for only a very few specific run sizes. This paper describes a new method of constructing blocked three-level second-order response surface designs with several desirable properties.

The type of application which motivated this work includes experiments in food processing, in which the use of highly variable biological materials means that large run-to-run variation is common. Two particular applications, which illustrate the typical size of experiments we are considering, are as follows. [25] reported the results of an experiment to optimize the pre-treatment and drying conditions for the production of high quality potato cubes. Dehydration is one of the

Table 1: Factors and levels for potato cubes experiment

		Levels		
Factor	Units	-1	0	1
Blanching time	min	2	4	6
Sulfiting time	min	2	6	10
Initial drying time	min	40	60	80
Puffing time	s	40	50	60

major methods of food preservation and demand from the food industry for dehydrated potatoes is high. High temperature puffing is a process that leads to better quality dehydrated potatoes. In this experiment, four factors, each at three levels, as described in Table 1, were studied in 36 runs.

[20] reported an experiment which used seven three-level factors in 96 runs, to investigate the effects of refining and supplementation on the viscosity and energy density of weaning maize porridge. The factors studied were the level of refining, flour concentration, milk concentration, quantity of groundnut, cooking time, feeding temperature and shear speed. In such applications, experiments with up to about 100 runs are perfectly normal and advisable. The work presented here was developed in that context.

The rest of this paper is organized as follows. In Section 2 some useful properties of response surface designs are discussed and methods for obtaining unblocked designs with these properties are reviewed. A new method of obtaining blocked designs with these properties is introduced in Section 3 and guidelines for applying it are given in Section 4. The blocked designs obtained directly by this method may not allow the estimation of all polynomial effects. It is therefore shown in Section 5 how, by augmenting the blocks, the estimability of all polynomial effects can be ensured. Moreover, it is shown by example that the augmented blocked designs can be more efficient than traditional blocked three-level response surface designs. Although large blocks are suitable for many applications, designs in smaller blocks are obtained in Section 6. Section 7 rounds off the paper with a discussion.

2. Desirable properties of designs

Response surface designs should be chosen to have several desirable properties - [5] list fourteen, but there are others that could be added - and which of these are important depends on the applied context. When sequences of small experiments are run, there is considerable flexibility to drop factors which seem unimportant or to find a well-fitting polynomial model of the appropriate order.

When larger experiments are run in a single stage, such decisions have to be made at the analysis stage and so model selection becomes much more important. Model selection is made more robust and efficient if parameters are estimated orthogonally to each other and if all parameters of the same type (linear, quadratic or interaction) are estimated with the same variance. Many standard designs do indeed have these properties, but most blocked designs in use do not.

The familiar second-order model for a response surface experiment with q factors describes the expected response μ at the settings $x_1, \ldots, x_q$ of the factors by the equation

$$\mu = \alpha + \sum_{s=1}^{q} \beta_s x_s + \sum_{s=1}^{q} \beta_{ss} x_s^2 + \sum_{s=1}^{q-1} \sum_{t=s+1}^{q} \beta_{st} x_s x_t, \tag{1}$$

where α is the intercept and the parameters β_s, β_{ss} and β_{st} describe the linear, quadratic and interaction effects of the factors, respectively. Jointly, the latter $p = 2q + q(q-1)/2$ parameters are referred to as the polynomial effects. The experimental design region for the factor settings considered in the present paper is the hypercube $[-1, 1]^q$ so that $x_1, \ldots, x_q$ are values between -1 and 1. Responses from different runs of the experiment are assumed to be uncorrelated with constant variance.

D-optimal continuous designs for fitting the second-order model in a cuboidal design region [19, 13] have a very specific structure in the variance-covariance matrix. First, they have support on $\{-1, 0, 1\}^q$, i.e. they use only three levels of each factor. Secondly, they are *partially orthogonal*, i.e. all parameters of the second-order model can be estimated orthogonally, except for the quadratic parameters, which are correlated with each other and with the intercept. This partial orthogonality is almost always the best that can be achieved. Full orthogonality of all parameter estimators is only achieveable in a few very special cases, since the requirements for quadratic parameters to be estimated orthogonally (as in three-level orthogonal arrays) conflict with the requirements for interaction parameters to be estimated orthogonally (as in two-level orthogonal arrays of strength 4). Finally, D-optimal continuous designs are *factorwise balanced* [14], i.e. the variance-covariance matrix is invariant under permutations of factor labels. Note that factorwise balance means that the properties of the design are invariant to relabelling of the factors. It does not imply any other form of balance.

These properties of D-optimal continuous designs, as well as their D-optimality, are very attractive for practical use, as they make model selection more efficient and robust and also make interpretation of the results simpler. However, the continuous optimal designs cannot be implemented directly because they have irrational weights and cannot usually be well-approximated by designs with integer numbers of replicates of the design points. If an algorithm is used to search for a near-optimal exact design (e.g. [2]), the restriction to three levels for each factor usually costs little in terms of efficiency, but the properties of partial orthogonality and factorwise balance are almost always lost.

Three-level response surface designs are very commonly used in practice, due to the practical simplicity of using only three levels. Common three level designs include central composite designs [7] with the axial points at $\alpha = 1$ (in the usual notation), also called face-centered cubes, and Box-Behnken designs [4]. [14] introduced the class of subset designs, which consists of subsets, labelled $S_0, \ldots, S_q$, of the 3^q full factorial design, where S_r consists of all points with r factors at levels ± 1 and $q - r$ factors at level 0. The class of subset designs includes both three-level central composite and several Box-Behnken designs but also many additional designs.

The variance-covariance matrices of subset designs share the same attractive structure as those of continuous D-optimal designs, although subset designs are not, in general, D-optimal exact designs. The partial orthogonality and factorwise balance of these designs makes them very attractive in practice and, indeed, they are used much more commonly than near-optimal exact designs.

The second-order model with q factors in b blocks has expected response given by

$$\mu = \alpha_i + \sum_{s=1}^{q} \beta_s x_s + \sum_{s=1}^{q} \beta_{ss} x_s^2 + \sum_{s=1}^{q-1} \sum_{t=s+1}^{q} \beta_{st} x_s x_t, \qquad (2)$$

where α_i is the block effect of block i and all other notations and assumptions are the same as in equation (1). D-optimal continuous blocked designs for the second-order model in the hypercube can be constructed as product designs (see, for example, [15], p. 67). These designs replicate an unblocked D-optimal continuous design for the second-order model in every block and consequently inherit most of the properties of the unblocked designs. In particular, except for the quadratic parameters, all polynomial effects can be estimated orthogonally. The estimates of the quadratic effects are correlated with each other and with the estimates of the block effects. In the context of blocked designs, we refer to this as partial orthogonality. These continuous designs are also factorwise balanced.

Apart from a very few situations in which orthogonal blocking is possible [4, 12], blocked exact designs are usually obtained using search algorithms. [9] and [1] proposed interchange algorithms for searching for D-optimally blocked designs. [24] suggested an algorithm for blocking a given treatment design which maximizes a weighted M-efficiency criterion which more directly emphasizes near orthogonality (though not partial orthogonality in our sense). The resulting optimally-blocked designs almost never have partial orthogonality or factorwise balance. Recently, there has been a renewed focus on classical designs with combinatorial constructions which ensure specific structures in the covariance matrix of parameter estimators. For example, so-called definitive screening designs [17, 18], choose designs in which linear effects can be estimated orthogonally, though unlike our designs they do not allow estimation of the full second-order model. Similar aims are met by designs based on combining orthogonal arrays [27, 28].

In this paper, we introduce a class of designs which preserve some or all of the structure of the variance-covariance matrix of the D-optimal continuous and unblocked subset designs. Part of this structure means that all main effects columns of the design matrix have a column sum of zero, are pairwise orthogonal and orthogonal to any two-factor interaction column as well as any quadratic effect column. Recently, [23] emphasized the usefulness of these structural features and incorporated them into the definition of their orthogonal minimally aliased response surface designs, or OMARS designs for short. The blocked designs proposed here also possess these properties but have, in addition, two-factor interaction columns which are pairwise orthogonal and orthogonal to the quadratic effects columns. Hence, our designs aim for estimation of the full model, whereas OMARS emphasise estimation of submodels in fewer factors.

An exact three-level design ξ for model (2) with q factors and b blocks is called *partially orthogonal* if all polynomial effects can be estimated and if the information matrix is of the form

$$\mathbf{M}(\xi) = \begin{pmatrix} \boldsymbol{\Delta}_1 & \mathbf{0} & \boldsymbol{\Gamma} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\Delta}_2 & \mathbf{0} & \mathbf{0} \\ \boldsymbol{\Gamma}' & \mathbf{0} & \boldsymbol{\Lambda} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \boldsymbol{\Delta}_3 \end{pmatrix}, \tag{3}$$

where $\boldsymbol{\Gamma}$ is a $b \times q$ matrix, $\boldsymbol{\Lambda}$ is a symmetric $q \times q$ matrix, and $\boldsymbol{\Delta}_1$, $\boldsymbol{\Delta}_2$ and $\boldsymbol{\Delta}_3$ are diagonal matrices of order b, q, and $q(q-1)/2$, respectively. Notice that the columns of the matrix in (3) are arranged in the sequence block, linear, quadratic and interaction effects. Often, partially orthogonal designs can be generated that are also factorwise balanced. In that case, $\boldsymbol{\Delta}_2$ and $\boldsymbol{\Delta}_3$ are multiples of the identity matrix and $\boldsymbol{\Lambda}$ is completely symmetric (i.e. all diagonal elements are equal and all off-diagonal elements are equal). Another feature that makes partially orthogonal designs attractive is that they often permit orthogonal or near-orthogonal blocking as will be shown below. In the former case, all estimates of the polynomial effects are not affected by the blocking and in the latter, the estimates of the linear and the interaction effects are not affected by the blocking.

We present a strategy for the construction of partially orthogonal designs which exploits well-known properties of regular fractional factorials in a novel way. Also, a method for generating partially orthogonal designs with small block sizes is given. Examples illustrate that the new designs are often considerably more efficient than more traditional designs. This class of designs also includes, as special cases, blocked versions of Box-Behnken and central composite designs with factorial portions of resolution V or higher and thus provides a unifying perspective on blocked three-level second-order response surface designs.

3. Construction

In this section, a new class of three-level designs for model (2) is introduced which contains many designs that are orthogonally or near-orthogonally blocked and that are partially orthogonal.

We first describe the construction of the designs and then establish their main structural properties. An example of an orthogonally blocked partially orthogonal design is provided at the end of the section.

In what follows we consider exact designs ξ which specify the settings of the factors for each experimental run and the block in which the run is to be performed. The complete design matrix in model (2) corresponding to an exact design ξ with N runs is denoted by $(\mathbf{Z}, \mathbf{X})$ where $\mathbf{Z}$ is the block indicator matrix of order $N \times b$ and $\mathbf{X}$ is the treatment design matrix of order $N \times p$. All elements of $\mathbf{Z}$ are either 0 or 1 with the entry in row r and column s being 1 if and only if the experimental run corresponding to row r belongs to block s. The columns of the treatment design matrix $\mathbf{X}$ are arranged so that the first q columns correspond to linear effects and the next q columns to quadratic effects which are then followed by the columns associated with interaction effects. For any exact design ξ, the information matrix for estimating all the block and polynomial effects is given by $\mathbf{M}(\xi) = (\mathbf{Z}, \mathbf{X})'(\mathbf{Z}, \mathbf{X})$. The information matrix for estimating only the polynomial effects, also known as the treatment information matrix, is denoted by $\mathbf{M}_\beta(\xi)$. This is the matrix which appears in the reduced normal equations which can be used to estimate only the treatment parameters. It is widely used with unstructured treatments [16], but less often with response surface models. Its use simplifies some of the following results.

In what follows, $\mathbf{I}_m$ is the identity matrix of order m and $\mathbf{1}_m$ is the $m \times 1$ vector with all elements equal to one. We will frequently make use of matrices of the form $\mathbf{P_H} = (\mathbf{h}^1 * \mathbf{h}^2, \ldots, \mathbf{h}^1 * \mathbf{h}^m, \mathbf{h}^2 * \mathbf{h}^3, \ldots, \mathbf{h}^2 * \mathbf{h}^m, \ldots, \mathbf{h}^{(m-1)} * \mathbf{h}^m)$ where $\mathbf{H}$ is an arbitrary matrix with columns $\mathbf{h}^1, \ldots, \mathbf{h}^m$ and the symbol '$*$' denotes the Hadamard (or elementwise) product of vectors and matrices.

The designs proposed here are denoted by $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$. The construction of a design for q factors is organized around a matrix $\mathbf{B}$ with q columns and a fractional factorial $\mathbf{C}$ of resolution *III* or higher for $q-1$ two-level factors. In the simplest case, each block of the design is generated by multiplying $\mathbf{B}$ by a diagonal matrix which is defined in terms of a different row of $\mathbf{C}$.

Let $\mathbf{B} = (b_{i,j})$ be a $k \times q$ matrix with elements in $\{-1, 0, 1\}$ such that the first column of $\mathbf{B}$ is orthogonal to $\mathbf{A} = (|b_{i,j}|)$. In order to avoid trivialities, assume that $\mathbf{B} \neq \mathbf{0}$. Furthermore, let $\mathbf{C}$ be a regular fractional factorial design of resolution *III* or higher for $q-1$ two-level factors in n runs. Suppose that the elements in $\mathbf{C}$ are coded as ± 1. Let $\mathbf{D} = (\mathbf{1}_n, \mathbf{C})$. Denote the jth row of $\mathbf{D}$ by $\mathbf{d}_j$ and let $\mathbf{D}_j = \mathrm{diag}(\mathbf{d}_j)$ be the corresponding diagonal matrix. Define

$$\mathbf{B}_j = \mathbf{B}\mathbf{D}_j \tag{4}$$

for $j = 1, \ldots, n$. Let $\mathcal{S} = \{S_1, \ldots, S_b\}$ be a partition of $\{1, \ldots, n\}$ into b nonempty sets S_i of size n_i, $i = 1, \ldots, b$. For every $i \in \{1, \ldots, b\}$ define the $kn_i \times q$ matrix $\tilde{\mathbf{B}}_i$ by stacking the $\mathbf{B}_j$ with $j \in S_i$ on top of each other. The design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ is then the three-level design defined by the blocks $\tilde{\mathbf{B}}_1, \ldots, \tilde{\mathbf{B}}_b$.

The requirement imposed that the first column of $\mathbf{B}$ is orthogonal to $\mathbf{A}$ is crucial for achieving an information matrix with the structure in (3). Moreover, the construction of a design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ for model (2) with q factors requires a fractional factorial with $q-1$ factors. The reason is that, although the above construction could also be carried out when using as the matrix $\mathbf{D}$ a fractional factorial of resolution *III* or higher for q factors, the approach is much more widely applicable when a fraction $\mathbf{C}$ for $q-1$ factors is employed, as this will usually yield designs with smaller blocks. The purpose of the partition $\mathcal{S}$ is also to provide extra flexibility in the construction by combining the matrices in (4) into the desired number of blocks. Furthermore, the use of $\mathcal{S}$ often facilitates the orthogonal blocking of $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$.

The following theorem, which is proved in the Appendix, gives an information matrix $\mathbf{M}(\xi_{\mathbf{B},\mathbf{C},\mathcal{S}})$ which differs from the form in (3) only by having some additional non-zero elements. Subsequent results will then show how some remaining nonzero portions in the matrix can be eliminated by a proper choice of $\mathbf{B}$ and $\mathbf{C}$.

Theorem 1. *Let $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ be defined by the $k \times q$ matrix $\mathbf{B} = (b_{i,j})$, the $n \times (q-1)$ fractional factorial $\mathbf{C}$ and the partition $\mathcal{S} = \{S_1, \ldots, S_b\}$ with $|S_i| = n_i$ for $i = 1, \ldots, b$.*

(i) If $\mathbf{C}$ is of resolution III or higher, then

$$\mathbf{M}(\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}) = \begin{pmatrix} k\,\mathrm{diag}(\mathbf{v}) & \mathbf{E} & \mathbf{v}'\mathbf{w} & \tilde{\mathbf{E}} \\ \mathbf{E}' & n\,\mathrm{diag}(\mathbf{w}) & \mathbf{0} & \mathbf{F} \\ \mathbf{w}'\mathbf{v} & \mathbf{0} & n\mathbf{A}'\mathbf{A} & \mathbf{0} \\ \tilde{\mathbf{E}}' & \mathbf{F}' & \mathbf{0} & \mathbf{G} \end{pmatrix}, \tag{5}$$

where $\mathbf{v} = (n_1, \ldots, n_b)$, $\mathbf{A} = (|b_{i,j}|)$, $\mathbf{w} = \mathbf{1}_k'\mathbf{A}$, $\mathbf{F} = (\mathbf{B}'\mathbf{P_B}) * (\mathbf{D}'\mathbf{P_D})$, $\mathbf{D} = (\mathbf{1}_n, \mathbf{C})$ and $\mathbf{G} = (\mathbf{P}_\mathbf{B}'\mathbf{P_B}) * (\mathbf{P}_\mathbf{D}'\mathbf{P_D})$. The matrices $\mathbf{E}$ and $\tilde{\mathbf{E}}$ have rows $(\mathbf{1}_k'\mathbf{B}) * \sum_{j \in S_i} \mathbf{d}_j$ and $(\mathbf{1}_k'\mathbf{P_B}) * \sum_{j \in S_i} \tilde{\mathbf{d}}_j$, $i = 1, \ldots, b$, where $\mathbf{d}_j$ and $\tilde{\mathbf{d}}_j$ denote the jth row of $\mathbf{D}$ and $\mathbf{P_D}$, respectively. If, in addition, $\mathbf{B} = (\mathbf{H}', -\mathbf{H}')'$ or $\mathbf{B} = (\mathbf{H}', -\mathbf{H}', \mathbf{0})'$ for some matrix $\mathbf{H}$ and a zero vector $\mathbf{0}$, then $\mathbf{F} = \mathbf{0}$.

(ii) If $\mathbf{C}$ is of resolution IV or higher, then in (5) additionally $\mathbf{F} = \mathbf{0}$.

(iii) If $\mathbf{C}$ is of resolution V or higher, then in (5) additionally $\mathbf{F} = \mathbf{0}$ and $\mathbf{G} = n(\mathbf{P}_\mathbf{B}'\mathbf{P_B}) * \mathbf{I}_{q(q-1)/2}$ is diagonal.

Part (i) of Theorem 1 makes clear that every submatrix $\mathbf{U}$ of the information matrix (5) that is structurally different from its counterpart in (3) can be factorized into the elementwise product $\mathbf{U} = \mathbf{U_B} * \mathbf{U_C}$ of a matrix $\mathbf{U_B}$ which depends only on $\mathbf{B}$ and another matrix $\mathbf{U_C}$ which depends only on $\mathbf{C}$. In particular, this applies to $\mathbf{E}$, $\tilde{\mathbf{E}}$ and $\mathbf{F}$ which correspond to zero matrices in (3) and $\mathbf{G}$ whose counterpart is the diagonal matrix $\boldsymbol{\Delta}_3$. The important consequence of the factorization is then that the elements of these matrices can be obtained by multiplying the corresponding elements of the factors. Thus, in order to achieve a zero element in, for example, $\mathbf{E} = \mathbf{E_B} * \mathbf{E_C}$, it is sufficient that only one of the factors $\mathbf{E_B}$ or $\mathbf{E_C}$ has a zero in the corresponding position. Consequently, conditions which ensure that the information matrix $\mathbf{M}(\xi_{\mathbf{B},\mathbf{C},\mathcal{S}})$ exhibits the pattern in (3) can be expressed in terms of properties of the matrix $\mathbf{B}$ and the fractional factorial $\mathbf{C}$. The next result shows that the factorization also facilitates orthogonal blocking.

Corollary 1. *A design* $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ *is orthogonally blocked if and only if* $(\mathbf{1}_k'\mathbf{B}) * \sum_{j\in S_i} \mathbf{d}_j = \mathbf{0}$ *and* $(\mathbf{1}_k'\mathbf{P}_\mathbf{B}) * \sum_{j\in S_i} \tilde{\mathbf{d}}_j = \mathbf{0}$ *for* $i = 1, \dots, b$.

The blocks of a design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ are thus orthogonal if and only if $\mathbf{E}$ and $\tilde{\mathbf{E}}$ in (5) are zero matrices. Moreover, the condition for orthogonal blocking in Corollary 1 is equivalent to requiring that each block $\tilde{\mathbf{B}}_1, \dots, \tilde{\mathbf{B}}_b$ of the design has orthogonal columns which sum to zero. However, as stated, the condition is much more helpful for choosing an appropriate matrix $\mathbf{B}$ and selecting the partition $\mathcal{S}$ in view of the factorization argument. To illustrate, suppose that $\mathbf{B}$ has orthogonal columns so that $\mathbf{1}_k'\mathbf{P}_\mathbf{B}$ is a zero vector. In this case, the condition in Corollary 1 reduces to $(\mathbf{1}_k'\mathbf{B}) * \sum_{j\in S_i} \mathbf{d}_j = \mathbf{0}$ for $i = 1, \dots, b$. Hence orthogonal blocks can be achieved by choosing a matrix $\mathbf{B}$ whose columns add up to zero or by partitioning the set $\{1, \dots, n\}$ in such a way that for every i the sum of the rows $\mathbf{c}_j$ of $\mathbf{C}$ with j in S_i is a zero vector. Moreover, orthogonal blocking of the design is possible even when only some of the column sums of $\mathbf{B}$ are zero and the partition $\mathcal{S}$ can be so chosen that for every i all components of $\sum_{j\in S_i} \mathbf{d}_j$ that correspond to a nonzero column sum in $\mathbf{B}$ vanish. Similar remarks apply when not all columns of $\mathbf{B}$ are mutually orthogonal.

For an orthogonally blocked design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ that has been constructed by means of a fractional factorial $\mathbf{C}$ of resolution V or more, the information matrix $\mathbf{M}(\xi_{\mathbf{B},\mathbf{C},\mathcal{S}})$ exhibits the structure in (3). The matrix $\mathbf{F}$ in (5) is then a zero matrix and $\mathbf{G}$ is diagonal, so that $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ is partially orthogonal if all polynomial effects can be estimated. In general, $\mathbf{F}$ will 'almost' be a zero matrix and $\mathbf{G}$ will 'almost' be diagonal, even when $\mathbf{C}$ is of lower resolution. The following result makes this statement more precise by relating the number of nonzero elements in $\mathbf{F}$ and the number of nonzero off-diagonal elements in $\mathbf{G}$ to the wordlength pattern associated with $\mathbf{C}$. Subsequently, it is shown how elements in either matrix that cannot be guaranteed to be zero by means of the choice of $\mathbf{C}$ alone can be forced to vanish by an appropriate choice of the matrix $\mathbf{B}$. Finally, a condition is presented that ensures the estimability of the polynomial effects.

Corollary 2. *If the fractional factorial* $\mathbf{C}$ *has wordlength pattern* $(W_1, \dots, W_{q-1})$*, then the matrix* $\mathbf{F}$ *in (5) contains at most* $3W_3$ *nonzero elements and the number of nonzero off-diagonal elements of* $\mathbf{G}$ *in (5) is no larger than* $6(W_3 + W_4)$ *for* $q > 4$*, and less than or equal to* $6W_3$ *otherwise.*

Obviously, the only elements of $\mathbf{F} = (\mathbf{B}'\mathbf{P}_\mathbf{B}) * (\mathbf{D}'\mathbf{P}_\mathbf{D})$ that can be different from zero are those for which $\mathbf{D}'\mathbf{P}_\mathbf{D}$ has a nonzero element in the same position. The proof of Corollary 2 in the Appendix shows that the latter elements correspond to three-factor interactions in the defining contrast group of $\mathbf{C}$. Similarly, a necessary condition for an off-diagonal element of $\mathbf{G} = (\mathbf{P}_\mathbf{B}'\mathbf{P}_\mathbf{B}) * (\mathbf{P}_\mathbf{D}'\mathbf{P}_\mathbf{D})$ to be nonzero is that the corresponding element of $\mathbf{P}_\mathbf{D}'\mathbf{P}_\mathbf{D}$ is nonzero. Moreover, nonzero elements of $\mathbf{P}_\mathbf{D}'\mathbf{P}_\mathbf{D}$ are related to three- and four-factor interactions in the defining contrast group of $\mathbf{C}$. It is clear then that an element in $\mathbf{F}$ or $\mathbf{G}$, for which the corresponding element in $\mathbf{D}'\mathbf{P}_\mathbf{D}$ or $\mathbf{P}_\mathbf{D}'\mathbf{P}_\mathbf{D}$ is not a zero, can only be zero itself if the element in the same position of $\mathbf{B}'\mathbf{P}_\mathbf{B}$ or $\mathbf{P}_\mathbf{B}'\mathbf{P}_\mathbf{B}$ vanishes.

Every element of $\mathbf{B}'\mathbf{P_B}$ is the inner product of a column of $\mathbf{B}$ and a column of $\mathbf{P_B}$ and hence the sum of the elements in the componentwise product of three not necessarily distinct columns of $\mathbf{B}$. Similarly, every element of $\mathbf{P}'_\mathbf{B}\mathbf{P_B}$ is the inner product of two columns of $\mathbf{P_B}$ and thus the sum of the elements in the componentwise product of four not necessarily distinct columns of $\mathbf{B}$. Therefore the elements of $\mathbf{B}'\mathbf{P_B}$ and of $\mathbf{P}'_\mathbf{B}\mathbf{P_B}$ can be expressed in the form

$$s_{j_1,\ldots,j_l} = \sum_{i=1}^{k} b_{i,j_1}\cdots b_{i,j_l},$$

where $b_{i,j_1},\ldots,b_{i,j_l}$, $1 \le j_1 \le \ldots \le j_l \le q$, are elements of $\mathbf{B}$ and $l = 3$ or $l = 4$. Bearing in mind that each factor j of the fractional factorial $\mathbf{C}$ in $q-1$ factors influences the settings for factor $j+1$ in the design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$, it is easy to prove the following result which makes the correspondence between the defining contrast group of $\mathbf{C}$ and the elements of $\mathbf{B}$, $\mathbf{F}$ and $\mathbf{G}$ more explicit.

Corollary 3. *For $l = 3$ or $l = 4$, let the interaction of the factors $j_1 - 1 < \ldots < j_l - 1$, with $2 \le j_1,\ldots,j_l \le q$, be contained in the defining contrast group of the fractional factorial $\mathbf{C}$. If $l = 3$ and $s_{j_1,j_2,j_3} = 0$, the three elements of $\mathbf{F}$ in (5) that are the inner product of a column of the treatment design matrix $\mathbf{X}$, representing the linear effect of one of the factors j_1, j_2, j_3, and a column, representing the two-factor interaction of the remaining factors, vanish. Moreover, if $s_{1,j_1,j_2,j_3} = 0$, the six elements of $\mathbf{G}$ that are the inner product of a column representing the interaction of any two of the factors $1, j_1, j_2, j_3$ and a column corresponding to the interaction of the remaining two factors are zero. Similarly, if $l = 4$ and $s_{j_1,\ldots,j_4} = 0$, the six elements of $\mathbf{G}$, that are inner products of columns representing two-factor interactions of the factors $j_1,\ldots,j_4$, vanish.*

The preceding results indicate that, by identifying the three- and four-factor interactions in the defining contrast group of $\mathbf{C}$ and choosing $\mathbf{B}$ such that the corresponding elements of $\mathbf{B}'\mathbf{P_B}$ and $\mathbf{P}'_\mathbf{B}\mathbf{P_B}$ disappear, a design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ can be constructed for which $\mathbf{F} = \mathbf{0}$ in (5) and $\mathbf{G}$ is diagonal. If the design is orthogonally blocked, we additionally have $\mathbf{E} = \mathbf{0}$ and $\tilde{\mathbf{E}} = \mathbf{0}$. The design is partially orthogonal if the polynomial effects are estimable, and a sufficient condition for this is presented next. More about how to choose the matrix $\mathbf{B}$ and the fractional factorial $\mathbf{C}$ will be given in Section 4.

Corollary 4. *Suppose that $\mathbf{E}$, $\tilde{\mathbf{E}}$ and $\mathbf{F}$ in (5) are zero matrices and that $\mathbf{G}$ is diagonal. If $\mathbf{A}$ has rank q, if $\mathbf{1}_k$ is not contained in the column space of $\mathbf{A}$ and if all elements of $\mathbf{A}'\mathbf{A}$ are positive, then $\mathbf{M}(\xi_{\mathbf{B},\mathbf{C},\mathcal{S}})$ is invertible and the treatment information matrix is given by*

$$\mathbf{M}_\beta(\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}) = \begin{pmatrix} n\,\mathrm{diag}(\mathbf{w}) & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & n\mathbf{A}'(\mathbf{I}_k - \frac{1}{k}\mathbf{1}_k\mathbf{1}'_k)\mathbf{A} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{G} \end{pmatrix}.$$

Next, it is shown how the above results can be applied to generate an orthogonally blocked partially orthogonal design.

Example 1 We construct a design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ for $q = 4$ factors in $b = 4$ blocks of size 9. The matrix $\mathbf{B}$ is obtained by stacking the $W(4,3)$ weighing matrix

$$\mathbf{W} = \begin{pmatrix} 0 & -1 & -1 & -1 \\ 1 & 0 & 1 & -1 \\ 1 & -1 & 0 & 1 \\ 1 & 1 & -1 & 0 \end{pmatrix}$$

of order 4 and weight 3 on top of its foldover and adjoining a center point, to give

$$\mathbf{B} = \begin{pmatrix} \mathbf{W} \\ -\mathbf{W} \\ \mathbf{0} \end{pmatrix}. \tag{6}$$

It can easily be verified that the first column of $\mathbf{B}$ is orthogonal to $\mathbf{A}$, the matrix obtained by replacing every element of $\mathbf{B}$ with its absolute value. Thus $\mathbf{B}$ fulfills the requirement in the definition of $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$. For $\mathbf{C}$ in Theorem 1 we use the 2^{3-1}_{III} fractional factorial of resolution III in 4 runs with defining contrast $123 = I$, that is

$$\mathbf{C} = \begin{pmatrix} -1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & -1 \\ 1 & 1 & 1 \end{pmatrix}.$$

The partition $\mathcal{S} = \{\{1\},\{2\},\{3\},\{4\}\}$ then produces the required number of blocks. The resulting design is depicted in Table 2 where the level -1 is represented by a minus and the level 1 by a plus sign.

Since $\mathbf{W}$ has orthogonal columns, so does $\mathbf{B}$. The specific form of $\mathbf{B}$ in (6) implies that each column of $\mathbf{B}$ adds up to zero so that, according to Corollary 1, the design is orthogonally blocked and hence $\mathbf{E} = \mathbf{0}$ and $\tilde{\mathbf{E}} = \mathbf{0}$ in (5). Moreover, the choice of $\mathbf{B}$ implies $\mathbf{F} = \mathbf{0}$ by part (i) of Theorem 1. The defining contrast group of $\mathbf{C}$ is $\{I, 123\}$ and the corresponding wordlength pattern reads $(0,0,1)$. According to Corollary 2 the matrix $\mathbf{G}$ then contains at most six nonzero off-diagonal elements, which correspond to the three-factor interaction 123 in the defining contrast group of $\mathbf{C}$. By Corollary 3 the corresponding entries in $\mathbf{G}$ vanish if $s_{1234} = 0$. Obviously, this is the case since $\mathbf{W}$ contains a zero in every row. We note that, in the present situation, $\mathbf{F} = \mathbf{0}$ could also have been demonstrated by referring to Corollary 3. It follows that

$$\mathbf{M}(\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}) = \begin{pmatrix} 9\mathbf{I}_4 & \mathbf{0} & 6\mathbf{1}_4\mathbf{1}_4' & \mathbf{0} \\ \mathbf{0} & 24\mathbf{I}_4 & \mathbf{0} & \mathbf{0} \\ 6\mathbf{1}_4\mathbf{1}_4' & \mathbf{0} & 16\mathbf{1}_4\mathbf{1}_4' + 8\mathbf{I}_4 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & 16\mathbf{I}_6 \end{pmatrix}.$$

Table 2: Orthogonally blocked partially orthogonal design for four factors in four blocks

Blocks															
$\tilde{\mathbf{B}}_1$				$\tilde{\mathbf{B}}_2$				$\tilde{\mathbf{B}}_3$				$\tilde{\mathbf{B}}_4$			
0	+	+	−	0	+	−	+	0	−	+	+	0	−	−	−
+	0	−	−	+	0	+	+	+	0	−	+	+	0	+	−
+	+	0	+	+	+	0	−	+	−	0	−	+	−	0	+
+	−	+	0	+	−	−	0	+	+	+	0	+	+	−	0
0	−	−	+	0	−	+	−	0	+	−	−	0	+	+	+
−	0	+	+	−	0	−	−	−	0	+	−	−	0	−	+
−	−	0	−	−	−	0	+	−	+	0	+	−	+	0	−
−	+	−	0	−	+	+	0	−	−	−	0	−	−	+	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Finally, it can be easily checked that $\mathbf{A}$ has full rank q, that $\mathbf{1}_9$ is not contained in the image of $\mathbf{A}$ and that all elements of $\mathbf{A}'\mathbf{A}$ are positive. The information matrix $\mathbf{M}(\xi_{\mathbf{B},\mathbf{C},\mathcal{S}})$ is then invertible by Corollary 4 and the design is thus partially orthogonal with treatment information matrix

$$\mathbf{M}_\beta(\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}) = \begin{pmatrix} 24\mathbf{I}_4 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & 8\mathbf{I}_4 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & 16\mathbf{I}_6 \end{pmatrix}.$$

We note that the design in Table 2 has been derived previously by [12], who used a method based on complex-valued canonical contrasts introduced by [3], and by [11], who used the "remnant" of the 3^4 full factorial after removing the points of the Box-Behnken and central composite designs and blocked it using the confounding of three-level factorials.

4. Choosing B and C

The structure of the information matrix $\mathbf{M}(\xi_{\mathbf{B},\mathbf{C},\mathcal{S}})$ is determined on the one hand by the matrix $\mathbf{B}$ and on the other by the fractional factorial $\mathbf{C}$. The results of the previous section show that, in particular when $\mathbf{C}$ is of resolution *III* or *IV*, it is the interplay between $\mathbf{B}$ and $\mathbf{C}$ that can be fruitfully exploited to yield a design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ whose information matrix is of the form in (3). This section addresses in more detail how $\mathbf{B}$ and $\mathbf{C}$ can be chosen in order to generate designs with this property. Although in general $\mathbf{B}$ cannot be chosen without considering $\mathbf{C}$ and vice versa, we first discuss a few aspects regarding the choice of $\mathbf{B}$ that can be treated independently. Subsequently, we consider the choice of $\mathbf{C}$ and its implications for $\mathbf{B}$.

The definition of $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ requires $\mathbf{B}$ to be a matrix of order $k \times q$ with elements in $\{-1, 0, 1\}$ such that the first column of $\mathbf{B}$ is orthogonal to $\mathbf{A}$. The number of rows k can be chosen arbitrarily but determines the size of the blocks $\tilde{\mathbf{B}}_i$, $i = 1, \ldots, b$, of $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ via kn_i, where n_i is the size of the set S_i in the partition $\mathcal{S}$. Thus a matrix $\mathbf{B}$ with a small number of rows leads to greater flexibility in choosing block sizes.

Obviously, there are many ways to construct $\mathbf{B}$, but weighing matrices (e.g., [10]) and Hadamard matrices (e.g., [26]) appear to be particularly useful in this regard. Both types of matrices have orthogonal columns so that the whole matrix, or a submatrix of q columns, provides a suitable starting point for generating $\mathbf{B}$. Moreover, often the columns of such a matrix can be permuted so that the first column of the resulting matrix is orthogonal to the permuted matrix with every element replaced by its absolute value.

Previously it was noted that for a matrix $\mathbf{B}$ with orthogonal columns the condition $\mathbf{1}_k'\mathbf{B} = \mathbf{0}$ is sufficient for $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ to be orthogonally blocked, irrespective of the specific choice of $\mathbf{C}$ and the partition $\mathcal{S}$. Given a matrix $\mathbf{H}$ with elements in $\{-1, 0, 1\}$ and orthogonal columns, setting $\mathbf{B} = (\mathbf{H}', -\mathbf{H}')'$ or $\mathbf{B} = (\mathbf{H}', -\mathbf{H}', \mathbf{0})'$ always yields a matrix for which the above condition holds. Moreover, the first column of such a $\mathbf{B}$ will be orthogonal to $\mathbf{A}$ and so $\mathbf{F}$ in (5) will be a zero matrix. A matrix $\mathbf{B}$ of this kind with $\mathbf{H}$ defined by a weighing matrix was used to generate the design in Example 1.

The matrices with mutually orthogonal columns represent, however, only a comparatively small subset of the candidates from which $\mathbf{B}$ can be chosen. In particular, for generating designs with small blocks other options are available for which the number of rows k is smaller than the number of columns q and for which only some columns are orthogonal. An example of such a matrix will be presented in Section 5.

Next, we consider the choice of $\mathbf{C}$. When a fractional factorial of resolution V or higher with an acceptable number of runs is available, this will be the best choice in view of Theorem 1. Otherwise, a regular fraction of lower resolution with small numbers, W_3 and W_4, of three- and four-factor interactions, respectively, in its defining contrast group can be used. Corollaries 2 and 3 jointly imply that $\mathbf{B}$ then has to be chosen such that $s_{j_1,j_2,j_3} = s_{1,j_1,j_2,j_3} = 0$ for W_3 sets $\{j_1, j_2, j_3\} \subset \{2, \ldots, q\}$ and $s_{j_1,\ldots,j_4} = 0$ for W_4 sets $\{j_1, \ldots, j_4\} \subset \{2, \ldots, q\}$ in order to achieve a zero matrix $\mathbf{F}$ and a diagonal matrix $\mathbf{G}$ in (5). Often these requirements are easily fulfilled when, for each of the above sets $\{j_1, \ldots, j_l\}$ with $l = 3$ or $l = 4$, the submatrix of $\mathbf{B}$ consisting of the columns $j_1, \ldots, j_l$ contains a zero in every row. Similarly, permuting columns of a candidate matrix often yields a matrix $\mathbf{B}$ that satisfies the requirements.

In general, the computation of the numbers W_3 and W_4 for all regular fractions of a 2^f full factorial design requires the use of some algorithm. In what follows we restrict ourselves to the case $3 \leq f \leq 7$ and present results obtained by means of the algorithm of [21], for enumerating

Table 3: Wordlength patterns of two-level fractional factorials of resolution *III* in situations with up to seven factors where no regular fraction of higher resolution exists

Factors	Runs	Fractions	Wordlength pattern	Defining contrasts (example)
3	4	1	$(0, 0, 1)$	123
5	8	15	$(0, 0, 2, 1, 0)$	$123, 145$
6	8	30	$(0, 0, 4, 3, 0, 0)$	$123, 146, 245$
7	8	30	$(0, 0, 7, 7, 0, 0, 1)$	$123, 146, 245, 1247$

Table 4: Wordlength patterns of two-level minimum aberration designs in situations with up to seven factors where the highest achievable resolution is *IV*

Factors	Runs	Fractions	Wordlength pattern	Defining contrasts (example)
4	8	1	$(0, 0, 0, 1)$	1234
6	16	15	$(0, 0, 0, 3, 0, 0)$	$1234, 1256$
7	16	30	$(0, 0, 0, 7, 0, 0, 0)$	$1234, 1257, 1356$
	32	105	$(0, 0, 0, 1, 2, 0, 0)$	$1234, 12567$

all regular fractions of 2^f full factorial designs together with their wordlength patterns. Regular fractions of resolution *V* or higher for which, clearly, $W_3 = W_4 = 0$ are only available for the following combinations (f, n) of f factors and n runs and can be found in textbooks such as [26]: $(5, 16)$, $(6, 32)$ and $(7, 64)$. Tables 3 to 5 present wordlength patterns of resolution *III* and *IV* fractional factorials for all other factor-run combinations for which there exist fractions of resolution *III* or higher. For a given combination of factors and runs each table gives in its third column the number of different fractions that share the wordlength pattern in column four. The last column specifies a set of defining contrasts for generating one of these fractions.

Table 3 lists the wordlength patterns of all regular fractions of resolution *III* for the situations where no fractional factorials of higher resolution exist. For each of the factor-run combinations in the table there exists only a single wordlength pattern which means that all fractions in the third column of the table are equally suitable for constructing the corresponding design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$.

For combinations of factors and runs where the highest achievable resolution is *IV* a minimum aberration design represents the best choice for $\mathbf{C}$ among the fractions of resolution *IV* since then W_3 is equal to zero and W_4 is as small as possible. The corresponding wordlength patterns are given in Table 4. In general, however, a fraction that is most suitable for constructing the design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ is not necessarily optimal in terms of the aberration criterion. In fact, when the highest achievable resolution is *IV*, fractions of resolution *III* are often more appropriate.

Table 5 presents the wordlength patterns of all regular fractions of resolution *III* for the cases

Table 5: Wordlength patterns of two-level fractional factorials of resolution *III* in situations with up to seven factors where the highest achievable resolution is *IV*

Factors	Runs	Fractions	Wordlength pattern	Defining contrasts (example)
4	8	4	$(0,0,1,0)$	123
6	16	90	$(0,0,2,1,0,0)$	$123,145$
		10	$(0,0,2,0,0,1)$	$123,456$
		60	$(0,0,1,1,1,0)$	$123,1456$
7	16	210	$(0,0,4,3,0,0,0)$	$123,146,245$
		105	$(0,0,3,3,0,0,1)$	$123,145,167$
		630	$(0,0,3,2,1,1,0)$	$123,167,245$
		630	$(0,0,2,3,2,0,0)$	$123,245,1467$
	32	315	$(0,0,2,1,0,0,0)$	$123,145$
		70	$(0,0,2,0,0,1,0)$	$123,456$
		420	$(0,0,1,1,1,0,0)$	$123,1456$
		35	$(0,0,1,1,0,0,1)$	$123,4567$
		105	$(0,0,1,0,1,1,0)$	$123,14567$

where fractional factorials of resolution *IV* but not higher exist. In order to facilitate comparisons in the table, for each combination of factors and runs, the wordlength patterns are arranged in ascending order according to the minimum aberration criterion so that fractions corresponding to the last pattern presented have the least aberration. We illustrate the point that, for the purpose of constructing a design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$, regular fractions of resolution *III* are often to be preferred over minimum aberration designs of resolution *IV* by considering a special case. The general reasoning applies, however, to most of the other situations in the table.

As was already mentioned, for a given fractional factorial with specific values of W_3 and W_4, in order to obtain a zero matrix $\mathbf{F}$ and a diagonal matrix $\mathbf{G}$ in (5), the matrix $\mathbf{B}$ has to be chosen such that $s_{j_1,j_2,j_3} = s_{1,j_1,j_2,j_3} = 0$ for W_3 sets $\{j_1,j_2,j_3\} \subset \{2,\ldots,q\}$ and $s_{j_1,\ldots,j_4} = 0$ for W_4 sets $\{j_1,\ldots,j_4\} \subset \{2,\ldots,q\}$. In all, these represent $2W_3 + W_4$ constraints. Now consider the situation with $f = 6$ factors and $n = 16$ runs. The three patterns in Table 5 that exist for this situation impose five, four and three constraints on $\mathbf{B}$, respectively. Thus, among the fractions of resolution *III*, any design with wordlength pattern $(0,0,1,1,1,0)$, and consequently $W_3 = W_4 = 1$, imposes the least number of constraints on $\mathbf{B}$. For example, for the fraction generated by means of the defining contrasts $123 = I$ and $1456 = I$, the only three- and four-factor interactions in its defining contrast group are 123 and 1456, so that according to Corollary 3 a matrix $\mathbf{B}$ has to be constructed for which $s_{2,3,4} = s_{1,2,3,4} = 0$ and $s_{2,5,6,7} = 0$. The corresponding minimum aberration designs for

$f = 6$ and $n = 16$ in Table 4 all share the wordlength pattern $(0, 0, 0, 3, 0, 0)$. Since then $W_3 = 0$ and $W_4 = 3$, three constraints are implied for $\mathbf{B}$. The defining contrasts $1234 = I$ and $1256 = I$ in the last column of the table determine a regular fraction whose defining contrast group contains the interactions 1234, 1256 and 3456. Thus $\mathbf{B}$ has to be constructed to satisfy the constraints $s_{2,3,4,5} = s_{2,3,6,7} = s_{4,5,6,7} = 0$.

To sum up, the resolution *III* fraction in Table 5 imposes two constraints involving four columns and one constraint involving three columns of $\mathbf{B}$, whereas all three constraints imposed by the minimum aberration design in Table 4 involve four columns of the matrix. Since it is usually easier to satisfy constraints that refer to three columns of $\mathbf{B}$, the former fraction represents a more appropriate choice for $\mathbf{C}$ in the construction of a design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$.

5. Augmenting blocks

The previous sections have shown how orthogonally blocked designs $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ with information matrices having the attractive structure in (3) can be constructed and a sufficient condition for $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ to be partially orthogonal has been given in Corollary 4. Note, however, that the attractive structure of the information matrix is necessary, but not suffcient, for the covariance matrix to be non-singular and to ensure partial orthogonality. For such situations, in which the polynomial effects are not estimable by means of a design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$, partially orthogonal designs can be generated by adding additional points to the blocks. We do not only augment the initial blocks with axial or center points but also use sets of points which are based on the 2^2 and 2^3 full factorials. This additional flexibility allows the construction of many new designs, which can compete with more traditional designs in terms of both efficiency and overall size of the experiment.

The need for augmentation is to deal with the nonestimability, which arises from the nonorthogonality of the quadratic effects. Augmentation will always be necessary when for some integer $0 \leq r \leq q$ the points in the initial design all have r factors at levels ± 1 and the remaining $q - r$ factors at level 0, or when they are from only center points ($r = 0$) and one of factorial points ($r = q$) or axial points ($r = 1$). This essentially follows from the conditions of [14] for a subset design to allow estimation of the second-order model. However, with blocking, augmentation might also be necessary in other cases.

More precisely, consider the design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ with blocks $\tilde{\mathbf{B}}_1, \ldots, \tilde{\mathbf{B}}_b$. For $a = 1, 2, 3$ let $\mathbf{U}_a$ be a matrix of order $b \times C(q, a)$, where $C(q, a)$ designates the binomial coefficient and let $\mathbf{z} = (z_1, \ldots, z_b)$ be a vector such that all elements of $\mathbf{U}_a$ and $\mathbf{z}$ are nonnegative integers. Suppose that the columns of $\mathbf{U}_a$ are labeled with the subsets of size a of $\{1, \ldots, q\}$, enumerated in lexicographical order, and set $\mathcal{U} = \{\mathbf{U}_1, \mathbf{U}_2, \mathbf{U}_3\}$. Given this labeling of the columns the elements of $\mathbf{U}_1$, $\mathbf{U}_2$, $\mathbf{U}_3$ can be referred to as $u_{i,\{j_1\}}$, $u_{i,\{j_1,j_2\}}$ and $u_{i,\{j_1,j_2,j_3\}}$, respectively. For every $j_1 \in \{1, \ldots, q\}$ let $\mathbf{U}_{1,\{j_1\}}$ be the $2 \times q$ matrix with column j_1 given by the column vector $(-1, 1)'$ and all other elements equal to zero. Similarly, for every subset $\{j_1, j_2\} \subset \{1, \dots, q\}$ with $j_1 < j_2$ let $\mathbf{U}_{2,\{j_1,j_2\}}$ be the $4 \times q$ matrix with columns j_1 and j_2 being equal to the first and second columns of the 2^2 full factorial and all remaining elements being equal to zero. For example, if $q = 5$, then

$$\mathbf{U}_{2,\{1,4\}} = \begin{pmatrix} -1 & 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & 1 & 0 \end{pmatrix}.$$

Finally, for every subset $\{j_1, j_2, j_3\} \subset \{1, \dots, q\}$ with $j_1 < j_2 < j_3$ let $\mathbf{U}_{3,\{j_1,j_2,j_3\}}$ be the $8 \times q$ matrix the only nonzero elements of which can be found in columns j_1, j_2 and j_3 which are equal to the first, second and third column of the 2^3 full factorial. The augmented design $\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}}$ is then defined by adjoining $u_{i,\{j_1\}}$ times the matrix $\mathbf{U}_{1,\{j_1\}}$, $u_{i,\{j_1,j_2\}}$ times $\mathbf{U}_{2,\{j_1,j_2\}}$ and $u_{i,\{j_1,j_2,j_3\}}$ times $\mathbf{U}_{3,\{j_1,j_2,j_3\}}$, as well as z_i center points (i.e. zero vectors) to each block $\tilde{\mathbf{B}}_i$, $i = 1, \dots, b$, where the subsets $\{j_1\}$, $\{j_1, j_2\}$, and $\{j_1, j_2, j_3\}$ range over the columns of $\mathbf{U}_1, \mathbf{U}_2$ and $\mathbf{U}_3$, respectively.

The following theorem provides a set of sufficient conditions for such a design $\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}}$ to be partially orthogonal. The proof given in the Appendix shows that the requirements ensure the positive definiteness of the information matrix $\mathbf{M}(\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}})$. Subsequently it is considered how the conditions can be fulfilled when only axial or center points are used for augmenting the initial blocks of a design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$.

In order to be able to present $\mathbf{M}(\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}})$ in a concise way, some additional notation needs to be introduced. First, two $b \times q$ matrices, $\mathbf{V}_2 = (v_{2,i,\{j\}})$, where $v_{2,i,\{j\}} = \sum_{\{j_1,j_2\}:j\in\{j_1,j_2\}} u_{i,\{j_1,j_2\}}$, and $\mathbf{V}_3 = (v_{3,i,\{j\}})$, where $v_{3,i,\{j\}} = \sum_{\{j_1,j_2,j_3\}:j\in\{j_1,j_2,j_3\}} u_{i,\{j_1,j_2,j_3\}}$, for $i = 1, \dots, b$ and $j = 1, \dots, q$, are required for enumerating how often each of the q factors is involved in augmenting the ith block of the design, as specified by $\mathbf{U}_2$ and $\mathbf{U}_3$. Similarly, let $\mathbf{W}_3 = (w_{3,i,\{j,k\}})$ be a $b \times C(q, 2)$ matrix with columns labeled by the subsets of size two of $\{1, \dots, q\}$ in lexicographical order, whose elements $w_{3,i,\{j,k\}} = \sum_{\{j_1,j_2,j_3\}:\{j,k\}\subset\{j_1,j_2,j_3\}} u_{i,\{j_1,j_2,j_3\}}$ record how often the factors j and k are jointly involved in the augmentation of the ith block according to $\mathbf{U}_3$. Moreover, for brevity of notation in Theorem 2, we set $\mathbf{V}_1 = \mathbf{U}_1$, $\mathbf{W}_1 = \mathbf{0}$ and $\mathbf{W}_2 = \mathbf{U}_2$. Finally, for $a = 1, 2, 3$ denote by $\mathbf{N}_a$ the $q \times C(q, a)$ matrix with elements in $\{0, 1\}$ whose columns represent the subsets of size a of $\{1, \dots, q\}$ enumerated in lexicographical order.

Theorem 2. *Let $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ be a design such that the matrices $\mathbf{E}$, $\tilde{\mathbf{E}}$ and $\mathbf{F}$ in (5) are zero matrices and $\mathbf{G}$ is diagonal. If, for every diagonal element $g_{j,j}$ of $\mathbf{G}$ which is equal to zero, the jth column of $\mathbf{U}_2$ or $\mathbf{W}_3$ contains at least one positive element and if the matrix*

$$\mathbf{P} = \begin{pmatrix} \mathbf{A} \\ \mathrm{diag}(\mathbf{1}_b'\mathbf{U}_1) \\ \mathrm{diag}(\mathbf{1}_b'\mathbf{U}_2)\mathbf{N}_2' \\ \mathrm{diag}(\mathbf{1}_b'\mathbf{U}_3)\mathbf{N}_3' \end{pmatrix} \tag{7}$$

has rank q, then $\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}}$ or $\xi^{\mathcal{U},\tilde{\mathbf{z}}}_{\mathbf{B},\mathbf{C},\mathcal{S}}$, where $\tilde{\mathbf{z}} = \mathbf{z} + \mathbf{1}_b'$, is partially orthogonal. The information *matrix of* $\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}}$ *is*

$$\mathbf{M}(\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}}) =$$
$$\begin{pmatrix} \operatorname{diag}(k\mathbf{v}+\mathbf{z}+\sum 2^a \mathbf{1}'_{C(q,a)}\mathbf{U}'_a) & \mathbf{0} & \mathbf{v}'\mathbf{w}+\sum 2^a\mathbf{V}_a & \mathbf{0} \\ \mathbf{0} & \operatorname{diag}(n\mathbf{w}+\sum 2^a\mathbf{1}'_b\mathbf{V}_a) & \mathbf{0} & \mathbf{0} \\ \mathbf{w}'\mathbf{v}+\sum 2^a\mathbf{V}'_a & \mathbf{0} & n\mathbf{A}'\mathbf{A}+\sum 2^a\mathbf{N}_a\operatorname{diag}(\mathbf{1}'_b\mathbf{U}_a)\mathbf{N}'_a & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{G}+\operatorname{diag}(\sum 2^a\mathbf{1}'_b\mathbf{W}_a) \end{pmatrix}, \tag{8}$$

where all summations are taken over $a = 1, 2, 3$ *and* $\mathbf{A}$, k, n, $\mathbf{v}$ *and* $\mathbf{w}$ *are defined as in (5). The information matrix* $\mathbf{M}(\xi^{\mathcal{U},\tilde{\mathbf{z}}}_{\mathbf{B},\mathbf{C},\mathcal{S}})$ *of* $\xi^{\mathcal{U},\tilde{\mathbf{z}}}_{\mathbf{B},\mathbf{C},\mathcal{S}}$ *has the same form as* $\mathbf{M}(\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}})$ *with* $\tilde{\mathbf{z}}$ *in place of* $\mathbf{z}$.

The designs $\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}}$ and $\xi^{\mathcal{U},\tilde{\mathbf{z}}}_{\mathbf{B},\mathbf{C},\mathcal{S}}$ in the theorem are identical except that each block of the latter design contains an additional run at the center point. The number of center points within each block is, however, not necessarily the same. Moreover, by applying permutations of rows and columns, as in the proof of Theorem 2, to transform $\mathbf{M}(\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}})$ in (8) into block diagonal form and by using the formula for the inverse of a partitioned matrix, the treatment information matrix of any partially orthogonal augmented design $\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}}$ can be derived as follows.

Corollary 5. *If* $\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}}$ *is partially orthogonal, then*

$$\mathbf{M}_\beta(\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}}) = \begin{pmatrix} \operatorname{diag}(n\mathbf{w}+\sum 2^a\mathbf{1}'_b\mathbf{V}_a) & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{Q} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{G}+\operatorname{diag}(\sum 2^a\mathbf{1}'_b\mathbf{W}_a) \end{pmatrix}, \tag{9}$$

where

$$\begin{aligned} \mathbf{Q} \;=\;& n\mathbf{A}'\mathbf{A}+\sum 2^a\mathbf{N}_a\operatorname{diag}(\mathbf{1}'_b\mathbf{U}_a)\mathbf{N}'_a \\ & -(\mathbf{w}'\mathbf{v}+\sum 2^a\mathbf{V}'_a)\operatorname{diag}(k\mathbf{v}+\mathbf{z}+\sum 2^a\mathbf{1}'_{C(q,a)}\mathbf{U}'_a)^{-1}(\mathbf{v}'\mathbf{w}+\sum 2^a\mathbf{V}_a). \end{aligned} \tag{10}$$

The first requirement in Theorem 2 is automatically satisfied, when all elements of the matrix $\mathbf{A}'\mathbf{A}$ associated with a design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ are positive, since then all diagonal elements of $\mathbf{G}$ are positive. In this case, it needs only to be checked whether the matrix $\mathbf{P}$ in (7) has full rank q, which is particularly simple when the augmentation uses only center or axial points, so that $\mathbf{U}_2$ and $\mathbf{U}_3$ are zero matrices. More formally, we have the following result.

Corollary 6. *Let* $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ *be as in Theorem 2 and suppose that all elements of* $\mathbf{A}'\mathbf{A}$ *are positive. The requirements in Theorem 2 are fulfilled if* $\mathbf{A}$ *has rank* q *or if all components of* $\mathbf{1}'_b\mathbf{U}_1$ *are positive.*

The first condition in the corollary, that $\mathbf{A}$ has rank q, implies that adding a single center point to each block of an orthogonally blocked design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ will often be sufficient to generate a partially orthogonal design. Moreover, the blocks of the resulting design will remain orthogonal if and only if $kn/(kn + b) = kn_i/(kn_i + 1)$ for $i = 1, \ldots, b$, where, as before, n_i is the size of the element S_i of $\mathcal{S}$. In view of Corollary 4 augmenting the design might not be necessary at all, however. Similarly, the second condition that all components of $\mathbf{1}_b'\mathbf{U}_1$ are positive implies that a design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ with orthogonal blocks can frequently be turned into a partially orthogonal design by assigning the $2q$ different axial points arbitrarily to the blocks and possibly adding a single center point per block, as long as, with each occurrence of an axial point $\mathbf{x}$, also $-\mathbf{x}$ appears in the same block.

Example 2 Box and Behnken [4] present a second-order design for $q = 5$ factors which can be run in $b = 2$ orthogonal blocks of size 23. We generate a partially orthogonal design with blocks of the same size, which is considerably more efficient. To this end, first an orthogonally blocked design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ is constructed. Subsequently, the blocks are augmented to produce the final design.

Since $q = 5$, the construction of $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ requires a regular fraction $\mathbf{C}$ for $q - 1 = 4$ factors. Table 4 provides a fraction of resolution IV with $n = 8$ runs based on the defining contrast $1234 = I$. Adopting this fraction, we set

$$\mathbf{C} = \begin{pmatrix} -1 & -1 & -1 & -1 \\ -1 & -1 & 1 & 1 \\ -1 & 1 & -1 & 1 \\ -1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 \end{pmatrix}.$$

The construction will then give rise to eight matrices $\mathbf{B}_j$ as in (4). Since the overall size of the experiment is fixed at 46 it follows that only matrices $\mathbf{B}$ with at most five rows can be used. The matrices $\mathbf{B}_1, \ldots, \mathbf{B}_8$ are grouped into $b = 2$ blocks by means of a suitable partition $\mathcal{S} = \{S_1, S_2\}$. Here we use $S_1 = \{1, 2, 3, 4\}$ and $S_2 = \{5, 6, 7, 8\}$, which implies $(\mathbf{1}_k'\mathbf{B}) * \sum_{j \in S_i} \mathbf{d}_j = \mathbf{0}$, $i = 1, 2$, for any admissible choice of $\mathbf{B}$, that is any $\mathbf{B} = (b_{i,j})$ whose first column is orthogonal to $\mathbf{A} = (|b_{i,j}|)$, for which the elements in the second column of $\mathbf{B}$ add up to zero. Moreover, only the first component of both vectors $\sum_{j \in S_i} \tilde{\mathbf{d}}_j$, $i = 1, 2$, is different from zero. It follows from Corollary 1 that any design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$, for which the second column of the admissible matrix $\mathbf{B}$ consists entirely of zeros, is orthogonally blocked. Since $\mathbf{C}$ is of resolution IV the matrix $\mathbf{F}$ in (5) will be a zero matrix due to Theorem 1. Moreover, in order to achieve a diagonal $\mathbf{G}$ according to Corollary 3, the matrix $\mathbf{B}$ needs to be chosen such that $s_{2345} = 0$. A matrix satisfying all these requirements is

$$\mathbf{B} = \begin{pmatrix} -1 & 0 & -1 & 1 & 1 \\ 1 & 0 & 1 & -1 & 1 \end{pmatrix}.$$

The design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ is orthogonally blocked and the information matrix $\mathbf{M}(\xi_{\mathbf{B},\mathbf{C},\mathcal{S}})$ exhibits the pattern in (3) so that, in particular, $\mathbf{E}$, $\tilde{\mathbf{E}}$ and $\mathbf{F}$ in (5) are zero matrices and $\mathbf{G}$ is diagonal.

It is obvious that not all polynomial effects can be estimated from $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$. Also, it is clear that augmenting the design with axial and center points only is not sufficient to render all effects estimable. As to the first requirement in Theorem 2 we note that all zero elements on the diagonal of $\mathbf{G}$ correspond to interactions involving the second factor. Thus the requirement is fulfilled, for instance, for $\mathbf{U}_2$ with $u_{1,\{2,3\}} = u_{2,\{1,2\}} = u_{2,\{2,4\}} = u_{2,\{3,5\}} = 1$, $u_{1,\{2,5\}} = 2$ and $u_{i,\{j_1,j_2\}} = 0$ otherwise. Moreover, it can easily be checked that with this choice of $\mathbf{U}_2$ the matrix $\mathbf{P}$ in (7) has rank q regardless of which $\mathbf{U}_1$ and $\mathbf{U}_3$ are adopted. A possible allocation of the axial points to the blocks is specified by

$$\mathbf{U}_1 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

and $\mathbf{U}_3$ can be chosen to be a zero matrix. Finally, adding center points according to $\mathbf{z} = (1,3)$ gives the desired block size of 23 runs. The resulting augmented design $\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}}$ is partially orthogonal and shown in Table 6. Notice that the first eight rows in each block represent a block of the initial design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$.

The nonzero portions of the treatment information matrix of $\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}}$ in (9) are equal to $\mathrm{diag}(n\mathbf{w} + \sum 2^a \mathbf{1}_b' \mathbf{V}_a) = \mathrm{diag}(22, 20, 24, 20, 28)$,

$$\mathbf{Q} = \frac{1}{23} \begin{pmatrix} 262 & -124 & 104 & 144 & 64 \\ -124 & 252 & -148 & -100 & -104 \\ 104 & -148 & 264 & 128 & 124 \\ 144 & -100 & 128 & 252 & 96 \\ 64 & -104 & 124 & 96 & 244 \end{pmatrix}$$

and $\mathbf{G} + \mathrm{diag}(\sum 2^a \mathbf{1}_b' \mathbf{W}_a) = \mathrm{diag}(4, 16, 16, 16, 4, 4, 8, 16, 20, 16)$. Design 3 for $q = 5$ factors in Table 4 of Box and Behnken [4] is also partially orthogonal even though the method of construction is different from ours. Denoting the design by ξ_3 the treatment information matrix is

$$\mathbf{M}_\beta(\xi_3) = \begin{pmatrix} 16\mathbf{I}_5 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \frac{1}{23}(276\mathbf{I}_5 - 36\mathbf{1}_5\mathbf{1}_5') & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & 4\mathbf{I}_{10} \end{pmatrix}.$$

The relative D-efficiency $(\det \mathbf{M}_\beta(\xi_3) / \det \mathbf{M}_\beta(\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}}))^{1/20}$ of ξ_3, with respect to $\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}}$, for estimating the polynomial effects is equal to 0.605. Similarly, the relative A-efficiency of ξ_3 can be calculated as $\mathrm{trace}\,\mathbf{M}_\beta(\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}})^{-1} / \mathrm{trace}\,\mathbf{M}_\beta(\xi_3)^{-1} = 0.655$. The improved efficiency can be explained by the fact that all linear effects are estimated more precisely and all interaction effects are estimated at least as precisely when our design is used and that the precision for estimating the quadratic effects is only slightly lower than for the Box-Behnken design.

Table 6: Partially orthogonal design for five factors in two blocks

Blocks									
$\tilde{\mathbf{B}}_1$					$\tilde{\mathbf{B}}_2$				
$-$	0	$+$	$-$	$-$	$-$	0	$+$	$-$	$+$
$+$	0	$-$	$+$	$-$	$+$	0	$-$	$+$	$+$
$-$	0	$+$	$+$	$+$	$-$	0	$+$	$+$	$-$
$+$	0	$-$	$-$	$+$	$+$	0	$-$	$-$	$-$
$-$	0	$-$	$-$	$+$	$-$	0	$-$	$-$	$-$
$+$	0	$+$	$+$	$+$	$+$	0	$+$	$+$	$-$
$-$	0	$-$	$+$	$-$	$-$	0	$-$	$+$	$+$
$+$	0	$+$	$-$	$-$	$+$	0	$+$	$-$	$+$
0	$-$	$-$	0	0	$-$	$-$	0	0	0
0	$-$	$+$	0	0	$-$	$+$	0	0	0
0	$+$	$-$	0	0	$+$	$-$	0	0	0
0	$+$	$+$	0	0	$+$	$+$	0	0	0
0	$-$	0	0	$-$	0	$-$	0	$-$	0
0	$-$	0	0	$+$	0	$-$	0	$+$	0
0	$+$	0	0	$-$	0	$+$	0	$-$	0
0	$+$	0	0	$+$	0	$+$	0	$+$	0
0	$-$	0	0	$-$	0	0	$-$	0	$-$
0	$-$	0	0	$+$	0	0	$-$	0	$+$
0	$+$	0	0	$-$	0	0	$+$	0	$-$
0	$+$	0	0	$+$	0	0	$+$	0	$+$
$-$	0	0	0	0	0	0	0	0	0
$+$	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0

Although the augmented design already represents a sizable improvement there are other even more efficient augmentations. Also, there are other more efficient partially orthogonal designs in two blocks of 23 runs which are generated differently. For example, with regard to the central-composite-type design, which has the 2_V^{5-1} fractional factorial and seven center points in the first block and which repeats all axial points twice together with three center points in the second block, the relative D-efficiency of $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}^{\mathcal{U},\mathbf{z}}$ is equal to 0.891 and the relative A-efficiency is equal to 0.864. A closer investigation shows, however, that only four of the interaction effects are more accurately estimated when the central-composite-type design is used, whereas all other effects, in particular the quadratic effects, are more or as precisely estimated with $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}^{\mathcal{U},\mathbf{z}}$. We therefore want to emphasize that the purpose of the current example is not to advocate a particular design but to give an idea of the large number of competitive new designs that can be constructed as partially orthogonal designs.

6. Designs with small blocks

The design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ for $q = 5$ factors in two blocks of size eight, considered in Example 2, possesses a singular information matrix and does not allow the estimation of all $p = 20$ polynomial effects. One appealing feature of the design, however, is its apparently small block size. This section presents a method which uses designs of this kind for generating partially orthogonal designs with small blocks.

Suppose $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ is a design with b blocks $\tilde{\mathbf{B}}_1, \ldots, \tilde{\mathbf{B}}_b$ for which the portions $\mathbf{E}$, $\tilde{\mathbf{E}}$ and $\mathbf{F}$ of the information matrix in (5) are zero matrices and $\mathbf{G}$ is diagonal. We generate b additional blocks by applying the same permutation to the columns of each of the initial blocks. Formally, let π be a permutation of the numbers $1, \ldots, q$ and $\mathbf{P}_\pi$ be the corresponding permutation matrix. For $i = 1, \ldots, b$, set $\tilde{\mathbf{B}}_{b+i} = \tilde{\mathbf{B}}_i \mathbf{P}_\pi$. Enlarging $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ with the new blocks produces a design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S},\pi}$ consisting of the $2b$ blocks $\tilde{\mathbf{B}}_1, \ldots, \tilde{\mathbf{B}}_b, \tilde{\mathbf{B}}_{b+1}, \ldots, \tilde{\mathbf{B}}_{2b}$. Obviously, the procedure can be generalized to generate designs with rb blocks using $r-1$ permutations, but for simplicity only the case $r = 2$ is considered here.

The motivation behind the enlarged designs is that, if $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ is a design with b small blocks and singular information matrix of the form in (3), then the blocks of $\xi_{\mathbf{B},\mathbf{C},\mathcal{S},\pi}$ will also be small and the information matrix $\mathbf{M}(\xi_{\mathbf{B},\mathbf{C},\mathcal{S},\pi})$ will have the same structure, but might be invertible so that the enlarged design is partially orthogonal. Moreover, if the matrix $\mathbf{M}(\xi_{\mathbf{B},\mathbf{C},\mathcal{S},\pi})$ is singular, then an augmented partially orthogonal design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S},\pi}^{\mathcal{U},\mathbf{z}}$ can be generated exactly as in Section 5 where now, however, the common number of rows of the matrices $\mathbf{U}_1$, $\mathbf{U}_2$ and $\mathbf{U}_3$ in $\mathcal{U}$ and the length of the vector $\mathbf{z}$ are both equal to $2b$. We mention that a result similar to Theorem 2 could be formulated, but in the interest of space we only present an illustrative example.

Table 7: Partially orthogonal design for five factors in four small blocks

Blocks																			
$\tilde{\mathbf{B}}_1$					$\tilde{\mathbf{B}}_2$					$\tilde{\mathbf{B}}_3$					$\tilde{\mathbf{B}}_4$				
−	0	+	−	−	−	0	+	−	+	+	−	−	0	−	+	−	+	0	−
+	0	−	+	−	+	0	−	+	+	−	+	−	0	+	−	+	+	0	+
−	0	+	+	+	−	0	+	+	−	+	−	+	0	+	+	−	−	0	+
+	0	−	−	+	+	0	−	−	−	−	+	+	0	−	−	+	−	0	−
−	0	−	−	+	−	0	−	−	−	−	−	+	0	−	−	−	−	0	−
+	0	+	+	+	+	0	+	+	−	+	+	+	0	+	+	+	−	0	+
−	0	−	+	−	−	0	−	+	+	−	−	−	0	+	−	−	+	0	+
+	0	+	−	−	+	0	+	−	+	+	+	−	0	−	+	+	+	0	−
0	0	−	0	0	−	−	0	0	0	−	0	0	0	0	0	−	0	−	0
0	0	+	0	0	−	+	0	0	0	+	0	0	0	0	0	−	0	+	0
0	0	0	0	−	+	−	0	0	0						0	+	0	−	0
0	0	0	0	+	+	+	0	0	0						0	+	0	+	0

Example 3 Consider again the situation with $q = 5$ factors and suppose that the block size of 23 required by the partially orthogonal design in Table 6 cannot be realized due to practical constraints. Suppose further that the total number of 46 runs needed by the designs is acceptable, but that the experiment should be run in four blocks of almost equal size.

In this case an augmented partially orthogonal design $\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S},\pi}$, with three blocks of size 12 and one block of size 10, can be derived from the design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ considered in Example 2. To this end let $\tilde{\mathbf{B}}_1, \tilde{\mathbf{B}}_2$ be the blocks of $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ which consist of the first eight rows of the blocks depicted in Table 6. Two additional blocks $\tilde{\mathbf{B}}_3$ and $\tilde{\mathbf{B}}_4$ are obtained by rearranging the columns of $\tilde{\mathbf{B}}_1$ and $\tilde{\mathbf{B}}_2$ according to the permutation $\pi = (2, 4, 1, 5, 3)$ which, for example, takes the first column of $\tilde{\mathbf{B}}_1$ and $\tilde{\mathbf{B}}_2$ to the second column of $\tilde{\mathbf{B}}_3$ and $\tilde{\mathbf{B}}_4$, respectively. Finally, the blocks $\tilde{\mathbf{B}}_1, \ldots, \tilde{\mathbf{B}}_4$ are augmented as specified by $\mathcal{U} = \{\mathbf{U}_1, \mathbf{U}_2, \mathbf{U}_3\}$ and the vector $\mathbf{z} = (0, 0, 0, 0)$, where

$$\mathbf{U}_1 = \begin{pmatrix} 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$\mathbf{U}_2$ is a 4×10 matrix all elements of which are zero, except $u_{2,\{1,2\}} = u_{4,\{2,4\}} = 1$, and $\mathbf{U}_3$ is a zero matrix of order 4×10. Table 7 displays the resulting augmented design.

The treatment information matrix $\mathbf{M}_\beta(\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S},\pi})$ of the design is block-diagonal with nonzero portions diag$(38, 24, 34, 20, 34)$,

$$\frac{1}{15}\begin{pmatrix} 80 & 0 & 60 & 0 & 60 \\ 0 & 64 & -16 & -40 & -16 \\ 60 & -16 & 129 & 20 & 99 \\ 0 & -40 & 20 & 120 & 20 \\ 60 & -16 & 99 & 20 & 129 \end{pmatrix}$$

and diag$(20, 32, 16, 32, 16, 4, 16, 16, 32, 16)$, corresponding to the linear, quadratic, and interaction effects, respectively. From this the relative D-efficiency of the Box-Behnken design ξ_3 with respect to $\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S},\pi}$, for estimating the polynomial effects, can be calculated as 0.491 and the relative A-efficiency of ξ_3 is equal to 0.675. Thus, in addition to providing small almost equally sized blocks the partially orthogonal design possesses a considerably higher efficiency. Of course, if the small blocks are indeed successful in reducing within-block variance, then the increase in efficiency will be even greater. In practice, it will very often be advisable to have equal-sized blocks and this is easily achieved, without altering the partial orthogonality properties, by adding two center points to block 3 in Table 7.

7. Discussion

Running a response surface experiment in blocks is useful when high run-to-run variation can be expected. When orthogonal blocking of a given design is possible, parameter estimates for the polynomial effects are not affected by the blocking. Yet, when orthogonal blocking cannot be achieved, usually algorithms for arranging experimental runs into blocks that optimize some efficiency criterion have to be employed. The resulting designs, however, generally yield parameter estimates that are correlated to some extent.

For second-order response surface models this paper has introduced partially orthogonal designs as a new class of three-level designs. The notion of partially orthogonal designs is motivated by the observation that the information matrix of D-optimal continuous designs exhibits a specific structure in terms of a characteristic pattern of zero entries which correspond to uncorrelated effects. For the second-order model without blocks this pattern is also shared by central composite designs with a factorial portion of resolution V or higher and several Box-Behnken designs, as well as the more general class of subset designs [14]. This pattern makes model selection more robust, as well as aiding interpretation. Partially orthogonal designs then represent blocked designs which maintain this pattern. Often these designs permit orthogonal or near-orthogonal blocking.

For similar reasons, in particular robustness against model misspecification, [23] introduced OMARS designs, which are unblocked three-level response surface designs and which share several structural features with partially orthogonal designs (see Section 2). Although none of the two classes of designs is a subset of the other and the blocking of OMARS designs has not yet been investigated, there appears to be some overlap between OMARS and partially orthogonally designs, in particular when the sparsity constraints of OMARS designs are relaxed, which is mentioned as a possibility by Núñez Ares and Goos [23, p. 33]. Therefore the results in the present paper may lead to a better mathematical understanding of some of the algorithmically derived OMARS designs in the large catalogue of [23], which the authors mention as a possibility to improve their methods. Conversely, the OMARS designs found by [23] may inform the choice of the matrix $\mathbf{B}$ in the construction of the designs $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ in certain cases.

The emphasis on structural aspects of the designs does not preclude the study of efficiency or other statistical properties either within the class of partially orthogonal designs or compared with blocked designs generated by other methods. The examples presented herein demonstrate that partially orthogonal designs can be considerably more efficient than some traditional designs. The designs presented here are illustrative examples. We have studied multiple examples and found good designs of various sizes. A more systematic study could computationally generate a database of partially orthogonal designs and describe the statistical properties of every design by means of a characterization document similar to the one used by [23].

Besides statistical properties, the practical usefulness of any proposed design depends on the total number of runs that need to be performed. In the context of blocked experiments, additionally, the number of blocks and the block sizes need to be considered. Box-Behnken designs are only available for a very limited number of blocks and block sizes, whereas the designs considered here cover considerably more cases. Similarly, the augmented pairs designs [22] can only be run in two blocks which differ grossly in size. The examples in this paper show that partially orthogonal designs are more flexible and can be better tailored to the needs of the experiment.

The number of runs required by a design $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ equals the product of the number k of rows of the matrix $\mathbf{B}$ and the number n of runs of the fractional factorial $\mathbf{C}$. Augmented designs need additional runs. The number of blocks and the individual block sizes can be controlled by means of the partition $\mathcal{S}$. In general, for a given number of factors q it is usually possible to generate a partially orthogonal design with a larger number of small blocks or a design with a smaller number of large blocks. This also gives more freedom for constructing a design which fits the needs of the experiment.

Appendix A. Proof of Theorem 1

Block $\tilde{\mathbf{B}}_i$ of $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ consists of the rows of the n_i matrices $\mathbf{B}_j$, defined by (4), with $j \in S_i$, $i = 1, \ldots, b$. Without loss of generality, it can be assumed that the rows of $(\mathbf{Z}, \mathbf{X})$ are arranged according to blocks. Write $\mathbf{X} = (\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3)$ where $\mathbf{X}_1$, $\mathbf{X}_2$, $\mathbf{X}_3$ correspond to linear, quadratic and interaction effects, respectively. The information matrix can then be partitioned as

$$\mathbf{M}(\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}) = \begin{pmatrix} \mathbf{Z}'\mathbf{Z} & \mathbf{Z}'\mathbf{X}_1 & \mathbf{Z}'\mathbf{X}_2 & \mathbf{Z}'\mathbf{X}_3 \\ \mathbf{X}_1'\mathbf{Z} & \mathbf{X}_1'\mathbf{X}_1 & \mathbf{X}_1'\mathbf{X}_2 & \mathbf{X}_1'\mathbf{X}_3 \\ \mathbf{X}_2'\mathbf{Z} & \mathbf{X}_2'\mathbf{X}_1 & \mathbf{X}_2'\mathbf{X}_2 & \mathbf{X}_2'\mathbf{X}_3 \\ \mathbf{X}_3'\mathbf{Z} & \mathbf{X}_3'\mathbf{X}_1 & \mathbf{X}_3'\mathbf{X}_2 & \mathbf{X}_3'\mathbf{X}_3 \end{pmatrix},$$

with submatrices whose dimensions match those of the corresponding entries in (5).

(i) For $u = 1, 2, 3$ and every $i = 1, \dots, b$ let $\mathbf{X}_{u,i}$ denote the part of $\mathbf{X}_u$ corresponding to block number i. It is easy to see that $\mathbf{Z}'\mathbf{Z} = k \operatorname{diag}(\mathbf{v})$, $\mathbf{Z}'\mathbf{X}_2 = \mathbf{v}'\mathbf{w}$ and $\mathbf{X}_2'\mathbf{X}_2 = n\mathbf{A}'\mathbf{A}$. The ith row of $\mathbf{Z}'\mathbf{X}_1$ is equal to

$$\mathbf{1}_{kn_i}'\mathbf{X}_{1,i} = \sum_{j \in S_i} \mathbf{1}_k'\mathbf{B}\mathbf{D}_j = \mathbf{1}_k'\mathbf{B} \sum_{j \in S_i} \mathbf{D}_j = (\mathbf{1}_k'\mathbf{B}) * \sum_{j \in S_i} \mathbf{d}_j,$$

for every $i = 1, \dots, b$, which gives rise to $\mathbf{E}$ in (5). Similarly, it follows that $\mathbf{Z}'\mathbf{X}_3 = \tilde{\mathbf{E}}$, since

$$\mathbf{1}_{kn_i}'\mathbf{X}_{3,i} = \sum_{j \in S_i} \mathbf{1}_k'\mathbf{P}_{\mathbf{B}} \operatorname{diag}(\tilde{\mathbf{d}}_j) = \mathbf{1}_k'\mathbf{P}_{\mathbf{B}} \sum_{j \in S_i} \operatorname{diag}(\tilde{\mathbf{d}}_j) = (\mathbf{1}_k'\mathbf{P}_{\mathbf{B}}) * \sum_{j \in S_i} \tilde{\mathbf{d}}_j,$$

for every i. The part of $\mathbf{M}(\xi_{\mathbf{B},\mathbf{C},\mathcal{S}})$ corresponding to the linear effects is given by

$$\mathbf{X}_1'\mathbf{X}_1 = \sum_{i=1}^{b} \mathbf{X}_{1,i}'\mathbf{X}_{1,i} = \sum_{i=1}^{b} \sum_{j \in S_i} \mathbf{D}_j\mathbf{B}'\mathbf{B}\mathbf{D}_j,$$

from which it follows that the element $(\mathbf{X}_1'\mathbf{X}_1)_{r,s}$, in row $1 \le r \le q$ and column $1 \le s \le q$ of the matrix, is the product $(\mathbf{B}'\mathbf{B})_{r,s}(\mathbf{D}'\mathbf{D})_{r,s}$ of the corresponding elements of $\mathbf{B}'\mathbf{B}$ and $\mathbf{D}'\mathbf{D}$. Since $\mathbf{C}$ is of resolution *III* or higher, we have $\mathbf{D}'\mathbf{D} = n\mathbf{I}_q$. Consequently, $\mathbf{X}_1'\mathbf{X}_1$ is a diagonal matrix with diagonal elements $n(\mathbf{B}'\mathbf{B})_{r,r}$, which can be concisely written as $\mathbf{X}_1'\mathbf{X}_1 = n \operatorname{diag}(\mathbf{w})$.

Next it is shown that $\mathbf{X}_1'\mathbf{X}_2$ and $\mathbf{X}_2'\mathbf{X}_3$ are zero matrices. Consider first the matrix

$$\mathbf{X}_1'\mathbf{X}_2 = \sum_{i=1}^{b} \mathbf{X}_{1,i}'\mathbf{X}_{2,i} = \sum_{i=1}^{b} \sum_{j \in S_i} \mathbf{D}_j\mathbf{B}'\mathbf{A} = \operatorname{diag}(\mathbf{1}_n'\mathbf{D})\mathbf{B}'\mathbf{A}.$$

The rightmost term in this equation is a zero matrix since each column of $\mathbf{D}$, except the first, adds up to zero and the first row of $\mathbf{B}'\mathbf{A}$ is a zero vector, due to the requirement that the first column of $\mathbf{B}$ is orthogonal to $\mathbf{A}$. Similarly, it follows that

$$\mathbf{X}_2'\mathbf{X}_3 = \sum_{i=1}^{b} \mathbf{X}_{2,i}'\mathbf{X}_{3,i} = \sum_{i=1}^{b} \sum_{j \in S_i} \mathbf{A}'\mathbf{P}_{\mathbf{B}} \operatorname{diag}(\tilde{\mathbf{d}}_j) = \mathbf{A}'\mathbf{P}_{\mathbf{B}} \operatorname{diag}(\mathbf{1}_n'\mathbf{P}_{\mathbf{D}})$$

is a zero matrix, since $\mathbf{C}$ being a resolution *III* design implies $\mathbf{1}_n'\mathbf{P}_{\mathbf{D}} = \mathbf{0}$.

It remains to be shown that $\mathbf{X}_1'\mathbf{X}_3 = \mathbf{F}$ and $\mathbf{X}_3'\mathbf{X}_3 = \mathbf{G}$. From

$$\mathbf{X}_1'\mathbf{X}_3 = \sum_{i=1}^{b} \mathbf{X}_{1,i}'\mathbf{X}_{3,i} = \sum_{i=1}^{b}\sum_{j\in S_i} \mathbf{D}_j\mathbf{B}'\mathbf{P}_{\mathbf{B}}\,\mathrm{diag}(\tilde{\mathbf{d}}_j),$$

it follows that the element $(\mathbf{X}_1'\mathbf{X}_3)_{r,s}$ in row $1 \le r \le q$ and column $1 \le s \le q(q-1)/2$ of $\mathbf{X}_1'\mathbf{X}_3$ is given by

$$(\mathbf{X}_1'\mathbf{X}_3)_{r,s} = \sum_{i=1}^{b}\sum_{j\in S_i} d_{j,r}(\mathbf{B}'\mathbf{P}_{\mathbf{B}})_{r,s}\tilde{d}_{j,s} = (\mathbf{B}'\mathbf{P}_{\mathbf{B}})_{r,s}(\mathbf{D}'\mathbf{P}_{\mathbf{D}})_{r,s},$$

where $d_{j,r}$ and $\tilde{d}_{j,s}$ are the rth and sth element of $\mathbf{d}_j$ and $\tilde{\mathbf{d}}_j$, respectively. Here, $(\mathbf{B}'\mathbf{P}_{\mathbf{B}})_{r,s}$ and $(\mathbf{D}'\mathbf{P}_{\mathbf{D}})_{r,s}$ denote the elements in row r and column s of $\mathbf{B}'\mathbf{P}_{\mathbf{B}}$ and $\mathbf{D}'\mathbf{P}_{\mathbf{D}}$. Thus, $\mathbf{X}_1'\mathbf{X}_3 = (\mathbf{B}'\mathbf{P}_{\mathbf{B}}) * (\mathbf{D}'\mathbf{P}_{\mathbf{D}}) = \mathbf{F}$. Similarly, it can be shown that $\mathbf{X}_3'\mathbf{X}_3 = (\mathbf{P}_{\mathbf{B}}'\mathbf{P}_{\mathbf{B}}) * (\mathbf{P}_{\mathbf{D}}'\mathbf{P}_{\mathbf{D}}) = \mathbf{G}$. Finally, if $\mathbf{B} = (\mathbf{H}', -\mathbf{H}')'$ or $\mathbf{B} = (\mathbf{H}', -\mathbf{H}', \mathbf{0})'$, it follows that $\mathbf{B}'\mathbf{P}_{\mathbf{B}} = \mathbf{H}'\mathbf{P}_{\mathbf{H}} - \mathbf{H}'\mathbf{P}_{\mathbf{H}} = \mathbf{0}$ and hence $\mathbf{F} = \mathbf{0}$.

(ii) If $\mathbf{C}$ is of resolution *IV*, all elements of $\mathbf{D}'\mathbf{P}_{\mathbf{D}}$ are equal to zero except $(\mathbf{D}'\mathbf{P}_{\mathbf{D}})_{r,r-1}$, $r = 2, \ldots, q$. Since the first column of $\mathbf{B}$ is orthogonal to $\mathbf{A}$, the corresponding elements $(\mathbf{B}'\mathbf{P}_{\mathbf{B}})_{r,r-1}$ of $\mathbf{B}'\mathbf{P}_{\mathbf{B}}$ vanish. Consequently, $\mathbf{F} = (\mathbf{B}'\mathbf{P}_{\mathbf{B}}) * (\mathbf{D}'\mathbf{P}_{\mathbf{D}}) = \mathbf{0}$.

(iii) Only the statement regarding $\mathbf{G}$ needs to be proved because of (ii). Clearly, $\mathbf{C}$ having resolution *V* implies $\mathbf{P}_{\mathbf{D}}'\mathbf{P}_{\mathbf{D}} = n\mathbf{I}_{q(q-1)/2}$ so that $\mathbf{G} = (\mathbf{P}_{\mathbf{B}}'\mathbf{P}_{\mathbf{B}}) * (\mathbf{P}_{\mathbf{D}}'\mathbf{P}_{\mathbf{D}}) = n(\mathbf{P}_{\mathbf{B}}'\mathbf{P}_{\mathbf{B}}) * \mathbf{I}_{q(q-1)/2}$.

Appendix B. Proof of Corollary 1

Using the same notation as before, it has to be shown [6, 15] that

$$\frac{1}{kn}\sum_{a=1}^{b} \mathbf{1}_{kn_a}'\mathbf{X}_{u,a} = \frac{1}{kn_i}\mathbf{1}_{kn_i}'\mathbf{X}_{u,i}, \tag{B.1}$$

for every $u = 1, 2, 3$ and every $i = 1, \ldots, b$, is equivalent to the requirement that both $(\mathbf{1}_k'\mathbf{B}) * \sum_{j\in S_i}\mathbf{d}_j$ and $(\mathbf{1}_k'\mathbf{P}_{\mathbf{B}}) * \sum_{j\in S_i}\tilde{\mathbf{d}}_j$ are zero vectors, for every $i = 1, \ldots, b$. For $u = 2$ condition (B.1) is always fulfilled without making any assumptions since $\mathbf{1}_{kn_i}'\mathbf{X}_{2,i} = n_i\mathbf{1}_k'\mathbf{A}$, for every i. If $u = 1$, the sum on the left-hand side of (B.1) is equal to $\mathbf{1}_b'\mathbf{E} = (\mathbf{1}_k'\mathbf{B}) * (\mathbf{1}_n'\mathbf{D})$. Since $\mathbf{C}$ is of resolution *III* or higher, only the first element of $\mathbf{1}_n'\mathbf{D}$ is different from zero. Also, the first element of $\mathbf{1}_k'\mathbf{B}$ is zero as the construction of the design requires the first column of $\mathbf{B}$ to be orthogonal to $\mathbf{A}$. Consequently, $(\mathbf{1}_k'\mathbf{B}) * (\mathbf{1}_n'\mathbf{D}) = \mathbf{0}$. Hence condition (B.1) is satisfied, for $u = 1$ and every i, if and only if each column of every block has column sum zero which is equivalent to $(\mathbf{1}_k'\mathbf{B}) * \sum_{j\in S_i}\mathbf{d}_j = \mathbf{0}$, for $i = 1, \ldots, b$. Similarly, if $u = 3$, it follows that $\sum_{a=1}^{b}\mathbf{1}_{kn_a}'\mathbf{X}_{3,a} = \mathbf{1}_b'\tilde{\mathbf{E}} = (\mathbf{1}_k'\mathbf{P}_{\mathbf{B}}) * (\mathbf{1}_n'\mathbf{P}_{\mathbf{D}}) = \mathbf{0}$, since $\mathbf{1}_n'\mathbf{P}_{\mathbf{D}} = \mathbf{0}$. Thus, for $u = 3$ and every i, condition (B.1) is equivalent to $(\mathbf{1}_k'\mathbf{P}_{\mathbf{B}}) * \sum_{j\in S_i}\tilde{\mathbf{d}}_j = \mathbf{0}$.

Appendix C. Proof of Corollary 2

Every element in $\mathbf{F} = (\mathbf{B}'\mathbf{P_B}) * (\mathbf{D}'\mathbf{P_D})$ corresponds to the inner product of a column in the treatment design matrix $\mathbf{X}$ that represents a linear effect and a column representing a two-factor interaction. All inner products involving the linear effect of the first factor vanish, because the corresponding entry of $\mathbf{D}'\mathbf{P_D}$ equals zero, due to $\mathbf{C}$ having resolution *III*. For factors other than the first one, the inner product will be zero for the same reason, when the product corresponds to the linear effect of a factor and an interaction involving the same factor but not the first factor. Moreover, $\mathbf{C}$ having resolution *III* also gives rise to zero elements in $\mathbf{F}$, whenever the first factor is involved in the interaction with some factor and the linear effect corresponds to yet another factor.

When the interaction of the first factor with another factor that also defines a linear effect is considered, the corresponding element of $\mathbf{B}'\mathbf{P_B}$ and hence of $\mathbf{F}$ is equal to zero since the first column of $\mathbf{B}$ is orthogonal to $\mathbf{A}$. Finally, elements of $\mathbf{F}$ corresponding to three different factors $2 \leq j_1, j_2, j_3 \leq q$ vanish if the three-factor interaction of the factors j_1-1, j_2-1, j_3-1 is not contained in the defining contrast group of $\mathbf{C}$. Otherwise, there are three elements in $\mathbf{F}$ involving the factors j_1, j_2, j_3 that can be different from zero. More specifically, each element of $\mathbf{D}'\mathbf{P_D}$ corresponding to the factors j_1, j_2, j_3 is a sum of products of elements in the columns j_1-1, j_2-1, j_3-1 of $\mathbf{C}$, which equals zero if and only if the interaction of the factors j_1-1, j_2-1, j_3-1 is not contained in the defining contrast group of $\mathbf{C}$ (see, for example, [8], 2003). The proof is completed by noting that the number of three-factor interactions in the defining contrast group is given by the component W_3 of the wordlength pattern of $\mathbf{C}$. The proof of the statement regarding $\mathbf{G}$ is analogous and is therefore omitted.

Appendix D. Proof of Corollary 4

Under the assumptions regarding $\mathbf{E}$, $\tilde{\mathbf{E}}$, $\mathbf{F}$, and $\mathbf{G}$, the determinant of $\mathbf{M}(\xi_{\mathbf{B},\mathbf{C},\mathcal{S}})$ is equal to

$$\det \mathbf{M}(\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}) = k^b n^{2q} \prod_{i=1}^{b} n_i \prod_{j=1}^{q} w_j \det(\mathbf{A}'(\mathbf{I}_k - \tfrac{1}{k}\mathbf{1}_k\mathbf{1}_k')\mathbf{A}) \det \mathbf{G},$$

where w_j represents the jth component of the vector $\mathbf{w} = \mathbf{1}_k'\mathbf{A}$. All w_j and $\det \mathbf{G}$ are positive, because $\mathbf{A}'\mathbf{A}$ contains only positive elements. The matrix $\mathbf{I}_k - \frac{1}{k}\mathbf{1}_k\mathbf{1}_k'$ is idempotent with null space $\{\lambda\mathbf{1}_k : \lambda \in \mathbb{R}\}$. Since $\mathbf{A}$ has rank q and $\mathbf{1}_k$ is not contained in the column space of $\mathbf{A}$, it follows that $\mathbf{A}'(\mathbf{I}_k - \frac{1}{k}\mathbf{1}_k\mathbf{1}_k')\mathbf{A}$ is positive definite and $\det \mathbf{M}(\xi_{\mathbf{B},\mathbf{C},\mathcal{S}})$ is thus positive. The treatment information matrix is readily obtained by using the well-known formula for the inverse of a partitioned matrix.

Appendix E. Proof of Theorem 2

Denote the treatment design matrix for $\xi_{\mathbf{B},\mathbf{C},\mathcal{S}}$ by $\mathbf{X}$ and the corresponding block indicator matrix by $\mathbf{Z}$. Similarly, let $\mathbf{X}^*$ and $\mathbf{Z}^*$ be the treatment design and block indicator matrices for the additional points in $\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}}$. Stacking $(\mathbf{Z},\mathbf{X})$ on top of $(\mathbf{Z}^*,\mathbf{X}^*)$ then yields the design matrix for the augmented design in model (2). It follows that

$$\mathbf{M}(\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}}) = \mathbf{M}(\xi_{\mathbf{B},\mathbf{C},\mathcal{S}})+$$

$$\begin{pmatrix} \mathrm{diag}(\mathbf{z}+\sum 2^a\mathbf{1}'_{C(q,a)}\mathbf{U}'_a) & \mathbf{0} & \sum 2^a\mathbf{V}_a & \mathbf{0} \\ \mathbf{0} & \mathrm{diag}(\sum 2^a\mathbf{1}'_b\mathbf{V}_a) & \mathbf{0} & \mathbf{0} \\ \sum 2^a\mathbf{V}'_a & \mathbf{0} & \sum 2^a\mathbf{N}_a\,\mathrm{diag}(\mathbf{1}'_b\mathbf{U}_a)\mathbf{N}'_a & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathrm{diag}(\sum 2^a\mathbf{1}'_b\mathbf{W}_a) \end{pmatrix},$$

where all summations are taken over $a=1,2,3$. All matrices $\mathbf{U}_a$, $\mathbf{V}_a$ and $\mathbf{W}_a$, $a=1,2,3$, are defined as stated before Theorem 2, in particular $\mathbf{V}_1=\mathbf{U}_1$, $\mathbf{W}_1=\mathbf{0}$ and $\mathbf{W}_2=\mathbf{U}_2$. Under the assumptions of Theorem 2 regarding the matrices $\mathbf{E}$, $\tilde{\mathbf{E}}$, $\mathbf{F}$ and $\mathbf{G}$, it follows from (5) that $\mathbf{M}(\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}})$ is equal to (8).

By multiplying $\mathbf{M}(\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}})$ from the left with a permutation matrix $\mathbf{\Pi}$ and from the right with $\mathbf{\Pi}'$, one obtains a block diagonal matrix with diagonal blocks

$$\begin{pmatrix} \mathrm{diag}(k\mathbf{v}+\mathbf{z}+\sum 2^a\mathbf{1}'_{C(q,a)}\mathbf{U}'_a) & \mathbf{v}'\mathbf{w}+\sum 2^a\mathbf{V}_a \\ \mathbf{w}'\mathbf{v}+\sum 2^a\mathbf{V}'_a & n\mathbf{A}'\mathbf{A}+\sum 2^a\mathbf{N}_a\,\mathrm{diag}(\mathbf{1}'_b\mathbf{U}_a)\mathbf{N}'_a \end{pmatrix}, \tag{E.1}$$

in which $\mathbf{A}$, k, n, $\mathbf{v}$ and $\mathbf{w}$ are defined as in (5), $\mathrm{diag}(n\mathbf{w}+\sum 2^a\mathbf{1}'_b\mathbf{V}_a)$ and $\mathbf{G}+\mathrm{diag}(\sum 2^a\mathbf{1}'_b\mathbf{W}_a)$. Since $\det\mathbf{\Pi}\det\mathbf{\Pi}'=1$, it then follows that the determinant of $\mathbf{M}(\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}})$ is equal to the product of the determinants of the matrices $\mathrm{diag}(n\mathbf{w}+\sum 2^a\mathbf{1}'_b\mathbf{V}_a)$, $\mathbf{G}+\mathrm{diag}(\sum 2^a\mathbf{1}'_b\mathbf{W}_a)$ and (E.1).

The requirement regarding the diagonal elements of $\mathbf{G}$ implies that all components of $n\mathbf{w}+\sum 2^a\mathbf{1}'_b\mathbf{V}_a$ and all diagonal elements of the matrix $\mathbf{G}+\mathrm{diag}(\sum 2^a\mathbf{1}'_b\mathbf{W}_a)$ are positive. Consequently, both $\mathrm{diag}(n\mathbf{w}+\sum 2^a\mathbf{1}'_b\mathbf{V}_a)$ and $\mathbf{G}+\mathrm{diag}(\sum 2^a\mathbf{1}'_b\mathbf{W}_a)$ have positive determinants. Also, $\det\mathrm{diag}(k\mathbf{v}+\mathbf{z}+\sum 2^a\mathbf{1}'_{C(q,a)}\mathbf{U}'_a)>0$, since the diagonal elements of the matrix are the block sizes. By the well-known formula for the determinant of a partitioned matrix, it follows that the determinant of the matrix in (E.1) is equal to $\det\mathrm{diag}(k\mathbf{v}+\mathbf{z}+\sum 2^a\mathbf{1}'_{C(q,a)}\mathbf{U}'_a)\det\mathbf{Q}$, where, as in (10),

$$\begin{aligned}\mathbf{Q} \;=\;& n\mathbf{A}'\mathbf{A}+\sum 2^a\mathbf{N}_a\,\mathrm{diag}(\mathbf{1}'_b\mathbf{U}_a)\mathbf{N}'_a \\ & -(\mathbf{w}'\mathbf{v}+\sum 2^a\mathbf{V}'_a)\,\mathrm{diag}(k\mathbf{v}+\mathbf{z}+\sum 2^a\mathbf{1}'_{C(q,a)}\mathbf{U}'_a)^{-1}(\mathbf{v}'\mathbf{w}+\sum 2^a\mathbf{V}_a).\end{aligned}$$

Now, rearrange the rows of the treatment design matrix of $\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}}$ in accordance with the blocks and denote the part of the resulting matrix corresponding to the quadratic effects in the ith block by $\tilde{\mathbf{X}}_{2,i}$, $i = 1, \ldots, b$. From the representation of the information matrix $\mathbf{M}(\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}})$, it is easy to see that

$$\mathbf{Q} = \sum_{i=1}^{b} (\tilde{\mathbf{X}}'_{2,i}\tilde{\mathbf{X}}_{2,i} - \tfrac{1}{k_i}\tilde{\mathbf{X}}'_{2,i}\mathbf{1}_{k_i}\mathbf{1}'_{k_i}\tilde{\mathbf{X}}_{2,i}) = \sum_{i=1}^{b} \tilde{\mathbf{X}}'_{2,i}(\mathbf{I}_{k_i} - \tfrac{1}{k_i}\mathbf{1}_{k_i}\mathbf{1}'_{k_i})\tilde{\mathbf{X}}_{2,i},$$

where $k_1, \ldots, k_b$ are the block sizes of the augmented design. The rightmost expression in this equation shows that $\mathbf{Q}$ is positive semi-definite.

If $\mathbf{Q}$ is positive definite, so that $\det \mathbf{Q} > 0$, it immediately follows that the augmented design is partially orthogonal since then $\det \mathbf{M}(\xi^{\mathcal{U},\mathbf{z}}_{\mathbf{B},\mathbf{C},\mathcal{S}}) > 0$. If, by contrast, $\det \mathbf{Q} = 0$, then there exists a column vector $\mathbf{x} \neq \mathbf{0}$ with $\mathbf{x}'\mathbf{Q}\mathbf{x} = 0$. The requirement that $\mathbf{P}$ has rank q ensures that $n\mathbf{A}'\mathbf{A} + \sum 2^a \mathbf{N}_a \operatorname{diag}(\mathbf{1}'_b\mathbf{U}_a)\mathbf{N}'_a$ is positive definite. Consequently, replacing $\mathbf{z}$ in (10) with $\tilde{\mathbf{z}} = \mathbf{z} + \mathbf{1}'_b$, that is adding a center point to each block, implies $\mathbf{x}'\mathbf{Q}\mathbf{x} > 0$ for every column vector $\mathbf{x} \neq \mathbf{0}$, so that $\mathbf{Q}$ is positive definite and the augmented design $\xi^{\mathcal{U},\tilde{\mathbf{z}}}_{\mathbf{B},\mathbf{C},\mathcal{S}}$ is partially orthogonal.

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