Regular Fractions of Factorial Arrays

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Abstract For symmetric arrays of two-level factors, a regular fraction is a well-defined concept, which has been generalized in various ways to arrays of s-level factors with s a prime or prime power, and also to mixed-level arrays with arbitrary numbers of factor levels. This paper introduces three further related definitions of a regular fraction for a general array, based on squared canonical correlations or the commuting of projectors. All classical regularity definitions imply regularity under the new definitions, which also permit further arrays to be considered regular. As a particularly natural example, non-cyclic Latin squares, which are not regular under several classical regularity definitions, are regular fractions under the proposed definitions. This and further examples illustrate the different regularity concepts.

1 Introduction

An array is an $N \times n$ (N rows, n columns) table of symbols, for which the ith column contains s_i symbols. The columns are also called factors, the symbols are also called levels. If $s_1 = \cdots = s_n$, the array is called symmetric, otherwise mixed-level or asymmetric. A full factorial would have (a multiple of) $s_1 \times \cdots \times s_n$ rows; we consider a fraction with N rows. In a balanced array, each column contains each of its symbols equally often. If in addition each pair of columns contains each of its pairs of symbols equally often, the array is an orthogonal array (OA). We only consider balanced arrays, and in most cases OAs. Now we consider three established regularity definitions in more detail:

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Table 1 Two Latin squares: a cyclic one for 4-level factors and a non-cyclic one for 5-level factors; entries show the level of factor C for each AB combination

4-level factors		*B*				5-level factors		*B*				
		0	**1**	**2**	**3**			**0**	**1**	**2**	**3**	**4**
A	**0**	0	1	2	3	*A*	**0**	0	1	2	3	4
	1	1	2	3	0		**1**	1	0	3	4	2
	2	2	3	0	1		**2**	2	3	4	0	1
	3	3	0	1	2		**3**	3	4	1	2	0
							4	4	2	0	1	3

Cyclic group regularity or Abelian group regularity refers to arrays for which the s_i levels of the ith factor can be given in terms of the cyclic group $\mathbb{Z}/s_i\mathbb{Z}$ or, more generally, an Abelian group of order s_i, such that the fraction is a coset of a subgroup of the direct product of all these groups (i.e., of the full factorial).

Pseudo-factor regularity refers to arrays created using defining relations among prime-level pseudo-factors: any factor with non-prime number of levels is viewed as a full factorial in so-called pseudo-factors whose numbers of levels are primes. These arrays can also be characterized by the existence of a coding based on pseudo-factors such that the rows form a coset of a subgroup of an Abelian group, i.e., they are a special case of Abelian group regular arrays. Kobilinsky, Monod and Bailey [12] recently described algorithms for creating such arrays; these are implemented in the R package **planor** (Kobilinsky, Bouvier and Monod [11]).

GF regularity refers to symmetric arrays with all factors at q levels, q a prime power, that can be created through defining equations for fractionating, also called generators, based on additive contrasts in the Galois field $GF(q)$. If q is prime, addition in $GF(q)$ coincides with addition modulo q, while it is different otherwise, see e.g. Dey and Mukerjee [5]. Equivalently, GF regularity can be characterized by labeling the q levels of each factor such that the rows form an affine subspace of the n-dimensional affine space over GF(q). This is the concept discussed by Bose [3] and implies all other types of regularity.

For symmetric 2-level or 3-level arrays, all these regularity types are equivalent. With more than three levels, they need no longer coincide, not even for symmetric arrays with number of levels a prime power. For example, the 4-level array, arranged as a Latin square in Table 1, is Abelian group regular but not GF or pseudo-factor regular. Latin squares also provide examples for which it appears anti-intuitive to consider them non-regular, but which are not regular according to the classic criteria: the 5-level array in Table 1 (the first array from Eendebak and Schoen [6]) is neither GF regular nor pseudo-factor regular nor Abelian group regular (but will be considered regular according to our proposed criteria).

Regularity is closely related to orthogonality. OAs are a widely known orthogonal structure; an even weaker one was introduced by Tjur [15] and termed “Tjur block structure” by Bailey [1]. Tjur block structures consist of factors orthogonal in the sense that projectors onto the corresponding subspaces commute, with the trivial 1-level factor and the supremum of any pair of factors always included (see Table 4 for an example of the supremum). All OAs are Tjur block structures, but the reverse is not true (see e.g. Table 4). If the supremum is not included, it can be added without destroying orthogonality, so that closure under suprema is a lesser issue, and we will call a structure that requires addition of suprema a *weak Tjur block structure*. All examples in this paper are at least weak Tjur block structures.

We propose a regularity definition based on commuting projectors, called "geometric regularity". The recent work by Grömping and Xu [9] offers the possibility for two further regularity definitions, based on model matrices but nevertheless coding-invariant. One definition, called "CC-regularity", is based on the individual so-called squared canonical correlations (SCCs) for the main effect of each factor, whereas a stricter definition ("R^2 regularity") requires that the average R^2 value for explaining each degree of freedom for a main effect be either 0 or 1. The building blocks of CC-regularity and R^2 regularity are introduced in the next section, before the three new regularity definitions and their interrelations are presented in Section 3. Section 4 summarizes the relations among the criteria and discusses practical issues regarding their assessment.

2 Generalized Word Length Patterns, SCCs, and R^2 values

Definition 1 defines notation regarding model matrices and projectors. Definition 2 defines concepts in connection with the generalized word length pattern (GWLP), which was introduced by Xu and Wu [16] and generalizes the well-known word length pattern (WLP) for symmetric 2-level arrays.

Definition 1. Consider an $N \times n$ array with the ith column at s_i levels for $i = 1, \dots, n$.

(i) $\mathbf{1}_N$ denotes a column of ones.
(ii) For $j = 0, \dots, n$, a *j-factor set* is a subset of j columns of the array, and $\mathscr{S}_j = \{S \subseteq \{1, \dots, n\} : |S| = j\}$ denotes the set of all j-factor sets.
(iii) For $S \in \mathscr{S}_j$, $\mathbf{X}_S$ denotes the $N \times c_{\text{full}}$ model matrix of a full model with all main effects and interactions up to degree j, where $c_{\text{full}} = \prod_{i \in S} s_i$; $\mathbf{X}_S$ consists of suitably assembled rows of the matrix that would be used in the full factorial. The first column of $\mathbf{X}_S$ is assumed to be $\mathbf{1}_N$, and $\mathbf{X}_{\{\}} = \mathbf{1}_N$.
(iv) $\mathbf{P}_S = \mathbf{X}_S(\mathbf{X}_S'\mathbf{X}_S)^{-}\mathbf{X}_S'$ is the orthogonal projector onto the column span of $\mathbf{X}_S$.
(v) For factor i, $\mathbf{X}_{\{i\}}$ denotes the $N \times s_i$ model matrix including $\mathbf{1}_N$, and $\mathbf{X}_i$ denotes the $N \times (s_i - 1)$ sub-matrix without $\mathbf{1}_N$. The columns of $\mathbf{X}_i$ are centered.
(vi) Factor i is said to be in *normalized orthogonal coding* if $\mathbf{X}_i'\mathbf{X}_i = N\mathbf{I}_{s_i-1}$.
(vii) The full model matrix $\mathbf{X}_S$ is said to be in *normalized orthogonal coding*, if all individual factors are in normalized orthogonal coding and interaction columns are constructed as products of main effects columns.
(viii) The matrix of the $\prod_{i \in S}(s_i - 1)$ highest order interaction columns from $\mathbf{X}_S$ in normalized orthogonal coding is called $\mathbf{X}_{\mathscr{I}(S)}$. Thus $\mathbf{X}_{\mathscr{I}(\{i\})} = \mathbf{X}_i$ in normalized orthogonal coding, and $\mathbf{X}_{\mathscr{I}(\{\})} = \mathbf{1}_N$.

Table 2 Non-regular 16×3 resolution 3 array from Eendebak and Schoen [6] (transposed)

The transposed array																	Squared canonical correlations		
Run	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16		for A and B	for C
A	0	0	0	0	1	1	1	1	2	2	2	2	3	3	3	3	first	0.5	1
B	0	1	2	3	0	1	2	3	0	1	2	3	0	1	2	3	second	0.5	
C	0	0	1	1	0	1	0	1	1	0	1	0	1	1	0	0	third	0	

Definition 2. Consider an $N \times n$ array with the ith column at s_i levels for $i = 1, \ldots, n$.

(i) For $S \in \mathscr{S}_j$, $a_j(S) = (\mathbf{1}_N' \mathbf{X}_{\mathscr{I}(S)})(\mathbf{1}_N' \mathbf{X}_{\mathscr{I}(S)})'$ denotes the *projected a_j value*.
(ii) The *Generalized Word Length Pattern* (GWLP) $(A_0, A_1, A_2, \ldots, A_n)$ of the array is defined by $A_j = \sum_{S \in \mathscr{S}_j} a_j(S)$ for $j = 0, \ldots, n$.
(iii) The *resolution R* of the array is the smallest j such that $j > 0$ and $A_j > 0$.
(iv) A j-factor subset with resolution j is called a *full resolution subset*.

All OAs have resolution at least 3. Therefore, the GWLP for OAs is usually specified starting with A_3. For resolution 3 arrays, main effects can be estimated orthogonally to each other but may be confounded with interactions of two or more factors. For resolution $R > 3$, main effects are also orthogonal to interactions among up to $R-2$ factors. As one usually assumes lower order effects likely to be stronger than higher order effects, the entry A_R of the GWLP is the most important one. As it is the sum of the projected a_R values $a_R(S)$ over all R-factor sets S, these deserve attention. Grömping and Xu [9] provided two statistical interpretations for these, which are given below. Note that R without square always denotes the resolution, while R^2 denotes the coefficient of determination.

Lemma 1. *Let $S \in \mathscr{S}_R$. For a particular $i \in S$, $a_R(S)$ is the sum of*

(i) the $s_i - 1$ SCCs between the main effects model matrix $\mathbf{X}_i$ and the full model matrix $\mathbf{X}_{S-\{i\}}$;
(ii) the $s_i - 1$ R^2 values from regressing the $s_i - 1$ columns of $\mathbf{X}_i$ on $\mathbf{X}_{S-\{i\}}$, where $\mathbf{X}_i$ is in normalized orthogonal coding.

While the sums in Lemma 1 are identical, no matter which factor i in S is chosen, the individual summands can be different (see Table 2, where the sum is 1 for all factors). The individual R^2 values in (ii) also depend on the choice of normalized orthogonal coding and are therefore not further considered. Note that the SCCs are closely related to the *canonical efficiency factors* introduced by James and Wilkinson [10]; the latter are used in the literature on incomplete block designs and are implemented in the R package **dae** by Brien [4].

According to [9], a factor i in a resolution R array is fully confounded within an R-factor set S, if the respective $a_R(S)$ is equal to $s_i - 1$. This is the case exactly if all SCCs are 1 for this factor singled out as the main effects factor, or, equivalently, if all R^2 values from explaining the columns of $\mathbf{X}_i$ through $\mathbf{X}_{S-\{i\}}$ are 1. On the other hand, if all SCCs are zero, or, equivalently, if all R^2 values from explaining the columns of $\mathbf{X}_i$ through $\mathbf{X}_{S-\{i\}}$ are 0, the set S does not contribute anything to A_R.

Consider factor i in a j-factor set S. If all SCCs between $\mathbf{X}_i$ and $\mathbf{X}_{S-\{i\}}$ are in $\{0,1\}$ then there is a coding for factor i such that each column of $\mathbf{X}_i$ is either fully explained by or uncorrelated with $\mathbf{X}_{S-\{i\}}$. Contrary to most results stated in [9], this insight applies to any j-factor set S regardless of its resolution. This makes the idea of using the SCCs for the assessment of array regularity worth pursuing. Also, the average R^2 value from regressing the columns of $\mathbf{X}_i$ (regardless of coding) onto those of $\mathbf{X}_{S-\{i\}}$ is 1 or 0 exactly if the entire factor is fully explained or not explained at all by the factors in $S-\{i\}$, i.e. this is a stricter variant of no partial confounding. These two versions of regularity are now formally defined, along with geometric regularity.

3 The New Regularity Definitions

Definition 3. A balanced $N \times n$ array is *CC regular*, if the following holds: for every subset S of at least two of the n factors, for every $i \in S$, all SCCs between $\mathbf{X}_i$ and $\mathbf{X}_{S-\{i\}}$ are 0 or 1 only.

Definition 4. A balanced $N \times n$ array is R^2 *regular*, if the following holds: for every subset S of at least two of the n factors, for every $i \in S$, the R^2 values obtained from regressing the columns of $\mathbf{X}_i$ on $\mathbf{X}_{S-\{i\}}$ are all 0 or all 1.

The expressions “CC regular” and “R^2 regular” have been inspired by their correspondence to 0/1 only SCC frequency tables and average R^2 frequency tables, as proposed in [7].

Theorem 1. *The following relations hold.*

(i) R^2 regularity implies CC regularity.
(ii) For symmetric 2-level arrays, R^2 regularity and CC regularity are equivalent.

Proof. Consider a set $S \subseteq \{1,\ldots,n\}$, and a factor $i \in S$.

(i) R^2 regularity implies that the span of $\mathbf{X}_i$ is either contained in the span of $\mathbf{X}_{S-\{i\}}$ (which implies that all SCCs are 1), or is orthogonal to that space (which implies that all SCCs are 0).

(ii) The single R^2 value equals the single SCC for each pair $\mathbf{X}_{\{i\}}$ and $\mathbf{X}_{S-\{i\}}$. □

Definition 4 is equivalent to each factor’s *average* R^2 value being 0 or 1, respectively. Note that R^2 regularity is possible only for symmetric arrays, as the sum of SCCs is the same for all factors in a set and coincides with the sum of R^2 values in the case of full resolution; this restriction does not hold for trivial cases, i.e. for mixed-level arrays that are obtained by crossing or nesting R^2 regular symmetric arrays with different numbers of levels. Furthermore, note that CC regularity and R^2 regularity request the 0/1 property for *all* sets of factors, which is much more than was investigated for generalized resolution (see [9]), where considerations for resolution R arrays were restricted to R-factor sets. Table 3 gives an example of a

Table 3 24×13 array of resolution 3 from Kuhfeld [13] (transposed)

Run	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
A	1	1	1	1	1	1	1	1	1	1	1	1	2	2	2	2	2	2	2	2	2	2	2	2
B	1	1	1	1	1	1	2	2	2	2	2	2	1	1	1	1	1	1	2	2	2	2	2	2
C	1	1	1	2	2	2	1	1	1	2	2	2	1	1	1	2	2	2	1	1	1	2	2	2
D	1	2	2	1	1	2	1	1	2	1	2	2	1	1	2	1	2	2	1	2	2	1	1	2
E	2	1	1	1	2	2	1	2	2	1	1	2	1	2	2	1	1	2	1	1	2	2	2	1
F	1	1	2	2	2	1	2	1	2	1	1	2	1	2	2	1	2	1	2	1	1	1	2	2
G	1	2	2	1	2	1	1	2	1	2	1	2	1	2	1	2	1	2	2	1	2	1	1	2
H	2	1	2	2	1	1	1	2	1	1	2	2	1	1	2	2	1	2	2	2	1	1	2	1
J	1	2	1	2	1	2	2	2	1	1	1	2	1	2	2	2	1	1	1	2	1	2	1	2
K	2	2	1	2	1	1	1	1	2	2	1	2	1	2	1	1	2	2	2	2	1	2	1	1
L	2	2	1	1	2	1	2	1	1	1	2	2	1	1	2	2	2	1	2	1	2	2	1	1
M	2	1	2	1	1	2	2	1	1	2	1	2	1	2	1	2	2	1	1	2	2	1	2	1
N	7	6	3	5	2	11	8	4	12	9	10	1	1	10	9	12	4	8	11	2	5	3	6	7

Squared canonical correlations for 3 factor sets		for 4 factor sets of resolution 4	
SCC	frequency	SCC	frequency
0	1320	1/9	1980
1	198		

resolution 3 array that has regular 3-factor sets only, but contains partial confounding for 4-factor sets of resolution 4. Thus, it is not sufficient to restrict attention to R-factor sets when assessing CC regularity. We conjecture that it is sufficient to check all full resolution sets. For R^2 regularity, the proof is straightforward: for a full resolution set S and $i \in S$, all SCCs between $\mathbf{X}_i$ and $\mathbf{X}_{S-\{i\}}$ are 1; moreover, for $T \supset S$, all SCCs between $\mathbf{X}_i$ and $\mathbf{X}_{T-\{i\}}$ are 1; for $k \in T - S$, either all SCCs between $\mathbf{X}_k$ and $\mathbf{X}_{T-\{k\}}$ are 0, or k is part of another full resolution set which is independently assessed. For CC regularity, we have so far not found a proof for the conjecture.

We now define *geometric regularity*, using the fact that two projectors commute if and only if their column spans are are geometrically orthogonal in the sense of [15]. It is a more lenient variant of the orthogonal block structures introduced by Bailey [1].

Definition 5. A balanced $N \times n$ array is *geometrically regular*, if the following holds: for any two subsets S and T of the n factors, $\mathbf{P}_S$ and $\mathbf{P}_T$ commute.

$S \subseteq T$ implies $\mathbf{P}_S\mathbf{P}_T = \mathbf{P}_T\mathbf{P}_S = \mathbf{P}_S$, i.e., such pairs of sets need not be checked. The following theorem, which follows from equivalence of 0/1 canonical correlations to projector commuting, shows the close relationship between CC regularity and geometric regularity.

Theorem 2. *Let $i \in \{1,\ldots,n\}$, and $\emptyset \neq S,T \subseteq \{1,\ldots n\}$. A balanced $N \times n$ array*

(i) is CC regular *iff $\mathbf{P}_{\{i\}}$ and $\mathbf{P}_S$ commute for all pairs i and S with $i \notin S$;*
(ii) is R^2 regular *iff $\mathbf{P}_{\{i\}}\mathbf{P}_S \in \{\mathbf{0},\mathbf{P}_{\{i\}}\}$ for all pairs i and S with $i \notin S$;*

(iii) is geometrically regular *iff all SCCs between* $\mathbf{X}_S$ *and* $\mathbf{X}_T$ *are in* $\{0,1\}$ *for all pairs S and T.*

Proof. All parts of the theorem follow from two linear algebra results: projectors commute iff the eigenvalues of their product are all in $\{0,1\}$ (follows from Fact 3.9.16 in [2] and Prop. 18.11 in [14]), and the non-zero SCCs of two column-centered matrices $\mathbf{M}$ and $\mathbf{N}$ coincide with the non-zero eigenvalues of the product of the corresponding orthogonal projectors $\mathbf{P_M P_N}$ (also in Prop. 18.11 in [14]). □

Theorem 2 shows that geometric regularity implies CC regularity. The reverse is not true: geometric regularity is stricter than CC regularity in that it requires orthogonality (in the geometric or 0/1 canonical correlation sense) between all effects, not only between main effects and other effects. For example, a CC regular (and even R^2 regular) but not geometrically regular array be constructed as a Latin cube from the 5-level Latin square of Table 1 by crossing a 5-level height factor H (levels 0 to 4) with the Latin square and modifying the original Latin square factor C by taking its sum with H modulo 5; for this Latin cube, the projectors $\mathbf{P}_{\{H,A\}}$ and $\mathbf{P}_{\{B,C\}}$ do not commute, even though it is CC regular and R^2 regular. For symmetric 2-level arrays, however, geometric regularity is equivalent to the other regularity definitions.

Table 4 CC regular and projector commute regular resolution 2 array

The transposed array		Squared canonical correlations	
Run	1 2 3 4 5 6 7 8	SCC	frequency
A	0 0 1 1 2 2 3 3	0	12
B	0 1 0 1 2 3 2 3	1	2
C	0 1 1 0 0 1 1 0		
The supremum of factors *A* and *B*			
H	0 0 0 0 1 1 1 1		

The next example illustrates the generality of the proposed regularity concepts. Table 4 shows an array that has resolution 2 only (no OA) and is a weak Tjur block structure; the main effects of the two 4-level factors have one completely confounded df each (0/1 vs 2/3 for *A* is confounded with 0/1 vs 2/3 for *B*); these give rise to the two SCCs of 1. Thus, this array is CC regular and pseudo-factor regular. As the overlap between *A* and *B* main effects splits into a parallel portion and a portion orthogonal to it, projectors onto the spaces spanned by *A* and *B* commute. All other projectors commute as well so that the array is geometrically regular. It is also Abelian group regular, but not R^2 regular or GF regular.

4 Final Remarks

We have extended GF regularity, pseudo-factor regularity and cyclic / Abelian group regularity with three new regularity definitions. The following hierarchy holds: GF regularity ⇒ pseudo-factor regularity ⇒ Abelian group regularity ⇒ geometric regularity⇒ CC regularity. Furthermore, GF regularity ⇒ R^2 regularity ⇒ CC regularity. The reverse is not true: this is obvious for GF regularity and pseudo-factor regularity, or R^2 regularity and CC regularity, and follows from the examples discussed throughout the paper for the other implications. The new proposals thus provide weaker regularity requirements than the established ones. Their weakness is welcome, because it allows us to consider the 5-level Latin square of Table 1 as a regular array. Whether or not one also wants to consider as regular the Latin cube that can be constructed from it yields the distinction between CC or R^2 regularity on the one hand, and geometric regularity on the other hand.

All three new regularity definitions can be checked post-hoc without knowledge of the array construction principle. However, even with a moderate number of factors, the effort can be tremendous; nevertheless, checking remains more manageable than trying to verify construction-based regularity for unknown construction and level labeling. We mentioned that R^2 regularity can be established by considering only full resolution sets, and conjectured the same to hold for CC regularity. For feasibility reasons, the R package **DoE.base** [8] includes a check for R^2 or CC regularity based on full resolution sets only. Should the conjecture prove wrong, this check only provides for CC regularity within all lowest order factor sets. Checks for geometric regularity have so far not been implemented. Work is in progress on technical conditions, in addition to excluding pairs of subsets related by inclusion, that would reduce the computational burden of checking all pairs of subsets.

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