

## GENERALIZED RESOLUTION FOR ORTHOGONAL ARRAYS

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The generalized word length pattern of an orthogonal array allows a ranking of orthogonal arrays in terms of the generalized minimum aberration criterion (Xu and Wu [Ann. Statist. **29** (2001) 1066–1077]). We provide a statistical interpretation for the number of shortest words of an orthogonal array in terms of sums of  $R^2$  values (based on orthogonal coding) or sums of squared canonical correlations (based on arbitrary coding). Directly related to these results, we derive two versions of generalized resolution for qualitative factors, both of which are generalizations of the generalized resolution by Deng and Tang [Statist. Sinica **9** (1999) 1071–1082] and Tang and Deng [Ann. Statist. **27** (1999) 1914–1926]. We provide a sufficient condition for one of these to attain its upper bound, and we provide explicit upper bounds for two classes of symmetric designs. Factor-wise generalized resolution values provide useful additional detail.

**1. Introduction.** Orthogonal arrays (OAs) are widely used for designing experiments. One of the most important criteria for assessing the usefulness of an array is the generalized word length pattern (GWLP) as proposed by Xu and Wu (2001):  $A_3, A_4, \dots$  are the numbers of (generalized) words of lengths 3, 4,  $\dots$ , and the design has resolution  $R$ , if  $A_i = 0$  for all  $i < R$  and  $A_R > 0$ . Analogously to the well-known minimum aberration criterion for regular fractional factorial designs [Fries and Hunter (1980)], the quality criterion based on the GWLP is generalized minimum aberration [GMA; Xu and Wu (2001)]: a design  $D_1$  has better generalized aberration than a design  $D_2$ , if its resolution is higher or—if both designs have resolution  $R$ —if its number  $A_R$  of shortest words is smaller; in case of ties in  $A_R$ , frequencies of successively longer words are compared, until a difference is encountered.

The definition of the  $A_i$  in Xu and Wu is very technical (see Section 2). One of the key results of this paper is to provide a statistical meaning for the number of shortest words,  $A_R$ : we will show that  $A_R$  is the sum of  $R^2$  values from

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linear models with main effects model matrix columns in orthogonal coding as dependent variables and full models in  $R - 1$  other factors on the explanatory side. For arbitrary factor coding, the “sum of  $R^2$ ” interpretation cannot be upheld, but it can be shown that  $A_R$  is the sum of squared canonical correlations [Hotelling (1936)] between a factor’s main effects model matrix columns in arbitrary coding and the full model matrix from  $R - 1$  other factors. These results will be derived in Section 2.

For regular fractional factorial 2-level designs, the GWLP coincides with the well-known word length pattern (WLP). An important difference between regular and nonregular designs is that factorial effects in regular fractional factorial designs are either completely aliased or not aliased at all, while nonregular designs can have partial aliasing, which can lead to noninteger entries in the GWLP. In fact, the absence of complete aliasing has been considered an advantage of nonregular designs [e.g., those by Plackett and Burman (1946)] for screening applications. Deng and Tang (1999) and Tang and Deng (1999) defined “generalized resolution” (GR) for nonregular designs with 2-level factors, in order to capture their advantage over complete confounding in a number. For example, the 12 run Plackett–Burman design has  $GR = 3.67$ , which indicates that it is resolution III, but does not have any triples of factors with complete aliasing. Evangelaras et al. (2005) have made a useful proposal for generalizing GR (called *GRes* by them) for designs in quantitative factors at 3 levels; in conjunction with Cheng and Ye (2004), their proposal can easily be generalized to cover designs with quantitative factors in general. However, there is so far no convincing proposal for designs with qualitative factors. The second goal of this paper is to close this gap, that is, to generalize Deng and Tang’s/Tang and Deng’s GR to OAs for qualitative factors. Any reasonable generalization of GR has to fulfill the following requirements: (i) it must be coding-invariant, that is, must not depend on the coding chosen for the experimental factors (this is a key difference vs. designs for quantitative factors), (ii) it must be applicable for symmetric and asymmetric designs (i.e., designs with a fixed number of levels and designs with mixed numbers of levels), (iii) like in the 2-level case,  $R + 1 > GR \geq R$  must hold, and  $GR = R$  must be equivalent to the presence of complete aliasing somewhere in the design, implying that  $R + 1 > GR > R$  indicates a resolution  $R$  design with no complete aliasing among projections of  $R$  factors. We offer two proposals that fulfill all these requirements and provide a rationale behind each of them, based on the relation of the GWLP to regression relations and canonical correlations among the columns of the model matrix.

The paper is organized as follows: Section 2 formally introduces the GWLP and provides a statistical meaning to its number of shortest words, as discussed above. Section 3 briefly introduces generalized resolution by Deng and Tang (1999) and Tang and Deng (1999) and generalizes it in two meaningful ways. Section 4 shows weak strength  $R$  [in a version modified from Xu (2003) to imply strength  $R - 1$ ] to be sufficient for maximizing one of the generalized resolutions in a resolution

$R$  design. Furthermore, it derives an explicit upper bound for the proposed generalized resolutions for two classes of symmetric designs. Section 5 derives factor wise versions of both types of generalized resolution and demonstrates that these provide useful additional detail to the overall values. The paper closes with a discussion and an outlook on future work.

Throughout the paper, we will use the following notation: An orthogonal array of resolution  $R = \text{strength } R - 1$  in  $N$  runs with  $n$  factors will be denoted as  $\text{OA}(N, s_1, \dots, s_n, R - 1)$ , with  $s_1, \dots, s_n$  the numbers of levels of the  $n$  factors (possibly but not necessarily distinct), or as  $\text{OA}(N, s_1^{n_1}, \dots, s_k^{n_k}, R - 1)$  with  $n_1$  factors at  $s_1$  levels,  $\dots$ ,  $n_k$  factors at  $s_k$  levels ( $s_1, \dots, s_k$  possibly but not necessarily distinct), whichever is more suitable for the purpose at hand. A subset of  $k$  indices that identifies a  $k$ -factor projection is denoted by  $\{u_1, \dots, u_k\} (\subseteq \{1, \dots, n\})$ . The unsquared letter  $R$  always refers to the resolution of a design, while  $R^2$  denotes the coefficient of determination.

**2. Projection frequencies and linear models.** Consider an  $\text{OA}(N, s_1, \dots, s_n, R - 1)$ . The resolution  $R$  implies that main effects can be confounded with interactions among  $R - 1$  factors, where the extent of confounding of degree  $R$  can be investigated on a global scale or in more detail: Following [Xu and Wu \(2001\)](#), the factors are coded in orthogonal contrasts with squared column length normalized to  $N$ . We will use the expression “normalized orthogonal coding” to refer to this coding; on the contrary, the expressions “orthogonal coding” or “orthogonal contrast coding” refer to main effects model matrix columns that have mean zero and are pairwise orthogonal, but need not be normalized. For later reference, note that for orthogonal coding (whether normalized or not) the main effects model matrix columns for an OA (of strength at least 2) are always uncorrelated.

We write the model matrix for the full model in normalized orthogonal coding as

$$(1) \quad \mathbf{M} = (\mathbf{M}_0, \mathbf{M}_1, \dots, \mathbf{M}_n),$$

where  $\mathbf{M}_0$  is a column of “+1”s,  $\mathbf{M}_1$  contains all main effects model matrices, and  $\mathbf{M}_k$  is the matrix of all  $\binom{n}{k}$   $k$ -factor interaction model matrices,  $k = 2, \dots, n$ . The portion  $\mathbf{X}_{u_1, \dots, u_k}$  of  $\mathbf{M}_k = (\mathbf{X}_{1, \dots, k}, \dots, \mathbf{X}_{n-k+1, \dots, n})$  denotes the model matrix for the particular  $k$ -factor interaction indexed by  $\{u_1, \dots, u_k\}$  and is obtained by all products from one main effects contrast column each from the  $k$  factors in the interaction. Note that the normalized orthogonal coding of the main effects implies that all columns of  $\mathbf{M}_k$  have squared length  $N$  for  $k \leq R - 1$ . Now, on the global scale, the overall number of words of length  $k$  can be obtained as the sum of squared column averages of  $\mathbf{M}_k$ , that is,  $A_k = \mathbf{1}_N^T \mathbf{M}_k \mathbf{M}_k^T \mathbf{1}_N / N^2$ . Obviously, this sum can be split into contributions from individual  $k$ -factor projections for more detailed considerations, that is,

$$(2) \quad A_k = \sum_{\substack{\{u_1, \dots, u_k\} \\ \subseteq \{1, \dots, n\}}} \mathbf{1}_N^T \mathbf{X}_{u_1, \dots, u_k} \mathbf{X}_{u_1, \dots, u_k}^T \mathbf{1}_N / N^2 =: \sum_{\substack{\{u_1, \dots, u_k\} \\ \subseteq \{1, \dots, n\}}} a_k(u_1, \dots, u_k),$$

where  $a_k(u_1, \dots, u_k)$  is simply the  $A_k$  value of the  $k$ -factor projection  $\{u_1, \dots, u_k\}$ . The summands  $a_k(u_1, \dots, u_k)$  are called “projection frequencies.”

EXAMPLE 1. For 3-level factors, normalized polynomial coding has the linear contrast coefficients  $-\sqrt{3/2}, 0, \sqrt{3/2}$  and the quadratic contrast coefficients  $\sqrt{1/2}, -\sqrt{2}, \sqrt{1/2}$ . For the regular design  $OA(9, 3^3, 2)$  with the defining relation  $C = A + B \pmod{3}$ , the model matrix  $\mathbf{M}$  has dimensions  $9 \times 27$ , including one column for  $\mathbf{M}_0$ , six for  $\mathbf{M}_1$ , twelve for  $\mathbf{M}_2$  and eight for  $\mathbf{M}_3$ . Like always, the column sum of  $\mathbf{M}_0$  is  $N$  (here: 9), and like for any orthogonal array, the column sums of  $\mathbf{M}_1$  and  $\mathbf{M}_2$  are 0, which implies  $A_0 = 1, A_1 = A_2 = 0$ . We now take a closer look at  $\mathbf{M}_3$ , arranging factor A as (0 0 0 1 1 1 2 2 2), factor B as (0 1 2 0 1 2 0 1 2) and factor C as their sum (mod 3), denoting linear contrast columns by the subscript  $l$  and quadratic contrast columns by the subscript  $q$ . Then

$$\mathbf{M}_3 = \begin{pmatrix} \text{contrast} & A_l B_l C_l & A_q B_l C_l & A_l B_q C_l & A_q B_q C_l & A_l B_l C_q & A_q B_l C_q & A_l B_q C_q & A_q B_q C_q \\ \hline & -\sqrt{\frac{27}{8}} & \sqrt{\frac{9}{8}} & \sqrt{\frac{9}{8}} & -\sqrt{\frac{3}{8}} & \sqrt{\frac{9}{8}} & -\sqrt{\frac{3}{8}} & -\sqrt{\frac{3}{8}} & \sqrt{\frac{1}{8}} \\ & 0 & 0 & 0 & 0 & 0 & 0 & -\sqrt{6} & \sqrt{2} \\ & -\sqrt{\frac{27}{8}} & \sqrt{\frac{9}{8}} & -\sqrt{\frac{9}{8}} & \sqrt{\frac{3}{8}} & -\sqrt{\frac{9}{8}} & \sqrt{\frac{3}{8}} & -\sqrt{\frac{3}{8}} & \sqrt{\frac{1}{8}} \\ & 0 & 0 & 0 & 0 & 0 & -\sqrt{6} & 0 & \sqrt{2} \\ & 0 & 0 & 0 & \sqrt{6} & 0 & 0 & 0 & \sqrt{2} \\ & 0 & \sqrt{\frac{9}{2}} & 0 & \sqrt{\frac{3}{2}} & 0 & -\sqrt{\frac{3}{2}} & 0 & -\sqrt{\frac{1}{2}} \\ & -\sqrt{\frac{27}{8}} & -\sqrt{\frac{9}{8}} & \sqrt{\frac{9}{8}} & \sqrt{\frac{3}{8}} & -\sqrt{\frac{9}{8}} & -\sqrt{\frac{3}{8}} & \sqrt{\frac{3}{8}} & \sqrt{\frac{1}{8}} \\ & 0 & 0 & \sqrt{\frac{9}{2}} & \sqrt{\frac{3}{2}} & 0 & 0 & -\sqrt{\frac{3}{2}} & -\sqrt{\frac{1}{2}} \\ & 0 & 0 & 0 & 0 & -\sqrt{\frac{9}{2}} & -\sqrt{\frac{3}{2}} & -\sqrt{\frac{3}{2}} & -\sqrt{\frac{1}{2}} \\ \hline \text{column sum} & -\sqrt{\frac{243}{8}} & \sqrt{\frac{81}{8}} & \sqrt{\frac{81}{8}} & \sqrt{\frac{243}{8}} & -\sqrt{\frac{81}{8}} & -\sqrt{\frac{243}{8}} & -\sqrt{\frac{243}{8}} & \sqrt{\frac{81}{8}} \end{pmatrix}.$$

Half of the squared column sums of  $\mathbf{M}_3$  are  $243/8$  and  $81/8$ , respectively. This implies that the sum of the squared column sums is  $A_3 = a_3(1, 2, 3) = (4 \cdot 243/8 + 4 \cdot 81/8)/81 = 2$ .

EXAMPLE 2. Table 1 displays the only  $OA(18, 2^1 3^2, 2)$  that cannot be obtained as a projection from the L18 design that was popularized by Taguchi (of

TABLE 1  
A partially confounded  $OA(18, 2^1 3^2, 2)$  (transposed)

A	0	1	1	0	0	1	0	1	0	1	1	0	1	0	0	1	0	1
B	0	0	0	0	0	0	1	1	1	1	1	2	2	2	2	2	2	2
C	0	1	2	1	2	0	0	2	0	1	1	2	2	1	2	0	1	0

course, this triple is not interesting as a stand-alone design, but as a projection from a design in more factors only; the Taguchi L18 is for convenience displayed in Table 4 below). The 3-level factors are coded like in Example 1, for the 2-level factor, normalized orthogonal coding is the customary  $-1/+1$  coding. Now, the model matrix  $\mathbf{M}$  has dimensions  $18 \times 18$ , including one column for  $\mathbf{M}_0$ , five for  $\mathbf{M}_1$ , eight for  $\mathbf{M}_2$  and four for  $\mathbf{M}_3$ . Again,  $A_0 = 1$ ,  $A_1 = A_2 = 0$ . The squared column sums of  $\mathbf{M}_3$  are  $9 (1 \times)$ ,  $27 (2 \times)$  and  $81 (1 \times)$ , respectively. Thus,  $A_3 = a_3(1, 2, 3) = (9 + 2 \cdot 27 + 81)/324 = 4/9$ .

The projection frequencies  $a_k(u_1, \dots, u_k)$  from equation (2) are the building blocks for the overall  $A_k$ . The  $a_R(u_1, \dots, u_R)$  will be instrumental in defining one version of generalized resolution. Theorem 1 provides them with an intuitive interpretation. The proof is given in the Appendix.

**THEOREM 1.** *In an  $\text{OA}(N, s_1, \dots, s_n, R - 1)$ , denote by  $\mathbf{X}_c$  the model matrix for the main effects of a particular factor  $c \in \{u_1, \dots, u_R\} \subseteq \{1, \dots, n\}$  in normalized orthogonal coding, and let  $C = \{u_1, \dots, u_R\} \setminus \{c\}$ . Then  $a_R(u_1, \dots, u_R)$  is the sum of the  $R^2$ -values from the  $s_c - 1$  regression models that explain the columns of  $\mathbf{X}_c$  by a full model in the factors from  $C$ .*

**REMARK 1.** (i) Theorem 1 holds regardless which factor is singled out for the left-hand side of the model. (ii) The proof simplifies by restriction to normalized orthogonal coding, but the result holds whenever the factor  $c$  is coded by any set of orthogonal contrasts, whether normalized or not. (iii) Individual  $R^2$  values are coding dependent, but the sum is not. (iv) In case of normalized orthogonal coding for all factors, the full model in the factors from  $C$  can be reduced to the  $R - 1$  factor interaction only, since the matrix  $\mathbf{X}_c$  is orthogonal to the model matrices for all lower degree effects in the other  $R - 1$  factors.

**EXAMPLE 1 (Continued).** The overall  $a_3(1, 2, 3) = 2$  is the sum of two  $R^2$  values which are 1, regardless which factor is singled out as the main effects factor for the left-hand sides of regression. This reflects that the level of each factor is uniquely determined by the level combination of the other two factors.

**EXAMPLE 2 (Continued).** The  $R^2$  from regressing the single model matrix column of the 2-level factor on the four model matrix columns for the interaction among the two 3-level factors is  $4/9$ . Alternatively, the  $R^2$ -values for the regression of the two main effects columns for factor B on the AC interaction columns are  $1/9$  and  $3/9$ , respectively, which also yields the sum  $4/9$  obtained above for  $a_3(1, 2, 3)$ . For factor B in dummy coding with reference level 0 instead of normalized polynomial coding, the two main effects model matrix columns for factor B

TABLE 2  
An OA(8, 4<sup>1</sup>2<sup>2</sup>, 2) (transposed)

A	0	0	0	0	1	1	1	1
B	0	0	1	1	0	0	1	1
C	0	2	1	3	3	1	2	0

have correlation 0.5; the sum of the  $R^2$  values from full models in A and C for explaining these two columns is  $1/3 + 1/3 = 2/3 \neq a_3(1, 2, 3) = 4/9$ . This demonstrates that Theorem 1 is not applicable if orthogonal coding [see Remark 1(ii)] is violated.

**COROLLARY 1.** *In an OA( $N, s_1, \dots, s_n, R - 1$ ), let  $\{u_1, \dots, u_R\} \subseteq \{1, \dots, n\}$ , with  $s_{\min} = \min_{i=1, \dots, R}(s_{u_i})$ .*

(i) *A factor  $c \in \{u_1, \dots, u_R\}$  in  $s_c$  levels is completely confounded by the factors in  $C = \{u_1, \dots, u_R\} \setminus \{c\}$ , if and only if  $a_R(u_1, \dots, u_R) = s_c - 1$ .*

(ii)  *$a_R(u_1, \dots, u_R) \leq s_{\min} - 1$ .*

(iii) *If several factors in  $\{u_1, \dots, u_R\}$  have  $s_{\min}$  levels, either all of them are or none of them is completely confounded by the respective other  $R - 1$  factors in  $\{u_1, \dots, u_R\}$ .*

(iv) *A factor with more than  $s_{\min}$  levels cannot be completely confounded by the other factors in  $\{u_1, \dots, u_R\}$ .*

Part (i) of Corollary 1 follows easily from Theorem 1, as  $a_R(u_1, \dots, u_R) = s_c - 1$  if and only if all  $R^2$  values for columns of the factor  $c$  main effects model matrix are 100%, that is, the factor  $c$  main effects model matrix is completely explained by the factors in C. Part (ii) follows, because the sum of  $R^2$  values is of course bounded by the minimum number of regressions conducted for any single factor  $c$ , which is  $s_{\min} - 1$ . Parts (iii) and (iv) follow directly from parts (i) and (ii). For symmetric  $s$ -level designs, part (ii) of the corollary has already been proven by Xu, Cheng and Wu (2004).

**EXAMPLE 3.** For the design of Table 2,  $s_{\min} = 2$ , and  $a_3(1, 2, 3) = 1$ , that is, both 2-level factors are completely confounded, while the 4-level factor is only partially confounded. The individual  $R^2$  values for the separate degrees of freedom of the 4-level factor main effect model matrix depend on the coding (e.g., 0.2, 0 and 0.8 for the linear, quadratic and cubic contrasts in normalized orthogonal polynomial coding), while their sum is 1, regardless of the chosen orthogonal coding.

**THEOREM 2.** *In an OA( $N, s_1, \dots, s_n, R - 1$ ), let  $\{u_1, \dots, u_R\} \subseteq \{1, \dots, n\}$  with  $s_{\min} = \min_{i=1, \dots, R}(s_{u_i})$ . Let  $c \in \{u_1, \dots, u_R\}$  with  $s_c = s_{\min}$ ,  $C = \{u_1, \dots,$*

$u_R\} \setminus \{c\}$ . Under normalized orthogonal coding denote by  $\mathbf{X}_c$  the main effects model matrix for factor  $c$  and by  $\mathbf{X}_C$  the  $R - 1$  factor interaction model matrix for the factors in  $C$ .

If  $a_R(u_1, \dots, u_R) = s_{\min} - 1$ ,  $\mathbf{X}_C$  can be orthogonally transformed (rotation and/or switching) such that  $s_{\min} - 1$  of its columns are collinear to the columns of  $\mathbf{X}_c$ .

PROOF.  $a_R(u_1, \dots, u_R) = s_{\min} - 1$  implies all  $s_{\min} - 1$  regressions of the columns of  $\mathbf{X}_c$  on the columns of  $\mathbf{X}_C$  have  $R^2 = 1$ . Then, each of the  $s_{\min} - 1$   $\mathbf{X}_c$  columns can be perfectly matched by a linear combination  $\mathbf{X}_C \mathbf{b}$  of the  $\mathbf{X}_C$  columns; since all columns have the same length, this linear transformation involves rotation and/or switching only. If necessary, these  $s_{\min} - 1$  orthogonal linear combinations can be supplemented by further length-preserving orthogonal linear combinations so that the dimension of  $\mathbf{X}_C$  remains intact.  $\square$

Theorems 1 and 2 are related to canonical correlation analysis, and the redundancy index discussed in that context [Stewart and Love (1968)]. In order to make the following comments digestible, a brief definition of canonical correlation analysis is included without going into any technical detail about the method; details can, for example, be found in Härdle and Simar [(2003), Chapter 14]. It will be helpful to think of the columns of the main effects model matrix of factor  $c$  as the  $Y$  variables and the columns of the full model matrix in the  $R - 1$  other factors from the set  $C$  (excluding the constant column of ones for the intercept) as the  $X$  variables of the following definition and explanation. As it would be unnatural to consider the model matrices from experimental designs as random variables, we directly define canonical correlation analysis in terms of data matrices  $\mathbf{X}$  and  $\mathbf{Y}$  ( $N$  rows each) and empirical covariance matrices  $\mathbf{S}_{xx} = \mathbf{X}^{*\text{T}}\mathbf{X}^*/(N - 1)$ ,  $\mathbf{S}_{yy} = \mathbf{Y}^{*\text{T}}\mathbf{Y}^*/(N - 1)$ ,  $\mathbf{S}_{xy} = \mathbf{X}^{*\text{T}}\mathbf{Y}^*/(N - 1)$  and  $\mathbf{S}_{yx} = \mathbf{Y}^{*\text{T}}\mathbf{X}^*/(N - 1)$ , where the superscript  $*$  denotes columnwise centering of a matrix. We do not attempt a minimal definition, but prioritize suitability for our purpose. Note that our  $\mathbf{S}_{xx}$  and  $\mathbf{S}_{yy}$  are nonsingular matrices, since the designs we consider have strength  $R - 1$ ; the covariance matrix  $(\mathbf{X}^*\mathbf{Y}^*)^{\text{T}}(\mathbf{X}^*\mathbf{Y}^*)/(N - 1)$  of the combined set of variables may, however, be singular, which does not pose a problem to canonical correlation analysis, even though some accounts request this matrix to be nonsingular.

DEFINITION 1. Consider a set of  $pX$ -variables and  $qY$ -variables. Let the  $N \times p$  matrix  $\mathbf{X}$  and the  $N \times q$  matrix  $\mathbf{Y}$  denote the data matrices of  $N$  observations, and  $\mathbf{S}_{xx}$ ,  $\mathbf{S}_{yy}$ ,  $\mathbf{S}_{xy}$  and  $\mathbf{S}_{yx}$  the empirical covariance matrices obtained from them, with positive definite  $\mathbf{S}_{xx}$  and  $\mathbf{S}_{yy}$ .

- (i) Canonical correlation analysis creates  $k = \min(p, q)$  pairs of linear combination vectors  $\mathbf{u}_i = \mathbf{X}\mathbf{a}_i$  and  $\mathbf{v}_i = \mathbf{Y}\mathbf{b}_i$  with  $p \times 1$  coefficient vectors  $\mathbf{a}_i$  and  $q \times 1$  coefficient vectors  $\mathbf{b}_i$ ,  $i = 1, \dots, k$ , such that:
  - (a) the  $\mathbf{u}_1, \dots, \mathbf{u}_k$  are uncorrelated to each other,
  - (b) the  $\mathbf{v}_1, \dots, \mathbf{v}_k$  are uncorrelated to each other,

- (c) the pair  $(\mathbf{u}_1, \mathbf{v}_1)$  has the maximum possible correlation for any pair of linear combinations of the  $\mathbf{X}$  and  $\mathbf{Y}$  columns, respectively,
- (d) the pairs  $(\mathbf{u}_i, \mathbf{v}_i)$ ,  $i = 2, \dots, k$  successively maximize the remaining correlation, given the constraints of (a) and (b).
- (ii) The correlations  $r_i = \text{cor}(\mathbf{u}_i, \mathbf{v}_i)$  are called “canonical correlations,” and the  $\mathbf{u}_i$  and  $\mathbf{v}_i$  are called “canonical variates.”

REMARK 2. (i) If the matrices  $\mathbf{X}$  and  $\mathbf{Y}$  are centered, that is,  $\mathbf{X} = \mathbf{X}^*$  and  $\mathbf{Y} = \mathbf{Y}^*$ , the  $\mathbf{u}$  and  $\mathbf{v}$  vectors also have zero means, and the uncorrelatedness in (a) and (b) is equivalent to orthogonality of the vectors. (ii) It is well known that the canonical correlations are the eigenvalues of the matrices  $\mathbf{Q}_1 = \mathbf{S}_{xx}^{-1}\mathbf{S}_{xy}\mathbf{S}_{yy}^{-1}\mathbf{S}_{yx}$  and  $\mathbf{Q}_2 = \mathbf{S}_{yy}^{-1}\mathbf{S}_{yx}\mathbf{S}_{xx}^{-1}\mathbf{S}_{xy}$  [the first  $\min(p, q)$  eigenvalues of both matrices are the same; the larger matrix has the appropriate number of additional zeroes] and the  $\mathbf{a}_i$  are the corresponding eigenvectors of  $\mathbf{Q}_1$ , the  $\mathbf{b}_i$  the corresponding eigenvectors of  $\mathbf{Q}_2$ .

According to the definition, the canonical correlations are nonnegative. It can also be shown that  $\mathbf{u}_i$  and  $\mathbf{v}_j$ ,  $i \neq j$ , are uncorrelated, and orthogonal in case of centered data matrices; thus, the pairs  $(\mathbf{u}_i, \mathbf{v}_i)$  decompose the relation between  $\mathbf{X}$  and  $\mathbf{Y}$  into uncorrelated components, much like the principal components decompose the total variance into uncorrelated components. In data analysis, canonical correlation analysis is often used for dimension reduction. Here, we retain the full dimensionality. For uncorrelated  $Y$  variables like the model matrix columns of  $\mathbf{X}_c$  in Theorem 1, it is straightforward to see that the sum of the  $R^2$  values from regressing each of the  $Y$  variables on all the  $X$  variables coincides with the sum of the squared canonical correlations. It is well known that the canonical correlations are invariant to arbitrary nonsingular affine transformations applied to the  $X$ - and  $Y$ -variables, which translate into nonsingular linear transformations applied to the centered  $\mathbf{X}$ - and  $\mathbf{Y}$ -matrices [cf., e.g., Härdle and Simar (2003), Theorem 14.3]. For our application, this implies invariance of the canonical correlations to factor coding. Unfortunately, this invariance property does not hold for the  $R^2$  values or their sum: according to Lazraq and Cléroux [(2001), Section 2] the aforementioned redundancy index—which is the average  $R^2$  value calculated as  $a_R(u_1, \dots, u_R)/(s_c - 1)$  in the situation of Theorem 1—is invariant to linear transformations of the centered  $\mathbf{X}$  matrix, but only to *orthonormal* transformations of the centered  $\mathbf{Y}$  matrix or scalar multiples thereof. For correlated  $Y$ -variables, the redundancy index contains some overlap between variables, as was already seen for Example 2, where the sum of the  $R^2$  values from dummy coding exceeded  $a_3(1, 2, 3)$ ; in that case, only the average or sum of the squared canonical correlations yields an adequate measure of the overall explanatory power of the  $X$ -variables on the  $Y$ -variables. Hence, for the case of arbitrary coding, Theorem 1 has to be restated in terms of squared canonical correlations.

THEOREM 3. In an  $\text{OA}(N, s_1, \dots, s_n, R - 1)$ , denote by  $\mathbf{X}_c$  the model matrix for the main effects of a particular factor  $c \in \{u_1, \dots, u_R\}$  in arbitrary coding,



and let  $C = \{u_1, \dots, u_R\} \setminus \{c\}$ . Then  $a_R(u_1, \dots, u_R)$  is the sum of the squared canonical correlations from a canonical correlation analysis of the columns of  $\mathbf{X}_c$  and the columns of the full model matrix  $\mathbf{F}_C$  in the factors from  $C$ .

EXAMPLE 1 (Continued).  $s_{\min} = 3, a_3(1, 2, 3) = 2$ , that is, the assumptions of Theorems 2 and 3 are fulfilled. Both canonical correlations must be 1, because the sum must be 2. The transformation of  $\mathbf{X}_C$  from Theorem 2 can be obtained from the canonical correlation analysis: For all factors in the role of  $Y$ ,  $\mathbf{v}_i \propto \mathbf{y}_i$  (with  $\mathbf{y}_i$  denoting the  $i$ th column of the main effects model matrix of the  $Y$ -variables factor) can be used. For the first or second factor in the role of  $Y$ , the corresponding canonical vectors on the  $X$  side fulfill

$$\mathbf{u}_1 \propto \mathbf{B}_q \mathbf{C}_l - \mathbf{B}_l \mathbf{C}_q - \sqrt{3} \mathbf{B}_l \mathbf{C}_l - \sqrt{3} \mathbf{B}_q \mathbf{C}_q,$$

$$\mathbf{u}_2 \propto \sqrt{3} \mathbf{B}_l \mathbf{C}_q - \sqrt{3} \mathbf{B}_q \mathbf{C}_l - \mathbf{B}_l \mathbf{C}_l - \mathbf{B}_q \mathbf{C}_q$$

(or  $\mathbf{B}$  replaced by  $\mathbf{A}$  for the second factor in the role of  $Y$ ),

with the indices  $l$  and  $q$  denoting the *normalized* linear and quadratic coding introduced above. For the third factor in the role of  $Y$ ,

$$\mathbf{u}_1 \propto -\sqrt{3} \mathbf{A}_l \mathbf{B}_l + \mathbf{A}_q \mathbf{B}_l + \mathbf{A}_l \mathbf{B}_q + \sqrt{3} \mathbf{A}_q \mathbf{B}_q,$$

$$\mathbf{u}_2 \propto -\mathbf{A}_l \mathbf{B}_l - \sqrt{3} \mathbf{A}_l \mathbf{B}_q - \sqrt{3} \mathbf{A}_q \mathbf{B}_l + \mathbf{A}_q \mathbf{B}_q.$$

EXAMPLE 1 (Now with dummy coding). When using the design of Example 1 for an experiment with qualitative factors, dummy coding is much more usual than orthogonal contrast coding. This example shows how Theorem 3 can be applied for arbitrary nonorthogonal coding:  $\mathbf{A}_1$  is 1 for  $\mathbf{A} = 1$  and 0 otherwise,  $\mathbf{A}_2$  is 1 for  $\mathbf{A} = 2$  and 0 otherwise,  $\mathbf{B}$  and  $\mathbf{C}$  are coded analogously; interaction matrix columns are obtained as products of the respective main effects columns. The main effect and two-factor interaction model matrix columns in this coding do not have column means zero and have to be centered first by subtracting  $1/3$  or  $1/9$ , respectively. As canonical correlations are invariant to affine transformations, dummy coding leads to the same canonical correlations as the previous normalized orthogonal polynomial coding. We consider the first factor in the role of  $Y$ ; the centered model matrix columns  $\mathbf{y}_1 = \mathbf{A}_1 - 1/3$  and  $\mathbf{y}_2 = \mathbf{A}_2 - 1/3$  are correlated, so that we must not choose both canonical variates for the  $Y$  side proportional to the original variates. One instance of the canonical variates for the  $Y$  side is  $\mathbf{v}_1 = -\mathbf{y}_1/\sqrt{2}, \mathbf{v}_2 = (\mathbf{y}_1 + 2\mathbf{y}_2)/\sqrt{6}$ ; these canonical vectors are unique up to rotation only, because the two canonical correlations have the same size. The corresponding canonical vectors on the  $X$  side are obtained from the centered full model matrix

$$\mathbf{F}_C = ((\mathbf{B}_1 - \frac{1}{3}), (\mathbf{B}_2 - \frac{1}{3}), (\mathbf{C}_1 - \frac{1}{3}), (\mathbf{C}_2 - \frac{1}{3}), (\mathbf{B}_1 \mathbf{C}_1 - \frac{1}{9}), (\mathbf{B}_2 \mathbf{C}_1 - \frac{1}{9}),$$

$$(\mathbf{B}_1 \mathbf{C}_2 - \frac{1}{9}), (\mathbf{B}_2 \mathbf{C}_2 - \frac{1}{9}))$$

as  $\mathbf{u}_1 = (-\mathbf{f}_2 - \mathbf{f}_3 + \mathbf{f}_5 + 2\mathbf{f}_6 - \mathbf{f}_7 + \mathbf{f}_8)/\sqrt{2}$  and  $\mathbf{u}_2 = (2\mathbf{f}_1 + \mathbf{f}_2 + \mathbf{f}_3 + 2\mathbf{f}_4 - 3\mathbf{f}_5 - 3\mathbf{f}_7 - 3\mathbf{f}_8)/\sqrt{6}$ , with  $\mathbf{f}_j$  denoting the  $j$ th column of  $\mathbf{F}_C$ .

Note that the canonical vectors  $\mathbf{u}_1$  and  $\mathbf{u}_2$  now contain contributions not only from the interaction part of the model matrix but also from the main effects part, that is, we do indeed need the full model matrix as stated in Theorem 3.

EXAMPLE 2 (Continued).  $s_{\min} = 2$ ,  $a_3(1, 2, 3) = 4/9$ , that is, the assumption of Theorem 2 is not fulfilled, the assumption of Theorem 3 is. The canonical correlation using the one column main effects model matrix of the 2-level factor A in the role of Y is 2/3, the canonical correlations using the main effects model matrix for the 3-level factor B in the role of Y are 2/3 and 0; in both cases, the sum of the squared canonical correlations is  $a_3(1, 2, 3) = 4/9$ . For any other coding, for example, the dummy coding for factor B considered earlier, the canonical correlations remain unchanged (2/3 and 0, resp.), since they are coding invariant; thus, the sum of the squared canonical correlations remains 4/9, even though the sum of the  $R^2$  values was found to be different. Of course, the linear combination coefficients for obtaining the canonical variates depend on the coding [see, e.g., Härdle and Simar (2003), Theorem 14.3].

Canonical correlation analysis can also be used to verify that a result analogous to Theorem 2 cannot be generalized to sets of R factors for which  $a_R(u_1, \dots, u_R) < s_{\min} - 1$ . For this, note that the number of nonzero canonical correlations indicates the dimension of the relationship between the X- and the Y-variables.

Table 3 displays the  $R^2$  values from two different orthogonal codings and the squared canonical correlations from the main effects matrix of the first factor (Y-variables) vs. the full model matrix of the other two factors (X-variables) for the ten nonisomorphic GMA OA(32, 4<sup>3</sup>, 2) obtained from Eendebak and Schoen

TABLE 3  
Main effects matrix of factor A regressed on full model in factors B and C for the 10 nonisomorphic GMA OA(32, 4<sup>3</sup>, 2)

L	R <sup>2</sup> values from polynomial coding			R <sup>2</sup> values from Helmert coding			Squared canonical correlations			A <sub>3</sub>	Designs
	Q	C		1	2	3	1	2	3		
0.8	0	0.2		0	2/3	1/3	1	0	0	1	1
0.65	0	0.35		1/8	13/24	1/3	0.75	0.25	0	1	2
0.5	0	0.5		1/4	5/12	1/3	0.5	0.5	0	1	3, 6, 8, 10
0.45	0.25	0.3		1/4	5/12	1/3	0.5	0.25	0.25	1	4, 5, 7
0.375	0.25	0.375		5/16	17/48	1/3	0.375	0.375	0.25	1	9

(2013). These designs have one generalized word of length 3, that is, they are non-regular. There are cases with one, two and three nonzero canonical correlations, that is, neither is it generally possible to collapse the linear dependence into a one-dimensional structure nor does the linear dependence generally involve more than one dimension.

**3. Generalized resolution.** Before presenting the new proposals for generalized resolution, we briefly review generalized resolution for symmetric 2-level designs by [Deng and Tang \(1999\)](#) and [Tang and Deng \(1999\)](#). For 2-level factors, each effect has a single degree of freedom (df) only, that is, all the  $\mathbf{X}$ 's in any  $\mathbf{M}_k$  [cf. equation (1)] are one-column matrices. [Deng and Tang \(1999\)](#) looked at the absolute sums of the columns of  $\mathbf{M}$ , which were termed  $J$ -characteristics by [Tang and Deng \(1999\)](#). Specifically, for a resolution  $R$  design, these authors introduced GR as

$$(3) \quad \text{GR} = R + 1 - \frac{\max J_R}{N},$$

where  $J_R = |\mathbf{1}_N^T \mathbf{M}_R|$  is the row vector of the  $J$ -characteristics  $|\mathbf{1}_N^T \mathbf{X}_{u_1, \dots, u_R}|$  obtained from the  $\binom{n}{R}$   $R$ -factor interaction model columns  $\mathbf{X}_{u_1, \dots, u_R}$ . For 2-level designs, it is straightforward to verify the following identities:

$$(4) \quad \begin{aligned} \text{GR} &= R + 1 - \sqrt{\max_{(u_1, \dots, u_R)} a_R(u_1, \dots, u_R)} \\ &= R + 1 - \max_{(u_1, \dots, u_R)} |\rho(X_{u_1}, X_{u_2, \dots, u_R})|, \end{aligned}$$

where  $\rho$  denotes the correlation; note that the correlation in (4) does not depend on which of the  $u_i$  takes the role of  $u_1$ . [Deng and Tang \[\(1999\), Proposition 2\]](#) proved a very convincing projection interpretation of their GR. Unfortunately, [Proposition 4.4 of Diestelkamp and Beder \(2002\)](#), in which a particular  $\text{OA}(18, 3^3, 2)$  is proven to be indecomposable into two  $\text{OA}(9, 3^3, 2)$ , implies that [Deng and Tang's](#) result cannot be generalized to more than two levels.

The quantitative approach by [Evangelaras et al. \[\(2005\), their equation \(4\)\]](#) generalized the correlation version of (4) by applying it to single df contrasts for the quantitative factors. For the qualitative factors considered here, any approach based on direct usage of single df contrasts is not acceptable because it is coding dependent. The approach for qualitative factors taken by [Evangelaras et al.](#) is unreasonable, as will be demonstrated in [Example 5](#). [Pang and Liu \(2010\)](#) also proposed a generalized resolution based on complex contrasts. For designs with more than 3 levels, permuting levels for one or more factors will lead to different generalized resolutions according to their definition, which is unacceptable for qualitative factors. For 2-level designs, their approach boils down to omitting the square root from  $\sqrt{\max_{(u_1, \dots, u_R)} a_R(u_1, \dots, u_R)}$  in (4), which implies that their proposal does not simplify to the well-grounded generalized resolution of [Deng and Tang](#)

(1999)/Tang and Deng (1999) for 2-level designs. This in itself makes their approach unconvincing. Example 5 will compare their approach to ours for 3-level designs. The results from the previous section can be used to create two adequate generalizations of GR for qualitative factors. These are introduced in the following two definitions.

For the first definition, an  $R$  factor projection is considered as completely aliased, whenever all the levels of at least one of the factors are completely determined by the level combination of the other  $R - 1$  factors. Thus, generalized resolution should be equal to  $R$ , if and only if there is at least one  $R$  factor projection with  $a_R(u_1, \dots, u_R) = s_{\min} - 1$ . The GR defined in Definition 2 guarantees this behavior and fulfills all requirements stated in the Introduction:

DEFINITION 2. For an  $OA(N, s_1, \dots, s_n, R - 1)$ ,

$$GR = R + 1 - \sqrt{\max_{\substack{\{u_1, \dots, u_R\} \\ \subseteq \{1, \dots, n\}}} \frac{a_R(u_1, \dots, u_R)}{\min_{i=1, \dots, R} s_{u_i} - 1}}$$

In words, GR increases the resolution by one minus the square root of the worst case average  $R^2$  obtained from any  $R$  factor projection, when regressing the main effects columns in orthogonal coding from a factor with the minimum number of levels on the other factors in the projection. It is straightforward to see that (4) is a special case of the definition, since the denominator is 1 for 2-level designs. Regarding the requirements stated in the Introduction, (i) GR from Definition 2 is coding invariant because the  $a_R(\cdot)$  are coding invariant according to Xu and Wu (2001). (ii) The technique is obviously applicable for symmetric and asymmetric designs alike, and (iii)  $GR < R + 1$  follows from the resolution,  $GR \geq R$  follows from part (ii) of Corollary 1,  $GR = R$  is equivalent to complete confounding in at least one  $R$ -factor projection according to part (i) of Corollary 1.

EXAMPLE 4. The GR values for the designs from Examples 1 and 3 are 3 ( $GR = R$ ), the GR value for the design from Example 2 is  $3 + 1 - \sqrt{4/9} = 3.33$ , and the GR values for all designs from Table 3 are  $3 + 1 - \sqrt{1/3} = 3.42$ .

Now, complete aliasing is considered regarding individual degrees of freedom (df). A coding invariant individual df approach considers a factor's main effect as completely aliased in an  $R$  factor projection, whenever there is at least one pair of canonical variates with correlation one. A projection is considered completely aliased, if at least one factor's main effect is completely aliased in this individual df sense. Note that it is now possible that factors with the same number of levels can show different extents of individual df aliasing within the same projection, as will be seen in Example 5 below.

DEFINITION 3. For an  $OA(N, s_1, \dots, s_n, R - 1)$  and tuples  $(c, C)$  with  $C = \{u_1, \dots, u_R\} \setminus \{c\}$ ,

$$GR_{ind} = R + 1 - \max_{\{u_1, \dots, u_R\} \subseteq \{1, \dots, n\}} \max_{c \in \{u_1, \dots, u_R\}} r_1(\mathbf{X}_c; \mathbf{F}_C)$$

with  $r_1(\mathbf{X}_c; \mathbf{F}_C)$  the largest canonical correlation between the main effects model matrix for factor  $c$  and the full model matrix of the factors in  $C$ .

In words,  $GR_{ind}$  is the worst case confounding for an individual main effects df in the design that can be obtained by the worst case coding (which corresponds to the  $\mathbf{v}_1$  vector associated with the worst canonical correlation). Obviously,  $GR_{ind}$  is thus a stricter criterion than  $GR$ . Formally, Theorem 3 implies that  $GR$  from Definition 2 can be written as

$$(5) \quad GR = R + 1 - \sqrt{\max_{\substack{(u_1, \dots, u_R): \\ \{u_1, \dots, u_R\} \subseteq \{1, \dots, n\}}} \frac{\sum_{j=1}^{s_{u_1}-1} r_j(\mathbf{X}_{u_1}; \mathbf{F}_{\{u_2, \dots, u_R\}})^2}{\min_i s_{u_i} - 1}}$$

Note that maximization in (5) is over tuples, so that it is ensured that the factor with the minimum number of levels does also get into the first position. Comparing (5) with Definition 3,  $GR_{ind} \leq GR$  is obvious, because  $r_1^2$  cannot be smaller than the average over all  $r_i^2$  (but can be equal, if all canonical correlations have the same size). This is stated in a theorem.

THEOREM 4. For  $GR$  from Definition 2 and  $GR_{ind}$  from Definition 3,  $GR_{ind} \leq GR$ .

REMARK 3. (i) Under normalized orthogonal coding, the full model matrix  $\mathbf{F}_C$  in Definition 3 can again be replaced by the  $R - 1$  factor interaction matrix  $\mathbf{X}_C$ . (ii) Definition 3 involves calculation of  $R \binom{n}{R}$  canonical correlations ( $R$  correlations for each  $R$  factor projection). In any projection with at least one 2-level factor, it is sufficient to calculate one single canonical correlation obtained with an arbitrary 2-level factor in the role of  $Y$ , because this is necessarily the worst case. Nevertheless, calculation of  $GR_{ind}$  carries some computational burden for designs with many factors.

Obviously, (4) is a special case of  $GR_{ind}$ , since the average  $R^2$  coincides with the only squared canonical correlation for projections of  $R$  2-level factors.  $GR_{ind}$  also fulfills all requirements stated in the Introduction: (i)  $GR_{ind}$  is coding invariant because the canonical correlations are invariant to affine transformations of the  $X$  and  $Y$  variables, as was discussed in Section 2. (ii) The technique is obviously applicable for symmetric and asymmetric designs alike, and (iii)  $GR_{ind} < R + 1$  again follows from the resolution,  $GR_{ind} \geq R$  follows from the properties of correlations, and  $GR_{ind} = R$  is obviously equivalent to complete confounding of at least one main effects contrast in at least one  $R$  factor projection, in the individual df sense discussed above.

TABLE 4  
The Taguchi L18 (transposed)

Column	Row																	
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	0	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1
2	0	0	0	1	1	1	2	2	2	0	0	0	1	1	1	2	2	2
3	0	1	2	0	1	2	0	1	2	0	1	2	0	1	2	0	1	2
4	0	1	2	0	1	2	1	2	0	2	0	1	1	2	0	2	0	1
5	0	1	2	1	2	0	0	1	2	2	0	1	2	0	1	1	2	0
6	0	1	2	1	2	0	2	0	1	1	2	0	0	1	2	2	0	1
7	0	1	2	2	0	1	1	2	0	1	2	0	2	0	1	0	1	2
8	0	1	2	2	0	1	2	0	1	0	1	2	1	2	0	1	2	0

EXAMPLE 5. We consider the three nonisomorphic  $OA(18, 3^3, 2)$  that can be obtained as projections from the well-known Taguchi L18 (see Table 4) by using columns 3, 4 and 5 ( $D_1$ ), columns 2, 3 and 6 ( $D_2$ ) or columns 2, 4 and 5 ( $D_3$ ). We have  $A_3(D_1) = 0.5$ ,  $A_3(D_2) = 1$  and  $A_3(D_3) = 2$ , and consequently  $GR(D_1) = 3.5$ ,  $GR(D_2) = 3.29$  and  $GR(D_3) = 3$ . For calculating  $GR_{ind}$ , the largest canonical correlations of all factors in the role of  $Y$  are needed. These are all 0.5 for  $D_1$  and all 1 for  $D_3$ , such that  $GR_{ind} = GR$  for these two designs. For  $D_2$ , the largest canonical correlation is 1 with the first factor (from column 2 of the L18) in the role of  $Y$ , while it is  $\sqrt{0.5}$  with either of the other two factors in the role of  $Y$ ; thus,  $GR_{ind} = 3 < GR = 3.29$ . The completely aliased 1 df contrast of the first factor is the contrast of the third level vs. the other two levels, which is apparent from Table 5: the contrast  $A = 2$  vs.  $A$  in  $(0, 1)$  is fully aliased with the contrast of one level of  $B$  vs. the other two, given a particular level of  $C$ . Regardless of factor coding, this direct aliasing is reflected by a canonical correlation “one” for the first canonical variate of the main effects contrast matrix of factor  $A$ .

Using this example, we now compare the GR introduced here to proposals by Evangelaras et al. (2005) and Pang and Liu (2010): The  $GR_{es}$  values reported by Evangelaras et al. (2005) for designs  $D_1$ ,  $D_2$  and  $D_3$  in the qualitative case are 3.75, 3.6464, 3.5, respectively; especially the 3.5 for the completely aliased design

TABLE 5  
Frequency table of columns 2 (= A), 3 (= B) and 6 (= C) of the Taguchi L18

		,, C = 0			,, C = 1				,, C = 2					
		B			B				B					
A		0	1	2	A	0	1	2	A	0	1	2		
	0	1	0	1		0	1	1	0		0	0	1	1
	1	1	0	1		1	1	1	0		1	0	1	1
	2	0	2	0		2	0	0	2		2	2	0	0

$D_3$  does not make sense. Pang and Liu reported values 3.75, 3.75 and 3, respectively; here, at least the completely aliased design  $D_3$  is assigned the value “3.” Introducing the square root, as was discussed in connection with equation (4), their generalized resolutions become 3.5, 3.5 and 3, respectively, that is, they coincide with our GR results for designs  $D_1$  and  $D_3$ . For design  $D_2$ , their value 3.5 is still different from our 3.29 for the following reason: our approach considers  $A_3 = a_3(1, 2, 3)$  as a sum of two  $R^2$ -values and subtracts the square root of their average or maximum (GR or GR<sub>ind</sub>, resp.), while Pang and Liu’s approach considers it as a sum of  $2^3 = 8$  summands, reflecting the potentially different linear combinations of the three factors in the Galois field sense, the (square root of the) maximum of which they subtract from  $R + 1$ .

**4. Properties of GR.** Let  $G$  be the set of all runs of an  $s_1 \times \dots \times s_n$  full factorial design, with  $|G| = \prod_{i=1}^n s_i$  the cardinality of  $G$ . For any design  $D$  in  $N$  runs for  $n$  factors at  $s_1, \dots, s_n$  levels, let  $N_{\mathbf{x}}$  be the number of times that a point  $\mathbf{x} \in G$  appears in  $D$ .  $\bar{N} = N/|G|$  denotes the average frequency for each point of  $G$  in the design  $D$ . We can measure the goodness of a fractional factorial design  $D$  by the uniformity of the design points of  $D$  in the set of all points in  $G$ , that is, the uniformity of the frequency distribution  $N_{\mathbf{x}}$ . One measure, suggested by Tang (2001) and Ai and Zhang (2004), is the variance

$$V(D) = \frac{1}{|G|} \sum_{\mathbf{x} \in G} (N_{\mathbf{x}} - \bar{N})^2 = \frac{1}{|G|} \sum_{\mathbf{x} \in G} N_{\mathbf{x}}^2 - \bar{N}^2.$$

Let  $N = q|G| + r$  with nonnegative integer  $q$  and  $r$  and  $0 \leq r < |G|$  (often  $q = 0$ ), that is,  $r = N \bmod |G|$  is the remainder of  $N$  when divided by  $|G|$ . Note that  $\sum_{\mathbf{x} \in G} N_{\mathbf{x}} = N$ , so  $V(D)$  is minimized if and only if each  $N_{\mathbf{x}}$  takes values on  $q$  or  $q + 1$  for any  $\mathbf{x} \in G$ . When  $r$  points in  $G$  appear  $q + 1$  times and the remaining  $|G| - r$  points appear  $q$  times,  $V(D)$  reaches the minimal value  $r(|G| - r)/|G|^2$ . Ai and Zhang (2004) showed that  $V(D)$  is a function of GWLP. In particular, if  $D$  has strength  $n - 1$ , their result implies that  $V(D) = \bar{N}^2 A_n(d)$ . Combining these results, and using the following definition, we obtain an upper bound for GR for some classes of designs and provide a necessary and sufficient condition under which this bound is achieved.

**DEFINITION 4** [Modified from Xu (2003)]. (i) A design  $D$  has maximum  $t$ -balance, if and only if the possible level combinations for all projections onto  $t$  columns occur as equally often as possible, that is, either  $q$  or  $q + 1$  times, where  $q$  is an integer such that  $N = q|G_{\text{proj}}| + r$  with  $G_{\text{proj}}$  the set of all runs for the full factorial design of each respective  $t$ -factor-projection and  $0 \leq r < |G_{\text{proj}}|$ .

(ii) An  $OA(N, s_1, \dots, s_n, t - 1)$  with  $n \geq t$  has weak strength  $t$  if and only if it has maximum  $t$ -balance. We denote weak strength  $t$  as  $OA(N, s_1, \dots, s_n, t^-)$ .

REMARK 4. Xu (2003) did not require strength  $t - 1$  in the definition of weak strength  $t$ , that is, the Xu (2003) definition of weak strength  $t$  corresponds to our definition of maximum  $t$ -balance. For the frequent case, for which all  $t$ -factor projections have  $q = 0$  or  $q = 1$  and  $r = 0$  in Definition 4(i), maximum  $t$ -balance is equivalent to the absence of repeated runs in any projection onto  $t$  factors. In that case, maximum  $t$ -balance implies maximum  $k$ -balance for  $k > t$ , and weak strength  $t$  is equivalent to strength  $t - 1$  with absence of repeated runs in any projection onto  $t$  or more factors.

THEOREM 5. Let  $D$  be an  $OA(N, s_1, \dots, s_R, R - 1)$ . Then  $A_R(D) \geq \frac{r(\prod_{i=1}^R s_i - r)}{N^2}$ , where  $r$  is the remainder when  $N$  is divided by  $\prod_{i=1}^R s_i$ . The equality holds if and only if  $D$  has weak strength  $R$ .

As all  $R$  factor projections of any  $OA(N, s_1, \dots, s_n, R^-)$  fulfill the necessary and sufficient condition of Theorem 5, we have the following corollary.

COROLLARY 2. Suppose that an  $OA(N, s_1, \dots, s_n, R)$  does not exist. Then any  $OA(N, s_1, \dots, s_n, R^-)$  has maximum GR among all  $OA(N, s_1, \dots, s_n, R - 1)$ .

COROLLARY 3. Suppose that an  $OA(N, s^n, R)$  does not exist. Let  $D$  be an  $OA(N, s^n, R - 1)$ . Then  $GR(D) \leq R + 1 - \sqrt{\frac{r(s^R - r)}{N^2(s - 1)}}$ , where  $r$  is the remainder when  $N$  is divided by  $s^R$ . The equality holds if and only if  $D$  has weak strength  $R$ .

EXAMPLE 6. (1) Any projection onto three 3-level columns from an  $OA(18, 6^1 3^6, 2)$  has 18 distinct runs ( $q = 0, r = N = 18$ ) and is an OA of weak strength 3, so it has  $A_3 = 1/2$  and  $GR = 4 - \sqrt{18 \cdot 9 / (18^2 \cdot 2)} = 3.5$ . (2) Any projection onto three or more  $s$ -level columns from an  $OA(s^2, s^{s+1}, 2)$  has  $GR = 3$ , since  $N = r = s^2$ , so that the upper limit from the corollary becomes  $GR = R = 3$ .

Using the following lemma according to Mukerjee and Wu (1995), Corollary 3 can be applied to a further class of designs.

LEMMA 1 [Mukerjee and Wu (1995)]. For a saturated  $OA(N, s_1^{n_1} s_2^{n_2}, 2)$  with  $n_1(s_1 - 1) + n_2(s_2 - 1) = N - 1$ , let  $\delta_i(a, b)$  be the number of coincidences of two distinct rows  $a$  and  $b$  in the  $n_i$  columns of  $s_i$  levels, for  $i = 1, 2$ . Then

$$s_1 \delta_1(a, b) + s_2 \delta_2(a, b) = n_1 + n_2 - 1.$$

Consider a saturated  $OA(2s^2, (2s)^1 s^{2s}, 2)$ , where  $r = N = 2s^2, s_1 = 2s, s_2 = s, n_1 = 1, n_2 = 2s$ . From Lemma 1, we have  $2\delta_1(a, b) + \delta_2(a, b) = 2$ . So any projection onto three or more  $s$ -level columns has no repeated runs, and thus it achieves the upper limit  $GR = 4 - \sqrt{(s - 2) / (2s - 2)}$  according to Corollary 3.



**COROLLARY 4.** For a saturated  $OA(2s^2, (2s)^1s^{2s}, 2)$ , any projection onto three or more  $s$ -level columns has  $GR = 4 - \sqrt{(s - 2)/(2s - 2)}$ , which is optimum among all possible OAs in  $2s^2$  runs.

**EXAMPLE 7.** Design 1 of Table 3 is isomorphic to a projection from a saturated  $OA(32, 8^14^8, 2)$ .  $A_3$  attains the lower bound from Theorem 5 ( $32 \cdot (64 - 32)/32^2 = 1$ ), and thus  $GR$  attains the upper bound  $4 - (1/3)^{1/2} = 3.42$  from the corollary.

Because of Theorem 4, any upper bound for  $GR$  is of course also an upper bound for  $GR_{ind}$ , that is, Corollaries 3 and 4 also provide upper bounds for  $GR_{ind}$ . However, for  $GR_{ind}$  the bounds are not tight in general; for example,  $GR_{ind} = 3$  for the design of Example 7 (see also Example 9 in the following section).

Butler (2005) previously showed that all projections onto  $s$ -level columns of  $OA(s^2, s^{s+1}, 2)$  or  $OA(2s^2, (2s)^1s^{2s}, 2)$  have GMA among all possible designs.

**5. Factor wise GR values.** In Section 3, two versions of overall generalized resolution were defined:  $GR$  and  $GR_{ind}$ . These take a worst case perspective: even if a single projection in a large design is completely confounded—in the case of mixed level designs or  $GR_{ind}$  affecting perhaps only one factor within that projection—the overall metric takes the worst case value  $R$ . It can therefore be useful to accompany  $GR$  and  $GR_{ind}$  by factor specific summaries. For the factor specific individual df perspective, one simply has to omit the maximization over the factors in each projection and has to use the factor of interest in the role of  $Y$  only. For a factor specific complete confounding perspective, one has to divide each projection’s  $a_R(\cdot)$  value by the factor’s df rather than the minimum df, in order to obtain the average  $R^2$  value for this particular factor. This leads to the following definition.

**DEFINITION 5.** For an  $OA(N, s_1, \dots, s_n, R - 1)$ , define

- (i)  $GR_{tot(i)} = R + 1 - \sqrt{\max_{\{u_2, \dots, u_R\} \subseteq \{1, \dots, n\} \setminus \{i\}} \frac{a_R(i, u_2, \dots, u_R)}{s_i - 1}}$ ,
- (ii)  $GR_{ind(i)} = R + 1 - \max_{\{i, u_2, \dots, u_R\} \subseteq \{1, \dots, n\}} r_1(\mathbf{X}_i; \mathbf{X}_{u_2, \dots, u_R})$ , with  $\mathbf{X}_i$  the model matrix of factor  $i$  and  $\mathbf{X}_{u_2, \dots, u_R}$  the  $R - 1$  factor interaction model matrix of the factors in  $\{u_2, \dots, u_R\}$  in normalized orthogonal coding, and  $r_1(\mathbf{Y}; \mathbf{X})$  the first canonical correlation between matrices  $\mathbf{X}$  and  $\mathbf{Y}$ .

It is straightforward to verify that  $GR$  and  $GR_{ind}$  can be calculated as the respective minima of the factor specific  $GR$  values from Definition 5.

**THEOREM 6.** For the quantities from Definitions 2, 3 and 5, we have

- (i)  $GR = \min_i GR_{tot(i)}$ ,

(ii)  $GR_{ind} = \min_i GR_{ind(i)}$ .

EXAMPLE 8. The Taguchi L18 has  $GR = GR_{ind} = 3$ , and the following  $GR_{ind(i)}$  and  $GR_{tot(i)}$  values ( $GR_{ind(i)} = GR_{tot(i)}$  for all  $i$ ): 3.18, 3, 3.29, 3, 3, 3.29, 3.29, 3.29. When omitting the second column, the remaining seven columns have  $GR = GR_{ind} = 3.18$ , again with  $GR_{ind(i)} = GR_{tot(i)}$  and the value for all 3-level factors at 3.42. When omitting the fourth column instead, the then remaining seven columns have  $GR = 3.18$ ,  $GR_{ind} = 3$ ,  $GR_{tot(i)}$  values 3.18, 3.29, 3.29, 3.42, 3.29, 3.29, 3.29 and  $GR_{ind(i)}$  values the same, except for the second column, which has  $GR_{ind(2)} = 3$ .

$GR$  from Definition 2 and  $GR_{ind}$  from Definition 3 are not the only possible generalizations of (4). It is also possible to define a  $GR_{tot}$ , by declaring only those  $R$  factor projections as completely confounded for which all factors are completely confounded. For this, the factor wise average  $R^2$  values for each projection—also used in  $GR_{tot(i)}$ —need to be considered. A projection is completely confounded, if these are all one, which can be formalized by requesting their minimum or their average to be one. The average appears more informative, leading to

$$(6) \quad GR_{tot} = R + 1 - \sqrt{\max_{\substack{\{u_1, \dots, u_R\} \\ \subseteq \{1, \dots, n\}}} \frac{1}{R} \sum_{i=1}^R \frac{a_R(u_1, \dots, u_R)}{s_{u_i} - 1}}$$

It is straightforward to see that  $GR_{tot} \geq GR$ , and that  $GR_{tot} = GR$  for symmetric designs. The asymmetric design of Table 2 (Example 3) has  $GR = 3$  and  $GR_{tot} = 3 + 1 - \sqrt{(1 + 1 + 1/3)/3} = 3.12 > 3$ , in spite of the fact that two of its factors are completely confounded. Of course, mixed level projections can never be completely confounded according to (6), which is the main reason why we have not pursued this approach.

The final example uses the designs of Table 3 to show that  $GR_{ind}$  and the  $GR_{ind(i)}$  can introduce meaningful differentiation between GMA designs.

EXAMPLE 9. All designs of Table 3 had  $A_3 = 1$  and  $GR = 3.42$ . The information provided in Table 3 is insufficient for determining  $GR_{ind}$ . Table 6 provides the necessary information: the largest canonical correlations are the same regardless which variable is chosen as the  $Y$  variable for seven designs, while they vary with the choice of the  $Y$  variable for three designs. There are five different  $GR_{ind}$  values for these 10 designs that were not further differentiated by  $A_3$  or  $GR$ , and in combination with the  $GR_{ind(i)}$ , seven different structures can be distinguished.

The differentiation achieved by  $GR_{ind}$  is meaningful, as can be seen by comparing frequency tables of the first, third and ninth design (see Table 7). The first and third design have  $GR_{ind} = 3$ , which is due to a very regular confounding pattern: in

TABLE 6  
*Largest canonical correlations,  $GR_{ind(i)}$  and  $GR_{ind}$  values for the GMA OA(32, 4<sup>3</sup>, 2)*

	$r_1(1; 23)$	$r_1(2; 13)$	$r_1(3; 12)$	$GR_{ind(1)}$	$GR_{ind(2)}$	$GR_{ind(3)}$	$GR_{ind}$
1	1.000	1.000	1.000	3.000	3.000	3.000	3.000
2	0.866	0.866	0.866	3.134	3.134	3.134	3.134
3	0.707	0.707	1.000	3.293	3.293	3.000	3.000
4	0.707	0.707	0.866	3.293	3.293	3.134	3.134
5	0.707	0.707	0.791	3.293	3.293	3.209	3.209
6	0.707	0.707	0.707	3.293	3.293	3.293	3.293
7	0.707	0.707	0.707	3.293	3.293	3.293	3.293
8	0.707	0.707	0.707	3.293	3.293	3.293	3.293
9	0.612	0.612	0.612	3.388	3.388	3.388	3.388
10	0.707	0.707	0.707	3.293	3.293	3.293	3.293

the first design, dichotomizing each factor into a 0/1 vs. 2/3 design yields a regular resolution III 2-level design (four different runs only), that is, each main effect contrast 0/1 vs. 2/3 is completely confounded by the two-factor interaction of the other two 0/1 vs. 2/3 contrasts; the third design shows this severe confounding for factor C only, whose 0/1 vs. 2/3 contrast is likewise completely confounded by the interaction between factors A and B. Design 9 is the best of all GMA designs in terms of  $GR_{ind}$ . It does not display such a strong regularity in behavior.  $GR_{ind}$  treats designs 1 and 3 alike, although design 1 is clearly more severely affected than design 3, which can be seen from the individual  $GR_{ind(i)}$ . However, as generalized resolution has always taken a “worst case” perspective, this way of handling things is appropriate in this context.

**6. Discussion.** We have provided a statistically meaningful interpretation for the building blocks of GWLP and have generalized resolution by Deng and Tang (1999) and Tang and Deng (1999) in two meaningful ways for qualitative factors. The complete confounding perspective of GR of Definition 2 appears to be more sensible than the individual df perspective of  $GR_{ind}$  as a primary criterion. However,  $GR_{ind}$  provides an interesting new aspect that may provide additional understanding of the structure of OAs and may help in ranking tied designs. The factor wise values of Section 5 add useful detail. It will be interesting to pursue concepts derived from the building blocks of  $GR_{tot(i)}$  and  $GR_{ind(i)}$  for the ranking of mixed level designs. As was demonstrated in Section 5, GR from Definition 2 and  $GR_{ind}$  from Definition 3 are not the only possible generalizations of (4) for qualitative factors. The alternative given in equation (6) appears too lenient and has therefore not been pursued. The concept of weak strength deserves further attention: For symmetric designs with weak strength  $t$  according to Definition 4, Xu [(2003), Theorem 3] showed that these have minimum moment aberration (MMA), and consequently GMA (as MMA is equivalent to GMA for symmetric designs)

TABLE 7  
Frequency tables of designs 1, 3 and 9 from Table 6

,, C = 0					,, C = 1					,, C = 2					,, C = 3								
Design 1					Design 1					Design 1					Design 1								
<b>B</b>					<b>B</b>					<b>B</b>					<b>B</b>								
<b>A</b>	<b>0</b>	<b>1</b>	<b>2</b>	<b>3</b>	<b>A</b>	<b>0</b>	<b>1</b>	<b>2</b>	<b>3</b>	<b>A</b>	<b>0</b>	<b>1</b>	<b>2</b>	<b>3</b>	<b>A</b>	<b>0</b>	<b>1</b>	<b>2</b>	<b>3</b>				
	0	1	1	0	0		0	1	1	0	0		0	0	0	1	1		0	0	0	1	1
	1	1	1	0	0		1	1	1	0	0		1	0	0	1	1		1	0	0	1	1
	2	0	0	1	1		2	0	0	1	1		2	1	1	0	0		2	1	1	0	0
	3	0	0	1	1		3	0	0	1	1		3	1	1	0	0		3	1	1	0	0
Design 3					Design 3					Design 3					Design 3								
<b>B</b>					<b>B</b>					<b>B</b>					<b>B</b>								
<b>A</b>	<b>0</b>	<b>1</b>	<b>2</b>	<b>3</b>	<b>A</b>	<b>0</b>	<b>1</b>	<b>2</b>	<b>3</b>	<b>A</b>	<b>0</b>	<b>1</b>	<b>2</b>	<b>3</b>	<b>A</b>	<b>0</b>	<b>1</b>	<b>2</b>	<b>3</b>				
	0	1	1	0	0		0	1	1	0	0		0	0	0	1	1		0	0	0	1	1
	1	1	0	1	0		1	1	0	1	0		1	0	1	0	1		1	0	1	0	1
	2	0	1	0	1		2	0	1	0	1		2	1	0	1	0		2	1	0	1	0
	3	0	0	1	1		3	0	0	1	1		3	1	1	0	0		3	1	1	0	0
Design 9					Design 9					Design 9					Design 9								
<b>B</b>					<b>B</b>					<b>B</b>					<b>B</b>								
<b>A</b>	<b>0</b>	<b>1</b>	<b>2</b>	<b>3</b>	<b>A</b>	<b>0</b>	<b>1</b>	<b>2</b>	<b>3</b>	<b>A</b>	<b>0</b>	<b>1</b>	<b>2</b>	<b>3</b>	<b>A</b>	<b>0</b>	<b>1</b>	<b>2</b>	<b>3</b>				
	0	1	1	0	0		0	1	0	1	0		0	0	1	0	1		0	0	0	1	1
	1	1	0	1	0		1	0	1	0	1		1	1	0	0	1		1	0	1	1	0
	2	0	0	1	1		2	1	1	0	0		2	0	1	1	0		2	1	0	0	1
	3	0	1	0	1		3	0	0	1	1		3	1	0	1	0		3	1	1	0	0

if they also have maximum  $k$ -balance for  $k = t + 1, \dots, n$ . In particular, this implies that an  $OA(N, s^n, t^-)$  with  $N \leq s^t$  has GMA, because of Remark 4. Here, we showed that designs of the highest possible resolution  $R$  maximize GR if they have weak strength  $R$ . It is likely that there are further beneficial consequences from the concept of weak strength.

APPENDIX: PROOF OF THEOREM 1

Let  $\mathbf{M}_C = (\mathbf{1}_N, \mathbf{M}_{1;C}, \dots, \mathbf{M}_{R-1;C})$ , with  $\mathbf{M}_{k;C}$  the model matrix for all  $k$ -factor interactions,  $k = 1, \dots, R - 1$ . The assumption that the resolution of the array is  $R$  and the chosen orthogonal contrasts imply  $\mathbf{X}_C^T \mathbf{M}_{k;C} = \mathbf{0}$  for  $k < R - 1$ , with  $\mathbf{X}_C$  as defined in the theorem. Denoting the  $R - 1$ -factor interaction matrix  $\mathbf{M}_{R-1;C}$  as  $\mathbf{X}_C$ , the predictions for the columns of  $\mathbf{X}_C$  can be written as

$$\hat{\mathbf{X}}_c = \mathbf{X}_C(\mathbf{X}_C^T \mathbf{X}_C)^{-1} \mathbf{X}_C^T \mathbf{X}_c = \frac{1}{N} \mathbf{X}_C \mathbf{X}_C^T \mathbf{X}_c,$$

since  $\mathbf{X}_C^T \mathbf{X}_C = N \mathbf{I}_{df(C)}$ . As the column averages of  $\hat{\mathbf{X}}_c$  are 0 because of the coding, the nominators for the  $R^2$  values are the diagonal elements of the matrix

$$\hat{\mathbf{X}}_c^T \hat{\mathbf{X}}_c = \frac{1}{N^2} \mathbf{X}_c^T \mathbf{X}_C \mathbf{X}_C^T \mathbf{X}_C \mathbf{X}_c^T \mathbf{X}_c = \frac{1}{N} \mathbf{X}_c^T \mathbf{X}_C \mathbf{X}_C^T \mathbf{X}_c.$$

Analogously, the corresponding denominators are the diagonal elements of

$$\mathbf{X}_c^T \mathbf{X}_c = N \mathbf{I}_{\text{df}(c)},$$

which are all identical to  $N$ . Thus, the sum of the  $R^2$  values is the trace of  $\frac{1}{N^2} \mathbf{X}_c^T \mathbf{X}_c \mathbf{X}_c^T \mathbf{X}_c$ , which can be written as

$$(7) \quad \text{tr} \left( \frac{1}{N^2} \mathbf{X}_c^T \mathbf{X}_c \mathbf{X}_c^T \mathbf{X}_c \right) = \frac{1}{N^2} \text{vec}(\mathbf{X}_c^T \mathbf{X}_c)^T \text{vec}(\mathbf{X}_c^T \mathbf{X}_c),$$

where the  $\text{vec}$  operator stacks the columns of a matrix on top of each other, that is, generates a column vector from all elements of a matrix [see, e.g., Bernstein (2009) for the rule connecting trace to  $\text{vec}$ ]. Now, realize that

$$\text{vec}(\mathbf{X}_c^T \mathbf{X}_c)^T = \text{vec} \left( \left( \sum_{i=1}^N \mathbf{X}_{c(i,f)} \mathbf{X}_{c(i,g)} \right)_{(f,g)} \right)^T = \mathbf{1}_{1 \times N} \mathbf{X}_{u_1, \dots, u_R},$$

where an index pair  $(i, j)$  stand for the  $i$ th row and  $j$ th column, respectively, and the columns in  $\mathbf{X}_{u_1, \dots, u_R}$  are assumed to appear in the order that corresponds to that in  $\text{vec}(\mathbf{X}_c^T \mathbf{X}_c)^T$  (w.l.o.g.). Then (7) becomes

$$\frac{1}{N^2} \mathbf{1}_{1 \times N} \mathbf{X}_{u_1, \dots, u_R} \mathbf{X}_{u_1, \dots, u_R}^T \mathbf{1}_{1 \times N} = a_R(u_1, \dots, u_R),$$

which proves the assertion.

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