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Algebraic solutions to the connectivity problem for m-way layouts: Interaction-contrast aliasing

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Abstract

An m-way layout, or design, is called complete if there is at least one observation per cell. Without any side conditions the parameters are *not* estimable but contrasts may be estimable and they are all estimable for the complete layout. For $m = 2$ the condition for estimability is the well-known connectivity condition: one can "walk" from any row to any other row, stepping on columns. The case $m > 2$ remains unsolved in some sense. The principal method used here is the Gröbner basis (G-basis) method introduced by Pistone and Wynn [1996. Generalised confounding with gröber bases. Biometrica 83, 653–666]. The problem is set up, using indicator functions, and necessary and sufficient conditions given for full estimability and various constructions using the G-basis method.
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1. The connectivity problem

The m-way layout, or table, is of considerable importance in statistics. A layout is complete if every cell has at least one observation. But incomplete tables are more complex entities. There are classical experimental designs, such as balanced incomplete blocks, designed to be incomplete, but for very incomplete tables there may be a lack of identifiability. In the language of linear models some *contrasts* may not be estimable. The condition for estimability for the 2-way table ($m=2$) is well known, namely the connectivity of the table; we shall discuss the details shortly. However, for $m > 2$ the conditions are more complex. This paper is a contribution to understanding this more complex problem. One might describe the problem as unsolved, but "not fully understood" would, perhaps, be a better description. We try, here, to give some insight taking advantage of the Gröbner basis (G-basis) method introduced by Pistone and Wynn (1996) and developed in Pistone et al. (2001).

Considerable effort has been devoted to the case of three factors: rows, columns and treatments. The interesting constructive methods of J.D and E.J Godolophin (Godolphin, 2004; Godolphin and Godolphin, 2001) should be mentioned. Earlier work is well represented by the important paper of Dodge et al. (1976). Ghosh (1989) developed a graphic method with a similar algebraic background. Weeks and Williams (1964) paper was one of the first papers

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to set the basic problem up and giving appropriate rank-based solutions. We can find one monograph: Butz (1982). Park and Shah (1995) and John and Williams (1995) cover the important block design case. The author has made some previous contributions: Wynn (1977) gives a solution in a special case and Dodge and Wynn (1988) cover the case $m = 3$ with connections to the last section of this paper.

The classical way to set up an m-way additive models is as follows. Let there be m independent factors $j = 1, \ldots, m$ where factor j has levels $i_j = 1, \ldots, n_j$. The factors form an m-way table with cells labelled $(i_1, \ldots, i_m)$. We consider the single replicate case where there is at most one observation per cell. We here call a cell "live" if it holds an observation $Y_{i_1,\ldots,i_m}$. Thus, a layout (table, design) is defined to be complete if and only if all cells are live.

For live cells the classical model is

$$Y_{i_1,\ldots,i_m} = \mu + \theta^{(1)}_{i_1} + \theta^{(2)}_{i_2} + \cdots + \theta^{(m)}_{i_m} + \varepsilon_{i_1,\ldots,i_m}, \tag{1}$$

where the errors, $\varepsilon_{i_1,\ldots,i_m}$, are uncorrelated with zero mean and non-zero, finite constant variance. Note that the estimability conditions of this paper are not dependent on constancy of variance.

A linear function of the parameters is defined to be estimable if it possesses a linear unbiased estimator. It is well known that in general, without further side assumptions, for a factor j the individual parameters $\theta^{(j)}_{i_j}$ are not estimable but that linear contrasts among the parameters, defined to be of the form

$$\sum_{i=1}^{n_j} c_i \theta^{(j)}_i, \tag{2}$$

with $\sum_i c_i = 0$, may or may not be estimable. This drives our definition.

Definition 1. In an m-way layout an index set $J \subseteq \{1, \ldots, m\}$ with standard additive model (1) layout is called J-connected if all the individual factor (2) contrasts for factors $j \in J$ are estimable. If all factor contrasts are estimable, that is $J = \{1, \ldots, m\}$, we call the design totally connected.

Note that in defining the term J-connected we are *not* restricting the full underlying model to just the factors in J. Rather, we retain the full model so that we are considering the factors in J, *in the presence of* the factors in the complement $J^c = \{1, \ldots, m\} \backslash J$. It is possible that a design can be J-connected without being totally connected. Note also that for a factor j to be estimable it is enough that all elementary contrasts of the form $\theta^{(j)}_i - \theta^{(j)}_k, i \neq k$ are estimable.

The condition for total connectivity in the case $m = 2$ is well known (see e.g. Weeks and Williams, 1964) and motivates Definition 1.

Theorem 2. *A 2-way layout* ($m = 2$) *is totally connected if every cell is connected to every other cell with a path which makes "steps" on live cells, moving in the rows* (*factor* 1) *or columns* (*factor* 2) *separately.*

The follow 3×3 table ($m = 2, n_1 = n_2 = 3$) is connected. The blank cells correspond to non-live cells and we have placed the observation in the live cells:

Y_{11}	Y_{12}	
	Y_{22}	Y_{23}
		Y_{33}

As an example, an unbiased linear estimator of the row contrast $\theta^{(1)}_1 - \theta^{(1)}_3$ is $Y_{12} - Y_{22} + Y_{23} - Y_{33}$.

In this paper, we adopt a somewhat algebraic approach, the starting point for which is the recasting of the model in terms of indicator functions. Thus, define the functions

$$x^{(j)}_i, \quad i = 1, \ldots, n_j, \quad j = 1, \ldots, m$$

with the side restrictions:

$$x_i^{(j)} = 0 \quad \text{or} \quad 1, \quad i = 1, \ldots, n_j, \quad j = 1, \ldots, m, \tag{3}$$

$$\sum_{i=1}^{n_j} x_i^{(j)} = 1, \quad j = 1, \ldots, m. \tag{4}$$

The variable $x_i^{(j)}$ is associated with the ith level of factor j and we can write model (1) as

$$Y_{i_1,\ldots,i_m} = \mu + \theta_{i_1}^{(1)} x_{i_1}^{(1)} + \theta_{i_2}^{(2)} x_{i_2}^{(2)} + \cdots + \theta_{i_m}^{(m)} x_{i_m}^{(m)} + \varepsilon_{i_1,\ldots,i_m}. \tag{5}$$

Condition (4) ensures that, for any j, no two $x_i^{(j)}$ and $x_{i'}^{(j)}$ $(i \neq i')$ can be equal to 1 at the same time, so that factor levels are distinguished.

The indicator function notation makes it easier, algebraically, to define interactions. For an extension of (1) to include interactions, the parameters need to hold all the information about which interaction is being considered. For example, a 2-way interaction corresponding to levels i_j and i_k for factors j and k needs a parameter $\theta_{i_j i_k}^{(jk)}$. But we can use the product form $\theta_{i_j i_k} x_{i_j}^{(j)} x_{i_k}^{(k)}$, with any suffix indexing, s, of the parameter so that the "responsibility" for describing which term is of interest is transferred to the monomials describing the main effects or interactions. It is important to note that, because of conditions (3) and (4), all the monomials which define interactions are square-free, or in other words multilinear. We will need this algebraic formulation to understand the G-basis methods in Section 2.

In Section 3 we shall show that q estimable interaction terms from a saturated model for a single replicate layout with m factors can be replaced (dummied) by a number of new (linear) factors so that all contrasts are estimable. Moreover the interactions terms given by the G-basis method provide an allocation of levels (treatments) to the cells of the original m-dimensional layout to achieve this. Additional levels can be added if there are more than single replicates. This is what is meant by *interaction-contrast aliasing* in the title of the paper.

2. The G-basis method for m-way layouts

The G-basis method is a systematic approach which for a given design and a given monomial ordering will give a saturated monomial regression basis. A key entity is a monomial in d indeterminants

$$x^\alpha = x_1^{\alpha_1} \cdots x_d^{\alpha_d}.$$

Here is a brief summary of the method.

1. We start with a polynomial ring $R[x] = R[x_1, \ldots, x_d]$ in d indeterminants $x_1, \ldots, x_d$. An experimental design, considered a finite discrete set D in $\mathcal{R}^d$ ($\mathcal{Q}^d$), is expressed as the solution of a set of polynomial equations. The set of all polynomials, with real coefficients and zeros on D, is the design ideal, $I(D)$.
2. A *monomial term ordering* τ is a total ordering of monomials $\prec_\tau$ such that for all $\gamma \geqslant 0$ ($\gamma_i \geqslant 0$, $i = 1, \ldots, d$):

   $$x^\alpha \prec_\tau x^\beta$$

   implies

   $$x^{\alpha+\gamma} \prec_\tau x^{\beta+\gamma}.$$

   A monomial ordering requires an *initial order* of the basic variables, such as

   $$1 \prec_\tau x_1 \prec_\tau x_2 \prec_\tau \cdots \prec_\tau x_d$$

   and the unit monomial 1 is always the first member of the order: $1 \prec_\tau x^\gamma$ for all $\gamma \geqslant 0$. A *total degree* ordering is one for which a monomial with higher degree is always higher in the ordering, defining degree as $\deg(x^\alpha) = \sum \alpha_i$.
3. Every polynomial has a unique leading term with respect to a monomial term ordering.

4. Find a G-basis for $I(D)$ with respect to τ. We omit the full definition of a Gröbner which can be found in O'Shea et al. (1996).
5. Take the quotient ring

$$R[x]/I(D).$$

This vector space is spanned by a special set of monomials: x^α, $\alpha \in L$, where the list L is unique given D and τ . These are all the monomials not divisible by the leading terms of the G-basis, and, moreover, the number of elements in L is the same as the sample size of the design D: $|L| = |D|$.
6. The set of multi-indices L has the "order ideal" property: $\alpha \in L$ implies $\beta \in L$ for any $0 \leqslant \beta \leqslant \alpha$, in the usual entry-wise sense, $\alpha_i \leqslant \beta_i$, $i = 1, \ldots, d$. In other words, we include all monomials dividing x^α.
7. Given L, any real "response" $y(x)$ has a unique polynomial interpolator given by

$$f(x) = \sum_{\alpha \in L} \theta_\alpha x^\alpha$$

such that $y(d) = f(d)$, $d \in D$. In statistical terms L provides a full rank saturated model.

Of particular interest will be total degree orderings. Heuristically, these favour the lower degrees of the monomial basis. For the m-way layout the G-basis method with a total degree ordering will yield (i) the constant term, (ii) a maximal set of linear terms and, if the sample size is large enough, (iii) some interaction terms. Because of the order ideal property, (6) above, if we obtain an interaction then we can also obtain all the interaction and the linear terms which divide that interaction. Thus, the G-basis method can be used directly to check identifiability because of its ability to deliver a unique basis given the design and monomial ordering.

We can state the relation to Definition 1 as a theorem.

Theorem 3. *An m-way layout is fully connected if and only if the G-basis with respect to a total degree ordering has exactly one linear element for each factor j. Moreover, in that case, the linear term is of the form* $\sum_{i=1}^{n_j} x_i^{(j)} - 1$.

Proof. Suppose that there is a single linear G-basis term associated with factor j. This will have one of the indicators for this factor as the leading term, say $x_k^{(j)}$. By the non-divisibility condition property (5), above, the basis $\{x^\alpha, \alpha \in L\}$ contains all $n_j - 1$ other terms $x_i^{(j)}$ except $x_k^{(j)}$, since none is divisible by $x_k^{(j)}$ (or any other term). Therefore we have estimability for this factor.

Conversely, assume that all the factors are estimable. We assume that the design is non-empty so that for any G-basis we have the constant term represented by 1. We know that if we include the constant term j must have at most $n_j - 1$ linear terms in a basis, because of the identity $\sum_i x_i^{(j)} - 1$. If there are less than $n_j - 1$ terms in the basis then there must be at least two distinct missing terms say $x_j^{(j)}$ and $x_k^{(j)}$, each of which is divisible by a leading term of a G-basis element, by property (5). The only candidates are $x_j^{(j)}$ and $x_k^{(j)}$ themselves. But they both cannot be leading terms in the same G-basis element, because of the total ordering property. Since we have chosen a total degree order, all other terms in the basis elements must be linear. This means that there are at least two linear conditions for $x_j^{(j)}$ and $x_k^{(j)}$ which hold (over the design). Moreover, the coefficient vectors must be linearly independent, because out of $x_j^{(j)}$ and $x_k^{(j)}$ the G-basis element with the leading terms lower in the initial ordering cannot contain the other leading term. Having two linear independent condition contracts estimability, so that there is at most one such linear term.

We need to show that there is exactly one linear G-basis element for factor j and that it is the condition $\sum_i x_i^{(j)} - 1$. List variables $x^{(j)}$ in the initial ordering with all of each factor's indicator variable adjacent and work up the initial ordering inductively. For the first factor, say $x^{(1)}$, we see that, applying the above argument, there must be exactly one linear term. For that, we have shown that there cannot be two, and if there are no linear terms then all the variables $x_j^{(1)}$ must be in the basis, which is impossible. In the induction assume that, for $j = 1, \ldots, k$, the property holds. For $x^{(k+1)}$ we cannot have any additional linear which is not $\sum_j x^{(k+1)} - 1$, and which involves only x_j^{k+1}. But nor can we have one which involves $x^{(j)}$ with $1 \leqslant j \leqslant k$, because, again, we would have a second linear basis element which is impossible. □

The calculations below were carried out in CoCoA (http://cocoa.dima.unige.it).

As an example consider the disconnected design in Shah and Khatri (1973) where $m = 3$, $n_1 = n_2 = 4$, $n_3 = 8$. The numbers in the cell refer to the levels of factor 3 (treatments).

1	2	5	6
3	4	7	8
8	6	1	3
7	5	2	4

If we take a total degree ordering the solution gives two linear terms for factor 1 and three each for factors 2 and 3. This leaves three interactions which are also listed. With our particular choice of ordering we obtain the full model basis:

$$\{1, x_3^{(1)}, x_4^{(1)}, x_2^{(2)}, x_3^{(2)}, x_4^{(2)}, x_2^{(3)}, x_3^{(3)}, x_4^{(3)}, x_5^{(3)}, x_6^{(3)}, x_7^{(3)}, x_8^{(3)}, x_3^{(2)} x_7^{(3)}, x_4^{(2)} x_4^{(3)}, x_4^{(2)} x_8^{(3)}\}.$$

In standard terminology the last three interactions are {column 3 × treatment 7}, {column 4 × treatment 4} and {column 4 × treatment 8}.

For comparison, the next design is given by Eccleston and Russell (1975) and is connected:

1	2	5	6
3	4	7	8
7	6	2	3
5	8	4	1

The basis is given below and confirms that each factor has three linear terms and there are two "spare" interactions:

$$\{1, x_2^{(1)}, x_3^{(1)}, x_4^{(1)}, x_2^{(2)}, x_3^{(2)}, x_4^{(2)}, x_2^{(3)}, x_3^{(3)}, x_4^{(3)}, x_5^{(3)}, x_6^{(3)}, x_7^{(3)}, x_8^{(3)}, x_3^{(2)} x_7^{(3)}, x_4^{(2)} x_8^{(3)}\}.$$

2.1. Interaction-contrast aliasing

This subsection discusses how to replace a maximal number q of interactions, given by the G-basis method, by linear factors.

Let X_j be the $n \times n_j$ design matrix for the linear terms of the jth factor, arising from the model produced by the G-basis method and let $\tilde{X}_m$ be the X-matrix for the interactions terms, from the method. Then we can write the fully saturated model in matrix form taking the indicator function approach as our starting point:

$$\mathrm{E}(Y) = \theta_0 + X_1\theta_1 + \cdots + X_m\theta_{m-1} + \tilde{X}_m\phi.$$

This matrix has full rank n, by construction, and let us assume that rank $\tilde{X}_m = q$, namely that there are q estimable interactions (we shall always use q in this way).

A naive form of dummying replaces every interaction parameter ϕ_s by a level s of factor m ($s = 1, \ldots, q$) allocating q parameters and adding an additional $(q + 1)$th level where there are no ϕ_s terms. But this may violate the indicator function condition for factor m that no two indicator functions can be equal to one for the same observation. A simple solution is to replace every column in $\tilde{X}$ by a 2-level factor column with level one where there is a one and level zero otherwise, leading to q 2-level factors. But in general we can use fewer factors with more levels as the following analysis reveals.

We begin with a small example. Suppose $m = 3$ and each factor has two levels and the basis contains the interaction $x_1^{(1)} x_1^{(2)} x_1^{(3)}$. Then, by the order ideal property it also contains the sub-interactions are $x_1^{(1)} x_1^{(2)}$, $x_1^{(1)} x_1^{(3)}$, $x_1^{(2)}$ and $x_1^{(3)}$. Consider the $\tilde{X}$ matrix. If there is a "1" in the $x_1^{(1)} x_1^{(2)} x_1^{(3)}$ interaction column, for some row, then $x_1^{(1)} = x_1^{(2)} = x_1^{(3)} = 1$ for this row. This implies that all the sub-interactions also have a one in this row. Column reduce $\tilde{X}$ by subtracting the $x_1^{(1)} x_1^{(2)} x_1^{(3)}$ column from the sub-interaction columns $\tilde{X}$ and hence remove all the ones for the sub-interactions, for this row. Other rows, where $x_1^{(1)} x_1^{(2)} x_1^{(3)} = 0$, are unaffected.

This points to a more general procedure. Using the monomial notation, if for any column x^α we have $x^\alpha = 1$ in some row then column reduce the row with any x^β column with $\alpha \leqslant \beta$ such that $x^\beta = 1$, if there is such an x^β column. If not, then leave this x^α, as it is. For the resulting matrix, we have one (or more) 1's in a row if there are columns with terms x^α, x^γ such that $x^\alpha = x^\gamma = 1$, but no dominating x^β with both $\alpha \leqslant \beta$ and $\gamma \leqslant \beta$. This is because $x^\alpha = 1$ and $x^\gamma = 1$ implies $x^\beta = 1$ where $\gamma = \alpha \vee \gamma \leqslant \beta$ for any such β, where $\alpha \vee \beta = (\max(\alpha_1, \beta_1), \ldots, \max(\alpha_m, \beta_m))$. The same approach applies when we have more than one "1" in the reduced $\tilde{X}$, after reduction.

Thus after the column reduction we are left with only special cases when we can have more than one "1" in a row. These arise from x^α which have no other dominating x^β (in the basis) with $\alpha \leqslant \beta$. The basic rule, then, is that (with one exception) when we assign linear factors we must not assign two or more un-dominated interactions to levels of the same factor.

The exception is when the indicator function property makes the two interactions automatically $\neq 1$ at the same time. For example, both interactions $x_1^{(1)}x_1^{(2)}x_1^{(3)}$ and $x_2^{(1)}x_1^{(2)}x_1^{(3)}$ cannot be "1" for the same row. We can decompose the problem to a series of disconnected problems where disconnected means not having different levels of the same factor, as in the above example. In the 2^m case the number of linear factors can be reduced to the maximal number of non-dominated interactions in the basis. For factors with more than one level we must maximise over the disconnected components.

We collect these results together.

Theorem 4. *For an $m-1$-way layout with q (algebraically) independent interactions from the G-basis method it is possible to replace these interaction terms with q^* factors where q^* does not exceed the maximal number of non-dominated interactions in any set of interaction terms, using no more than one level of each factor.*

Since the complete m-way layout has disconnected components, each with a single undominated m-way interaction, we can column reduce each $n \times (2^m - m - 1)$ submatrix for this interaction and all its sub-interactions so that it has a single "1" in each row. Then we can build up all the disconnected components to form one large factor. This gives:

Corollary 5. *For a complete $m-1$-way layout it is possible to replace the full set of interaction term by a single m-th factor with $q+1$ levels where $q = \prod_i^{m-1}(n_j - 1)$.*

3. Connectivity via the kernel

Let us take a standard partitioned standard regression model in expectation form

$$\mathrm{E}(Y) = X_1\theta + X_2\phi,$$

where X_1 is $n \times p_1$ and X_2 is $n \times p_2$. Let $\mathrm{rank}(X_1) = n - q$, with $q > 0$ and define a full rank kernel matrix (kernel for short) of X_1 is an $n \times q$ matrix K such that $X_1^{\mathrm{T}}K = 0$ and $\mathrm{rank}(K) = q$. We give the following without proof. It is implicit in much of the literature, see for example Dodge et al. (1976), and follows in any case from elementary theory.

Lemma 6. *A necessary and sufficient condition for ϕ to be estimable (in the full model (6)), with the kernel K just defined, is*

$$\mathrm{rank}(X_2^{\mathrm{T}}K) = p_2. \tag{6}$$

Let X_j be the $n \times n_j$ design matrix for the jth factor. Then we can write the full model in matrix form taking the indicator function approach as our starting point:

$$\mathrm{Y} = \mu + X_1\theta_1 + \cdots + X_m\theta_m.$$

Let $\mathbf{1}$ be the $n \times 1$ vector of ones and let K be a kernel matrix of

$$[\mathbf{1} : X_1 : \cdots : X_{m-1}].$$

Then, by adapting Lemma 6, the necessary and sufficient condition for the estimability of contrasts of the parameters θ_m of factor m is that

$$\operatorname{rank}(X_m^{\mathrm{T}} K) = n_m - 1. \tag{7}$$

Much of the rest of the paper is devoted to the consequences of this result and the starting point is that the G-basis method provides a guide to the construction of kernel matrices K.

3.1. The case $m = 2$

Suppose that the design is complete and balanced for factor 1 and there are say, k observations (replications) at every level of factor 1. Then we are interested in the kernel of $[1 : X_1]$. As an example take $k = 2, n_1 = 3$ giving:

$$[\mathbf{1}, X_1] = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \end{bmatrix}.$$

An example of a kernel is

$$K = \begin{bmatrix} 1 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & -1 \end{bmatrix}.$$

Now consider arranging the levels of the second factor to form X_2. Suppose $n_j = 4$, the maximum number of levels. It is clear that we need a connected chain of level assignments for factor 2 to estimate all factor 2 contrasts. A minimal allocation would be the 3×4 layout

*	*		
	*	*	
		*	*

where "$*$" represents an observation. The proof of Theorem 1 is simply an elaboration of this.

3.2. The case $m = 3$

One way to understand the $m = 3$ problem is to consider the columns of K as spread out in the table from the first two factors. In the case $m = 2$ we can see the structure of the K matrix from the orthogonality. Suppose that for the first two factors the layout is complete; then we can place the observations in a $n_1 \times n_2$ table of the first two factors. Code a typical column of K as $\{k_{ij}\}$, that is by the cells of the table. The kernel conditions on K are

$$\sum_i \sum_j k_{ij} = \sum_i k_{ij} = \sum_j k_{ij} = 0.$$

We can consider the corresponding $\{k_{ij}\}$ (for any column of K) as a balanced circuit. For example, for $n_1 = n_2 = 3$ we can take four independent circuits:

1	–1	0
–1	1	0
0	0	0

1	–1	0
0	0	0
–1	1	0

1	0	–1
–1	0	1
0	0	0

1	0	–1
0	0	0
–1	0	1

.

By Corollary 5 we may insert a maximal five treatments indexed by letters: A, B, C, D, E. We see that each table gives an estimable contrast. Here is one solution:

A	A	A
A	B	C
A	D	E

.

We allocate different letters B, C, D, E to each of the circuits where they did not intersect another circuit and then add more copies of A.

4. Construction of the kernel

The first two methods are based on the interaction matrix produced by the first $m - 1$ factors, from the G-basis method.

4.1. The "individual" method

Select a column, say x_s, of the full rank X-matrix for one of the interaction from the first $m - 1$ factors. We replace this by a vector k_s which is orthogonal to *all* other columns. Since this interaction matrix is full rank, this column is unique up to a scalar multiple. We can construct it easily as follows. Let $\tilde{X}_s$ be the submatrix for the full saturated $m - 1$ factor model (with interactions) consisting of all the columns except the chosen column, x_s. Then consider the projector onto the column space of $\tilde{X}_s$:

$$P_s = \tilde{X}_s(\tilde{X}_s^{\mathrm{T}}\tilde{X}_s)^{-1}\tilde{X}_s^{-1}.$$

Then we may take

$$k_s = (I - P_s)x_s,$$

where I is the $n \times n$ identity.

Note that if ϕ_s is the parameter associated with the given interaction then, in the saturated case, its least squares estimator is

$$\hat{\alpha}_s = \frac{k_s^{\mathrm{T}}Y}{k_s^{\mathrm{T}}k_s},$$

where Y is the vector of observations. Adjoining all such k_s columns gives a kernel matrix K since every column is orthogonal to the X-matrix for the original model, by construction. It can easily be shown also to be full rank.

As an example, consider the balanced incomplete block design represented by the 2-way layout:

*	*	*			
*			*	*	
	*		*		*
		*		*	*

.

Then the G-basis method with the initial ordering

$$1 \prec x_4^{(1)} \prec x_3^{(1)} \prec x_2^{(1)} \prec x_1^{(1)} \prec x_6^{(2)} \prec x_5^{(2)} \prec x_4^{(2)} \prec x_3^{(2)} \prec x_2^{(2)} \prec x_1^{(2)}$$

gives a basis with three interactions: namely

$$\{1, x_2^{(1)}, x_3^{(1)}, x_4^{(1)}, x_2^{(2)}, x_3^{(2)}, x_4^{(2)}, x_5^{(2)}, x_6^{(2)}, x_4^{(1)}x_6^{(2)}, x_4^{(1)}x_5^{(2)}, x_3^{(1)}x_4^{(2)}\}.$$

Notice that the interactions correspond to cells in the 2-way layout, and the corresponding columns have a single one for that cell. If we set up the basis and put the three k_s back the position of the design we have in order

0	–1	1			
0			0	0	
	1		0		–1
		–1		0	1

–1	0	1			
1			0	–1	
	0		0		0
		–1		1	0

1	–1	0			
–1			1	0	
	1		–1		0
		0		0	0

.

This "individual" method seems to be the simplest way of associating each kernel column with an estimable interaction. It is a nice exercise to allocated four levels of a new factor (treatments) which can be done following Theorem 4, since $q^* = 1$.

4.2. Bases with low complexity

Any computer programme which can give a null space will lead to a kernel matrix K. For example, the nullspace function on Maple^{TM} (Monagan et al., 2005). However, without care or further knowledge it is not always easy to predict which K will result. The following result shows that when the layout for the first $m-1$ factors is complete then we can find a K whose columns are particularly simple.

Theorem 7. *For any complete* $(m-1)$*-layout there is a kernel matrix whose columns have two ones*, *two minus ones and otherwise zero entries*.

Before proceeding to the proof an example is useful. Consider the case $m-1=3$ and $n_1 = n_2 = n_3 = 2$. In the notation of factorial design this is a 2^3 problem and we know that the rank of K is the number of interactions, namely four. For a particular choice of K (we have allowed ourself to rescale the columns to be integer), under the Theorem 7 the matrix $[X : K]$ is

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & -1 & -1 & 0 & -1 \\ 1 & 0 & 1 & 1 & 0 & 0 & 1 & -1 \\ 1 & 0 & 1 & 0 & -1 & 0 & -1 & 0 \\ 1 & 0 & 0 & 1 & 0 & -1 & -1 & 0 \\ 1 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \end{bmatrix}.$$

The interaction columns are in the order: $\{x_1x_3, x_1x_3, x_2x_3, x_1x_2x_3\}$.

The proof is in two parts. First we give the construction for the 2-level (2^{m-1}) case. Each column is geometrically associated with a given interaction terms. Since the layout for the $m-1$ factors is complete every interaction term is estimable.

For clarity consider 2-way interactions first. Consider the column of the interaction matrix $\tilde{X}_m$ corresponding to $x^{(i)}x^{(j)}$ $(i \neq j)$ (we have dropped the suffix for ease of expression). Then the construction rule for the corresponding column is: (i) set the entry equal to 1 if either (a) $x^{(i)}=x^{(j)}=1$, $x^{(k)}=0$, $k \neq i, j$ or (b) $x^{(i)}=x^{(j)}=0$, ; $x^{(k)}=0$, $k \neq i, j$; (ii) set the entry equal to -1 if either (a) $x^{(i)}=1$, $x^{(j)}=0$, $x^{(k)}=0$, $k \neq i, j$ or (b) $x^{(i)}=0$, $x^{(j)}=1$, $x^{(k)}=0$, $k \neq i, j$; (iii) set all other entries of the column equal to zero.

The column for a general interaction is constructed in a similar fashion. It is helpful to think of putting ones at opposite ends of diagonals of different lengths, which have one end at $(0, 0, \ldots, 0)$. Thus let $L \subseteq \{1, \ldots, m-1\}$ be an index set and consider an interaction: $\prod_{i\in L} x^{(i)}$ (again we have dropped the suffix). Then: (i) set the entry of the corresponding columns equal to 1 if either (a) $x^{(i)} = 1$, for all $i \in L$, $x^{(k)} = 0$, $k \notin L$ or (b) $x^{(i)} = 0$, for all $i \in L$, $x^{(k)} = 0$, $k \notin L$; (ii) select any $j \in L$ and allocate -1 if (a) $x^{(i)} = 1$, for all $i \notin L\backslash j$, $x^{(j)} = 0$, $x^{(k)} = 0$, $k \notin L$ or (b) $x^{(i)} = 0$, for all $i \in L\backslash j$, $x^{(j)} = 1$, $x^{(k)} = 0$, $k \notin L$; (iii) set all other entries of the column equal to zero. In the case that L is the interaction of all factors we ignore the $x^{(k)} = 0$, $k \notin L$ statement. In the example we have taken $j = 1$ in the construction for the interaction $x^{(1)}x^{(2)}x^{(3)}$.

We need to check orthogonality of K to the X-matrix from the first $m-1$ factors. This follows easily by confirming the sums for every one-dimensional margin of the $(m-1)$-dimensional layout are zero. The independence of the columns follows by ordering the columns of K rows by a non-decreasing number of entries and ordering the columns in a compatible fashion so that the bottom $q \times q$ matrix is upper triangular with ones on the diagonal. That all this is possible follows from the construction.

The second part of the theorem is to extend to factors with levels, respectively, $n_1, \ldots, n_{m-1} \geqslant 2$. The proof here is by induction using a copying operation. Start with 2-level factors. Then assume we have already successfully added factor levels up to $n'_1, \ldots, n'_{m-1}$, that K is the current kernel and we wish to add a new level to factor j. Then this adds $\prod_{i,i\neq j} n'_i$ rows to the X-matrix. Take any of the existing levels of factor j, say level k, and let K_2 be the corresponding submatrix of K. Let K_1 hold all other rows. Let K'_1 be the submatrix of K_1 omitting any column whose interaction includes the indicator function for level k of factor j, namely $x_k^{(j)}$; similarly for K_2. Then for the new level of factor j copy K'_1 and K'_2 in the arrangement shown below (after suitable ordering of rows and columns), where zero matrices are of suitable dimension.

$$\begin{bmatrix} K_1 & K'_1 \\ K_2 & 0 \\ 0 & K'_2 \end{bmatrix}.$$

This preserves the property of two 1's and two -1's in each column and gives the correct rank.

In the above 2^3 example, if a third level is added to the first factor then the result of the copying process is

$$\begin{bmatrix}
1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\
1 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\
1 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\
1 & 1 & 0 & 0 & 0 & -1 & -1 & 0 & -1 & -1 & -1 & -1 \\
1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & -1 & 0 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 1 & 0 & -1 & -1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\
1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\
1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\
1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\
1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1
\end{bmatrix}.$$

Note that the 4×3 submatrices K'_1 and K'_2 do not employ the eighth column of the original matrix corresponding to the interaction x_2x_3.

A simple counter example shows that when the $(m-1)$-factor design is not complete the property of two 1's and two -1's can fail. Consider the case $m - 1 = 2$, $n_1 = n_2 = 3$ and the incomplete layout:

*	*	
	*	*
*		*

.

Then, up to a scalar multiple, K has a single column and placing the entries in the 2-way layout we have

1	−1	
	1	−1
−1		1

.

4.3. Minimal lattice basis

For incomplete layouts one can reduce the complexity of the kernel by appealing to the so-called "minimal lattice basis" principle, as follows. The columns of the kernel K arising form the first $m-1$ factors are always rational and can be made integer by suitable scaling. So, without loss of generality take K integer. The columns $\{k_s\}$ generate an integer lattice in R^n:

$$\{r_1k_1 + \cdots + r_qk_q\},$$

where $r_1, \ldots, r_q$ range over all integers. The integer vectors generated in this way clearly lie in span$(k_1, \ldots, k_q)$, but there may be other integer vectors in the span. A minimal (also called reduced) lattice basis is a basis for the lattice which (i) generates all integer vectors in the basis (ii) is closest to the origin in some well-defined sense.

In the case when the layout for the first $m-1$ factors is incomplete, so that the result of Theorem 2 may not hold, we can still use a minimal lattice to reduce the complexity. There are a considerable number of lattice reduction methods and we only mention one of them here, perhaps the best known. In the LLL algorithm of Lenstra, Lenstra et al. (1982) each basis element, k_s in our case, is required to be the shortest in the two-dimensional projection generated by k_s and k_{s+1}. One can use the Maple `nullspace` procedure followed by the LLL algorithm, also available in Maple^{TM}.

We have seen for the "individual" method how every k_s is naturally associated to an interaction term given by the G- basis method. The exact relationship between a reduced lattice basis of the kernel based on the G-basis interaction terms and a basis produced by an automatic use of a lattice reduction method must be the subject of further research.

4.4. Contribution to the kernel from replication

In most of the examples above we did not allow any replication in the base $(m-1)$-factor layout. This makes it more difficult to construction kernel elements. However, with the case $m = 1$ we allowed replication because this is the only way to have a non-empty kernel. It is a simple matter to create low-complexity kernels to cover replication. The following principle applies for any point (combination of factors) from the $m-1$-factor layout replicated r times there can be assigned $r-1$ kernel (column) vectors k which only have a single 1 and -1, with the rest of the elements being zero. In the language of contrasts: $r-1$ independent residual contrasts can be associated with r-fold replication at a point.

These column vectors can be added to the kernel from the single replicate case to form the full kernel. So, *replication does not increase the complexity of the kernel*, in the sense of the last section. We can state this in a more positive fashion: the complexity of the kernel derives from the complexity of the single replicate design.

4.5. Using lower complexity kernels

A lower complexity kernel can be useful in understanding the placement of the levels of treatment m in relation to the other factors.

As a simple example consider the 2^3 example again and take letters A to E for the five levels of a fourth factor. Then clearly the allocation A, A, A, A, B, C, D, E, in the order in Section 4.1 will be connected. Each column of the kernel gives estimability for a particular contrast, which is the row of $X_m^{\mathrm{T}}K$. With an abuse of notation we can take the letters to represent parameters to obtain the contrasts:

$$A - A - A + B = B - A,$$
$$A - A - A + C = C - A,$$
$$A - A - A + D = D - A,$$
$$A - A - A + E = E - A.$$

We can generalise this idea and to restate the rank condition in slightly different form, close in spirit to Section 4.2.

Definition 8. Let X_m be the X-matrix for factor m and let K be an integer kernel derived from the first $m-1$ factors. Then the contrast lattice $\mathscr{L}$ for factor m (in the presence of factors $1,\ldots,m-1$) is the integer lattice generated by the columns of $X_m^{\mathrm{T}}K$.

The following is an extension to general m of a result for $m=3$ in Dodge and Wynn (1988). We state it without proof.

Theorem 9. *A contrast $\phi=\sum c_i\alpha_i^{(m)}$ with integer coefficients c_i for factor m is estimable if and only if some integer multiple $N\phi$ lies in the contrast lattice $\mathscr{L}$.*

This approach gives an interpretation of elementary contrasts. If we find a reduced lattice basis of the treatment lattice $\mathscr{L}$ (rather than from K) then typically we will obtain an elementary contrast basis.

Corollary 10. *An m-way layout is fully estimable for factor m if and only if there is a reduced lattice basis of the treatment lattice whose generators are elementary in having only one* 1 *and one* -1, *with all other elements zero.*

We complete this discussion with an attempt to understand connectivity as a generalisation the $m=2$ case of Theorem 1. We believe that in sofar as the connectivity problem remains "unsolved" it is because of the failure to give such a nice characterisation as in the $m=2$ case, even in the case $m=3$.

Here is a heuristic argument. In the case $m=2$ the connectivity can be seen as the ability to "step" from one level of, say, factor 2 to another level of factor 2, where the steps must be in the rows or columns. Now consider the m-way layout and assume that we already have the $(m-1)$-factor design and have computed a low-complexity kernel. Suppose we are interested in testing whether, for a particular allocation of factor m a particular elementary treatment contrast is estimable. Then by Theorem 9 we have an expression for the multiple of the contrast as an integer linear combination of the individual contrasts defined by the kernel lattice basis. If there is replication we may be able to achieve this with elementary contrasts, stepping within a particular cell in the $(m-1)$-dimensional layout and then between such cells. This is the simplest generalisation of Theorem 1. However, when there is little replication we may need to use kernel basis elements of greater complexity. The 2^4 problem in Section 4.1 is a revealing example. In such a case we argue that the basis elements of $\mathscr{L}$, or equivalently the factor m contrasts they define, can be considered as *generalised steps*. In summary, we can better understand the structure of a possible allocation of the levels of factor m by first reducing the complexity of the kernel K. In particular, when the $m-1$ level design is complete we can, according to Theorem 7, find a basis for $\mathscr{L}$, each element of which has at most four non-zero terms.

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