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Ulrike Grömping

An Interaction-Based Decomposition of Generalized Word Counts Suited to Assessing Combinatorial Equivalence of Factorial Designs

Eine wechselwirkungsbasierte Zerlegung verallgemeinerter Wort-Anzahlen, geeignet zur Bewertung kombinatorischer Äquivalenz faktorieller Pläne (englischsprachig)

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Ulrike Grömping

Beuth University of Applied Sciences, Berlin

Abstract

This paper provides new insights into coding invariance for designs with qualitative factors, including a coding invariant way of denoting the model coefficients. Furthermore, "interaction contributions" (ICs) are proposed for decomposing generalized word counts into contributions that neither depend on level allocation nor on the coding of factors in factorial designs. Combinatorially equivalent designs yield the same ICs, so that ICs are suitable for characterizing factorial designs with qualitative factors. ICs are based on singular value decomposition and are related to bias contributions by interaction degrees of freedom on the estimation of the intercept. The paper introduces ICs and their tabulations in interaction contribution frequency tables and illustrates their behavior in various examples. For situations where both are applicable, ICs are compared to the mean aberrations that were proposed Fontana, Rapallo and Rogantin (2016). The latter were introduced as a tool for assessing combinatorial equivalence of designs; ICs are more widely applicable for this purpose, particularly for designs with factors at more than three levels, for which the mean aberrations by Fontana et al. depend on the level coding.

1. Introduction

Two designs are called isomorphic, if they can be obtained from each other by swaps of columns and/or rows and/or *appropriate* relabelings of factor levels. Isomorphism has to be judged differently for designs with qualitative or quantitative factors: for designs with quantitative factors, isomorphism is sometimes called "geometric isomorphism" (see e.g. Cheng and Ye 2004); here, changes in level orderings can lead to non-isomorphic designs. For qualitative factors, on the other hand, each relabeling of factor levels leads to an isomorphic design; this type of isomorphism will be called "combinatorial equivalence" in this paper; the expression "non-isomorphic" will be taken to mean "not combinatorially equivalent". Criteria for assessing combinatorial equivalence have to be coding-invariant in two ways: they must not depend on swapping some levels in any design column, and for a given set of levels, they must not depend on a particular coding of a model matrix. In their seminal paper on generalized minimum aberration (GMA), Xu and Wu (2001) introduced the so-called normalized orthogonal coding (see Definition 2 below); this paper interprets coding invariance related to model matrices to mean invariance against the choice of a *normalized orthogonal* coding. This means, for example, that a coding invariant way of representing the model coefficients will be provided,

This paper is an extended and refocussed rewrite of Grömping (2016b).

Abbreviations: IC stands for "Interaction Contribution", $ICFT$ for "Interaction Contribution Frequency Table", PFT for "Projection Frequency Table", $MAFT$ for "Mean Aberration Frequency Table", $SCFT$ for squared canonical correlation frequency table, and $ARFT$ for "Average R^2 Frequency Table".

which is applicable for all choices of normalized orthogonal coding. Throughout the paper, the expression "coding invariant" will always be used in the sense outlined in this paragraph.

Xu and Wu (2001) introduced the generalized word length pattern ($GWLP$) which is now widely used as the basis of GMA: For a design with n factors, the $GWLP$ can be written as $(A_0, A_1, \ldots, A_n)$, where $A_0 = 1$ generally holds. For any $j > 0$, let $\mathcal{S}_j = \{S \subseteq \{1, \ldots, n\} : |S| = j\}$ denote the set of all j factor sets. The generalized count A_j of words of length j can be written as the sum of generalized word counts $a_j(S)$ from all such sets, i.e. as $A_j = \sum_{S \in \mathcal{S}_j} a_j(S)$. The $a_j(S)$ are called projected a_j values in the sequel. In many applications, the $GWLP$ is applied to orthogonal array designs, which implies that $A_1 = A_2 = 0$, so that the first interesting entry is A_3. In this paper, $A_1 = 0$ is assumed (i.e., level balance of all factors), and the number R with $A_1 = \cdots = A_{R-1} = 0$ and $A_R > 0$ is called the resolution of the design; this is in line with the conventional understanding of resolution (e.g. in Hedayat, Sloane and Stufken 1999 p.280) for $R \geq 3$ and extends the concept to $R = 2$, e.g. for supersaturated designs. Based on the projected a_3 values, Xu, Cheng and Wu (2004) proposed "minimum projection aberration" for resolution III designs with 3-level factors, and Schoen (2009) used frequency tables of projected a_3 values for the ranking of 18 run factorial designs. Frequency tables of projected a_j values will be called projection frequency tables (PFT_js) in this paper.

Xu and Wu (2001) discussed the statistical meaning of the a_j values in terms of the confounding between j factor interactions and the overall mean. Following a similar logic, Fontana, Rapallo and Rogantin (2016) decomposed the projected a_j values into "aberrations" for individual interaction degrees of freedom, using the complex contrasts that were introduced by Bailey (1982). Their paper is restricted to symmetric s-level designs, i.e. designs with all factors at s levels. They attempted to render the decompositions into aberrations invariant against level changes by permuting the levels of the individual interaction columns, which leads to tabulations of "mean aberrations"; the resulting tables will be called mean aberration frequency tables ($MAFT_j$s) in this paper. Unfortunately, $MAFT$s are not suitable for the assessment of combinatorial equivalence for $s > 3$, as can e.g. be verified by calculating the $MAFT_3$ for the cyclic 5-level Latin square (Fontana et al.'s design $\mathcal{F}_2$) after swapping the first two levels for the third factor; Example 3 will demonstrate that the $MAFT$ can also change after swapping two levels of a 4-level factor. Fontana et al.'s work gave rise to the research presented in this article; the interaction contributions (ICs) developed here are comparable to the mean aberrations, in the sense that both decompose generalized word counts into the same number of contributions, based on an interaction perspective. Contrary to the mean aberrations, ICs are invariant to level swaps and to choices of normalized orthogonal coding for all numbers of levels, and they also work for mixed-level designs.

The ICs are based on singular value decomposition (SVD); ambiguities arising from singular values with multiplicity larger than one are resolved in two different ways, which leads to two types of interaction contribution frequency tables ($ICFT$s). ICs have a statistical interpretation in terms of bias contributions of the interaction to estimation of the overall mean, and the $ICFT$s can be used for assessing combinatorial equivalence of designs. Note that, in spite of also using singular values, the approach of the present paper is quite different from the proposal by Katsaounis, Dean and Jones (2013) of using singular values for checking design equivalence for 2-level designs.

Recently, Grömping and Xu (2014) introduced two different decompositions of projected $a_R(S)$ values (with R the resolution), which work for full resolution sets S only, i.e. for R factor sets with at least resolution R. These decompositions are motivated by considering the impact of confounding in the R factor set S on estimation of each factor's main effects coefficients; Grömping (in press) investigated the use of tabulations based on those decompositions. Squared Canonical Correlation Frequency Tables ($SCFT$s) were found to be quite effective in assessing combinatorial equivalence of designs; the Example and Discussion sections will occasionally compare the discriminatory power of *ICFT*s and *MAFT*s with that of *SCFT*s.

In the following, Section 2 introduces notation and basic concepts, and Section 3 provides two fundamental theorems on coding invariance that may be useful for purposes beyond the development of ICs. Section 4 develops the bias on the sample mean for estimation of the intercept from the highest order interaction in a model with R factors based on a design of resolution R. Section 5 presents the decomposition results, relating them to previous insights on the bias. Section 6 provides several examples, and the final section discusses connections to further related work and reasonable future steps.

2. Notation and basic concepts

In this paper, experimental designs are taken to have N runs and n factors, with s_i levels for the ith factor. Before discussing the basics for factorial designs, some matrix products are defined and rules for them established. In the following, the superscript $\top$ denotes transposition, $\mathbf{1}_N$ and $\mathbf{0}_N$ denote column vectors of N ones or zeroes, respectively, $\mathbf{e}_i$ denotes a unit vector with the value "1" in position i and zeroes everywhere else, and $\mathbf{I}_N$ denotes an N-dimensional identity matrix. An orthogonal matrix $\mathbf{Q}$ is an $r \times r$ matrix with $\mathbf{Q}^\top \mathbf{Q} = \mathbf{Q}\mathbf{Q}^\top = \mathbf{I}_r$. Note that multiplication with an orthogonal matrix applies rotation and/or reflection operations only. This paper will use the term "rotation" for multiplication with any orthogonal matrix $\mathbf{Q}$, regardless whether $\mathbf{Q}$ involves only proper rotation ($det(\mathbf{Q}) = 1$) or not.

Definition 1 (Matrix Products)**.** The following matrix products are defined:

(i) For an $m \times n$ matrix $\mathbf{A}$ and an $r \times s$ matrix $\mathbf{B}$, the Kronecker product is defined as the $mr \times ns$ matrix $\mathbf{A} \otimes \mathbf{B} = (a_{ij}\mathbf{B})_{i=1,\ldots,m,j=1,\ldots,n}$.

(ii) For an $n_a \times N$ matrix $\mathbf{A}$ and an $n_b \times N$ matrix $\mathbf{B}$, the column wise Khatri-Rao product is defined as the $n_a n_b \times N$ matrix $\mathbf{A} \odot_c \mathbf{B} = (\mathbf{a}_1 \otimes \mathbf{b}_1, \ldots, \mathbf{a}_N \otimes \mathbf{b}_N)$, where $\mathbf{a}_i, \mathbf{b}_i, i = 1, \ldots, N$ denote the ith columns of $\mathbf{A}$ and $\mathbf{B}$, respectively, and $\otimes$ denotes the Kronecker product.

(iii) For an $N \times n_a$ matrix $\mathbf{C}$ and an $N \times n_b$ matrix $\mathbf{D}$, the row wise Khatri-Rao product is the $N \times n_a n_b$ matrix obtained as the transpose of the column wise Khatri-Rao product of their transposes: $\mathbf{C} \odot_r \mathbf{D} = (\mathbf{c}^1 \otimes \mathbf{d}^1, \ldots, \mathbf{c}^N \otimes \mathbf{d}^N)^\top$, where $\mathbf{c}^i$ and $\mathbf{d}^i$ denote the transposed ith rows of matrices $\mathbf{C}$ and $\mathbf{D}$, respectively.

(iv) For two $m \times n$ matrices $\mathbf{A}$ and $\mathbf{B}$, the Hadamard or Schur or element wise product is defined as $\mathbf{A} * \mathbf{B} = (a_{ij}b_{ij})_{i=1,\ldots,m,j=1,\ldots,n}$.

Lemma 1. *For an $N \times n_a$ matrix $\mathbf{A}$ and an $N \times n_b$ matrix $\mathbf{B}$:*

(i) $(\mathbf{A} \odot_r \mathbf{B})(\mathbf{A} \odot_r \mathbf{B})^\top = (\mathbf{A}\mathbf{A}^\top) * (\mathbf{B}\mathbf{B}^\top)$.

(ii) $(\mathbf{A} \odot_r \mathbf{B})^+ = (\mathbf{A} \odot_r \mathbf{B})^\top ((\mathbf{A}\mathbf{A}^\top) * (\mathbf{B}\mathbf{B}^\top))^+$*, where the superscript "+" denotes the Moore Penrose inverse.*

Lemma 1 (i) follows from $(\mathbf{A} \odot_c \mathbf{B})^\top (\mathbf{A} \odot_c \mathbf{B}) = (\mathbf{A}^\top \mathbf{A}) * (\mathbf{B}^\top \mathbf{B})$, which is a known result for the column wise Khatri Rao product and the Hadamard product (see e.g. Kolda and Bader 2009, Section 2.6), by applying it to $\mathbf{A}^\top$ and $\mathbf{B}^\top$ instead of $\mathbf{A}$ and $\mathbf{B}$. Lemma 1 (ii) follows from the Moore Penrose inverse for the column wise Khatri Rao product given in Kolda and Bader, or by checking the well-known Moore-Penrose conditions.

We now consider a factorial design with n factors in N runs. The ith factor has s_i levels, $i = 1, \ldots, n$, which occur equally often, i.e. all factors are level-balanced. A full factorial model can be written as follows:

$$E(Y) = \mu + \sum_{i=1}^{n} \mathbf{X}_i \boldsymbol{\beta}_i + \sum_{S \subseteq \{1,\ldots,n\}, |S| \geq 2} \mathbf{X}_{\mathcal{I}(S)} \boldsymbol{\beta}_{\mathcal{I}(S)} \tag{1}$$

with Y denoting the random $N \times 1$ vector of response values, $\mathbf{X}_i$ the main effects model matrix for factor i ($s_i - 1$ columns), $\mathbf{X}_{\mathcal{I}(S)}$ the interaction model matrix of the interaction among the factors in S ($\prod_{i \in S}(s_i - 1)$ columns), and $\boldsymbol{\beta}_{\text{effect}}$ the coefficient vector corresponding to the effect indicated in the subscript. Note that, in case of fractional factorial designs, the model (1) may contain more coefficients than there are runs in the experiment. In the following, the number of model matrix columns of matrix $\mathbf{X}_{\mathcal{I}(S)}$ in Equation(1) will be denoted as $df(S)$; in this paper, $df(S)$ refers to the degrees of freedom of the effect $\mathcal{I}(S)$ in the full factorial design and may be larger than the degrees of freedom available for the effect in a particular fractional design.

Definitions 2 and 3 provide the normalized orthogonal coding introduced by Xu and Wu (2001) and state Xu et al.'s (2004) definition of the a_j in the notation of this paper.

Definition 2 (normalized orthogonal coding)**.** Model (1) is said to be in normalized orthogonal coding, if

(i) the columns of $\mathbf{X}_i$ have mean 0, are orthogonal to each other and have squared length N,

(ii) for $S \in \mathcal{S}_j$, the interaction matrix $\mathbf{X}_{\mathcal{I}(S)}$ is the row wise Khatri-Rao product of the j main effects model matrices $\mathbf{X}_i, i \in S$.

Definition 3 (projected a_j values)**.** For $S \in \mathcal{S}_j$, with $\mathbf{X}_{\mathcal{I}(S)}$ the interaction model matrix in normalized orthogonal coding, $a_j(S) = \mathbf{1}_N^\top \mathbf{X}_{\mathcal{I}(S)} \mathbf{X}_{\mathcal{I}(S)}^\top \mathbf{1}_N / N^2$.

The next lemma relates main effects model matrices in different normalized orthogonal codings to each other.

Lemma 2. *If $\mathbf{X}_i$ and $\widetilde{\mathbf{X}}_i$ are both $N \times (s_i - 1)$ main effects model matrices in normalized orthogonal coding for factor i, there is an orthogonal $(s_i - 1) \times (s_i - 1)$ matrix $\mathbf{Q}$ such that $\widetilde{\mathbf{X}}_i = \mathbf{X}_i \mathbf{Q} \Leftrightarrow \widetilde{\mathbf{X}}_i \mathbf{Q}^\top = \mathbf{X}_i$.*

Lemma 2 is obvious from noting that different orthogonal bases for the factor i main effect with all columns of the same squared length N can only be obtained from each other by rotation and reflection operations. Note that results generalize to complex coding by changing the transpose to conjugate transpose.

The paper makes use of SVD: an $m \times n$ matrix $\mathbf{A}$ can be written as $\mathbf{UDV}^\top$ with orthogonal matrices $\mathbf{U}$ ($m \times m$) and $\mathbf{V}$ ($n \times n$), and an $m \times n$ diagonal matrix $\mathbf{D}$ of $min(m, n)$ non-negative singular values ζ_i. The columns of $\mathbf{U}$ and $\mathbf{V}$ are called left and right singular vectors, respectively. The non-zero squared singular values coincide with the non-zero eigen values of the positive semidefinite matrices $\mathbf{A}^\top\mathbf{A}$ and $\mathbf{A}\mathbf{A}^\top$. If all singular values are distinct, the first $min(m, n)$ columns of matrices $\mathbf{U}$ and $\mathbf{V}$ are unique, up to sign switches of corresponding column pairs $\mathbf{u}_i$ and $\mathbf{v}_i$. Where relevant, this paper enforces uniqueness by choosing signs such that the column means of $\mathbf{U}$ are non-negative. More serious ambiguities can arise from multiple singular values of the same size, which lead to non-unique groups of singular vectors: if $N \times r$ sub matrices $\mathbf{U}_{sub}$ and $\mathbf{V}_{sub}$ correspond to a singular value ζ with multiplicity $r > 1$, these can be replaced by the pair $\mathbf{L}_{sub}$ and $\mathbf{M}_{sub}$ with $\mathbf{L}_{sub} = \mathbf{U}_{sub}\mathbf{Q}$ and $\mathbf{M}_{sub} = \mathbf{V}_{sub}\mathbf{Q}$ with a suitable orthogonal $r \times r$ matrix $\mathbf{Q}$.

The final lemma of this section provides an auxiliary result that can be used to relate coding changes to SVDs.

Lemma 3. *Let* $\mathbf{X}$ *and* $\widetilde{\mathbf{X}}$ *be two different matrices with identical dimensions. The statements I and II are equivalent:*

I. $\mathbf{X}$ *and* $\widetilde{\mathbf{X}}$ *have SVDs with the same* $\mathbf{U}$ *and* $\mathbf{D}$ *and different* $\mathbf{V}$*.*
II. $\widetilde{\mathbf{X}} = \mathbf{X}\mathbf{Q}$ *with an orthogonal matrix* $\mathbf{Q} \neq \mathbf{I}$*.*

Proof. II implies I: Let $\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V_X}^\top$. Then $\widetilde{\mathbf{X}} = \mathbf{X}\mathbf{Q} = \mathbf{U}\mathbf{D}\mathbf{V}_\mathbf{X}^\top\mathbf{Q} = \mathbf{U}\mathbf{D}\mathbf{V}_{\widetilde{\mathbf{X}}}^\top$, with $\mathbf{V}_{\widetilde{\mathbf{X}}} = \mathbf{Q}^\top\mathbf{V}_\mathbf{X}$ an orthogonal matrix (since the product of two orthogonal matrices is again an orthogonal matrix).
I implies II: $\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}_\mathbf{X}^\top$ and $\widetilde{\mathbf{X}} = \mathbf{U}\mathbf{D}\mathbf{V}_{\widetilde{\mathbf{X}}}^\top$; choose the orthogonal matrix $\mathbf{Q} = \mathbf{V}_\mathbf{X}\mathbf{V}_{\widetilde{\mathbf{X}}}^\top$. □

3. Coding invariance

This section establishes two general results on coding invariance, which will constitute the basis for *ICFT*s: Theorem 1 shows the coding invariance of $\mathbf{X}_{\mathcal{I}(S)}\mathbf{X}_{\mathcal{I}(S)}^\top$; Corollary 1 states that matrices $\mathbf{U}$ and $\mathbf{D}$ of the SVD are coding invariant, while $\mathbf{V}$ depends on the coding; Corollary 2 makes clear that interaction model matrices for different codings can be obtained from each other by post-multiplication with an orthogonal matrix, and Theorem 2 introduces a coding invariant way of specifying the model coefficients.

Theorem 1. *The matrix* $\mathbf{X}_{\mathcal{I}(S)}\mathbf{X}_{\mathcal{I}(S)}^\top$ *does not depend on the choice of normalized orthogonal coding.*

Proof. According to Lemma 1, $\mathbf{X}_{\mathcal{I}(S)}\mathbf{X}_{\mathcal{I}(S)}^\top$ can be written as the Schur product of matrices $\mathbf{X}_i\mathbf{X}_i^\top$, $i \in S$, with $\mathbf{X}_i$ a main effects model matrix in normalized orthogonal coding. Because of Lemma 2, $\mathbf{X}_i\mathbf{X}_i^\top = \widetilde{\mathbf{X}}_i\widetilde{\mathbf{X}}_i^\top$ for two choices $\mathbf{X}_i$ and $\widetilde{\mathbf{X}}_i$ of normalized orthogonal coding for factor i. □

Corollary 1. For the SVD $\mathbf{X}_{\mathcal{I}(S)} = \mathbf{U}\mathbf{D}\mathbf{V}^\top$, the matrices $\mathbf{U}$ and $\mathbf{D}$ do not depend on the choice of normalized orthogonal coding, while $\mathbf{V}$ depends on that choice.

Proof. $\mathbf{X}_{\mathcal{I}(S)}\mathbf{X}_{\mathcal{I}(S)}^\top = \mathbf{U}\mathbf{D}\mathbf{V}^\top\mathbf{V}\mathbf{D}^\top\mathbf{U}^\top = \mathbf{U}\mathbf{D}\mathbf{D}^\top\mathbf{U}^\top$ is the eigen value decomposition of the coding invariant matrix $\mathbf{X}_{\mathcal{I}(S)}\mathbf{X}_{\mathcal{I}(S)}^\top$; $\mathbf{X}_{\mathcal{I}(S)}^\top\mathbf{X}_{\mathcal{I}(S)} = \mathbf{V}\mathbf{D}^\top\mathbf{U}^\top\mathbf{U}\mathbf{D}\mathbf{V}^\top = \mathbf{V}\mathbf{D}^\top\mathbf{D}\mathbf{V}^\top$ is the eigen value decomposition of the coding dependent matrix $\mathbf{X}_{\mathcal{I}(S)}^\top\mathbf{X}_{\mathcal{I}(S)}$. □

Corollary 2. Let $\mathbf{X}_{\mathcal{I}(S)}$ and $\widetilde{\mathbf{X}}_{\mathcal{I}(S)}$ denote two interaction model matrices for the factors in $S \subseteq \{1, \ldots, n\}$ in normalized orthogonal coding. There is an orthogonal matrix $\mathbf{Q}$ such that $\widetilde{\mathbf{X}}_{\mathcal{I}(S)} = \mathbf{X}_{\mathcal{I}(S)}\mathbf{Q}$.

Proof. The result follows immediately from Corollary 1 and Lemma 3. □

Theorem 2. *Consider model* (1) *denoted in normalized orthogonal coding for an unreplicated full factorial design in* $N = \prod_{i=1}^n s_i$ *runs, with* s_i *the number of levels for the* i*th factor. For an arbitrary effect "eff", denote the model matrix in any particular choice of normalized orthogonal coding as* $\mathbf{X}_{\mathit{eff}} = \mathbf{U}\mathbf{D}\mathbf{V}_\mathbf{X}^\top$ *and the corresponding coefficient vector as* $\boldsymbol{\beta}_{\mathit{eff}}$*.*
Define $\mathbf{c} = \mathbf{V}_\mathbf{X}^\top\boldsymbol{\beta}_{\mathit{eff}} \Leftrightarrow \boldsymbol{\beta}_{\mathit{eff}} = \mathbf{V}_\mathbf{X}\mathbf{c}$*. Then, the following holds:*

(i) The contribution of effect "eff" to Equation (1) *can be written as* $\mathbf{X}_{\mathit{eff}}\boldsymbol{\beta}_{\mathit{eff}} = \mathbf{U}\mathbf{D}\mathbf{c}$*.*
(ii) For a different normalized orthogonal coding with the model matrix $\widetilde{\mathbf{X}}_{\mathit{eff}}$ *and the corresponding coefficient vector* $\boldsymbol{\gamma}_{\mathit{eff}}$*, there is an SVD* $\widetilde{\mathbf{X}}_{\mathit{eff}} = \mathbf{U}\mathbf{D}\mathbf{V}_{\widetilde{\mathbf{X}}}^\top$ *such that* $\boldsymbol{\gamma}_{\mathit{eff}} = \mathbf{V}_{\widetilde{\mathbf{X}}}\mathbf{c}$ *with the same vector* $\mathbf{c}$*.*

Proof. Part (i) follows from $\mathbf{V}_{\mathbf{X}}^{\top}\mathbf{V}_{\mathbf{X}} = \mathbf{I}_{df(\text{eff})}$ after replacing $\mathbf{X}_{\text{eff}}$ with its SVD and $\boldsymbol{\beta}_{\text{eff}}$ with $\mathbf{V}_{\mathbf{X}}\mathbf{c}$: $\mathbf{X}_{\text{eff}}\boldsymbol{\beta}_{\text{eff}} = \mathbf{U}\mathbf{D}\mathbf{V}_{\mathbf{X}}^{\top}\mathbf{V}_{\mathbf{X}}\mathbf{c} = \mathbf{U}\mathbf{D}\mathbf{c}$. For part (ii), noting that $\widetilde{\mathbf{X}}_{\text{eff}} = \mathbf{X}_{\text{eff}}\mathbf{Q}$ for a suitable orthogonal matrix $\mathbf{Q}$ according to Lemma 2 or Corollary 2, Lemma 3 implies the existence of a $\mathbf{V}_{\widetilde{\mathbf{X}}}$ such that $\widetilde{\mathbf{X}}_{\text{eff}} = \mathbf{U}\mathbf{D}\mathbf{V}_{\widetilde{\mathbf{X}}}^{\top}$. Thus, $\widetilde{\mathbf{X}}_{\text{eff}}\boldsymbol{\gamma}_{\text{eff}} = \mathbf{U}\mathbf{D}\mathbf{V}_{\widetilde{\mathbf{X}}}^{\top}\boldsymbol{\gamma}_{\text{eff}}$. Inserting an identity matrix changes this into $\left(\mathbf{U}\mathbf{D}\mathbf{V}_{\widetilde{\mathbf{X}}}^{\top}\mathbf{V}_{\widetilde{\mathbf{X}}}\mathbf{V}_{\mathbf{X}}^{\top}\right)\left(\mathbf{V}_{\mathbf{X}}\mathbf{V}_{\widetilde{\mathbf{X}}}^{\top}\boldsymbol{\gamma}_{\text{eff}}\right) = \mathbf{X}_{\text{eff}}\mathbf{V}_{\mathbf{X}}\mathbf{V}_{\widetilde{\mathbf{X}}}^{\top}\boldsymbol{\gamma}_{\text{eff}}$. The matrix $\mathbf{X}_{\text{eff}}$ has full column rank, so that equality of both $\mathbf{X}_{\text{eff}}\boldsymbol{\beta}_{\text{eff}}$ and $\mathbf{X}_{\text{eff}}\mathbf{V}_{\mathbf{X}}\mathbf{V}_{\widetilde{\mathbf{X}}}^{\top}\boldsymbol{\gamma}_{\text{eff}}$ to $\mathbf{U}\mathbf{D}\mathbf{c}$ implies the equation $\boldsymbol{\beta}_{\text{eff}} = \mathbf{V}_{\mathbf{X}}\mathbf{V}_{\widetilde{\mathbf{X}}}^{\top}\boldsymbol{\gamma}_{\text{eff}}$, which is equivalent to $\boldsymbol{\gamma}_{\text{eff}} = \mathbf{V}_{\widetilde{\mathbf{X}}}\mathbf{V}_{\mathbf{X}}^{\top}\boldsymbol{\beta}_{\text{eff}} = \mathbf{V}_{\widetilde{\mathbf{X}}}\mathbf{c}$. □

Theorem 2 assumes a full factorial design in order to make sure that all effect model matrices in a full factorial model are of full column rank. The result holds without change for models with fewer runs, if their model matrices are chosen as appropriate subsets of rows of the full factorial model matrices. However, of course, there may be estimability issues with model coefficients due to rank deficiencies. Furthermore, note that the coding invariant representation $\mathbf{c}$ of the coefficient vector is unique up to sign changes only, if all singular values have multiplicity 1; as was mentioned in Section 2, this paper enforces uniqueness by choosing signs such that all column means of matrix $\mathbf{U}$ are non-negative. If there are singular values with multiplicity $r > 1$, there are more difficult ambiguities, because the matrices $\mathbf{U}$ and $\mathbf{V}$ are non-unique (see also Section 5.2); in those cases, matrix $\mathbf{U}$ and vector $\mathbf{c}$ have to be kept together in suitable pairs.

4. The bias of the intercept estimate

Now, assume that we have R factors (R the resolution), model (1) with $n = R$ is the true model, and we wrongly fit the smaller model

$$E(Y) = \mu + \sum_{i=1}^{R}\mathbf{X}_i\boldsymbol{\beta}_i + \sum_{S\subseteq\{1,\dots,R\},2\le|S|\le R-1}\mathbf{X}_{\mathcal{I}(S)}\boldsymbol{\beta}_{\mathcal{I}(S)} \tag{2}$$

omitting the highest order interaction (for $R = 2$, the third summand in (2) is omitted). The estimate for μ is $\bar{Y}$, with expectation $\mu + \mathbf{1}_N^{\top}\mathbf{X}_{\mathcal{I}(\{1,\dots,R\})}\boldsymbol{\beta}_{\mathcal{I}(\{1,\dots,R\})}/N$, i.e., bias $\mathbf{1}_N^{\top}\mathbf{X}_{\mathcal{I}(\{1,\dots,R\})}\boldsymbol{\beta}_{\mathcal{I}(\{1,\dots,R\})}/N$. Note that, because of the design's resolution, the omission of main effects or lower order interactions with any factor would not bias the intercept estimate, i.e., the bias would remain the same if we would, e.g., omit an entire factor instead of omitting only the R factor interaction. Of course, this bias strongly depends on the sizes of the unknown coefficients in $\boldsymbol{\beta}_{\mathcal{I}(\{1,\dots,R\})}$. According to Theorem 2, the effect of the unknown coefficients can be considered in terms of the coding invariant representation through the vector $\mathbf{c}$; it is customary to consider length 1 vectors. Note that $\boldsymbol{\beta} = \mathbf{V}\mathbf{c}$ has length 1 if and only if $\mathbf{c}$ has length 1.

As was already pointed out by Xu and Wu (2001), $a_R(\{1,\dots,R\})$ is an indicator of the bias for the intercept from the R factor interaction. In an overall way, according to Definition 3, $a_R(\{1,\dots,R\})$ is the sum of squares of the multipliers $\mathbf{1}_N^{\top}\mathbf{X}_{\mathcal{I}(\{1,\dots,R\})}/N$ with which the unknown interaction parameters in $\boldsymbol{\beta}_{\mathcal{I}(\{1,\dots,R\})}$ enter the bias; it is thus a Frobenius norm and as such provides an upper bound for the sum of squares of the bias vector: $||\mathbf{1}_N^{\top}\mathbf{X}_{\mathcal{I}(\{1,\dots,R\})}\boldsymbol{\beta}_{\mathcal{I}(\{1,\dots,R\})}/N||_2^2 \le a_R(\{1,\dots,R\})||\boldsymbol{\beta}_{\mathcal{I}(\{1,\dots,R\})}||_2^2$. The bound is exact for the worst-case $\boldsymbol{\beta}_{\mathcal{I}(\{1,\dots,R\})}$ which is collinear to $\mathbf{X}_{\mathcal{I}(\{1,\dots,R\})}^{\top}\mathbf{1}_N$ (because this is collinear to the first right singular vector of the row vector $\mathbf{1}_N^{\top}\mathbf{X}_{\mathcal{I}(\{1,\dots,R\})}$). That worst-case $\boldsymbol{\beta}_{\mathcal{I}(\{1,\dots,R\})}$ (of course) depends on the coding, while the worst-case bias directly depends on the model contribution $\mathbf{U}\mathbf{D}\mathbf{c}$ and is thus coding invariant; the details are given in Lemma 4.

Lemma 4. *Let the true model be model (1) with $n = R$, and $\mathbf{X}_{\mathcal{I}(\{1,\ldots,R\})} = \mathbf{UDV_X}$ the model matrix in normalized orthogonal coding for the interaction $\mathcal{I}(\{1,\ldots,R\})$, $\boldsymbol{\beta}_{\mathcal{I}(\{1,\ldots,R\})} = \mathbf{V_X c}$ the corresponding coefficient vector with $\mathbf{c}$ a $df(\{1,\ldots,R\}) \times 1$ vector, and $\bar{\mathbf{u}} = \mathbf{1}_N^\top \mathbf{U}/N$.*

(i) Then the bias for the estimation of μ by $\bar{Y} = \mathbf{1}_N^\top \mathbf{Y}/N$ can be written as $\bar{\mathbf{u}}\mathbf{Dc} = \sum_{i=1}^{min(N,df(\{1,\ldots,R\}))} c_i\zeta_i\bar{u}_i$ with $\bar{u}_i$ the average of the ith column of matrix $\mathbf{U}$.

(ii) The bias from (i) is coding invariant.

(iii) The worst-case squared bias for a length 1 vector $\boldsymbol{\beta}_{\mathcal{I}(\{1,\ldots,R\})}$ is $\bar{\mathbf{u}}\mathbf{DD}^\top\bar{\mathbf{u}}^\top$ and is attained for $\mathbf{c} = \mathbf{D}^\top\bar{\mathbf{u}}^\top/\sqrt{\bar{\mathbf{u}}\mathbf{DD}^\top\bar{\mathbf{u}}^\top}$.

Proof. In terms of $\mathbf{c}$, the bias can be written as
$\mathbf{1}_N^\top \mathbf{X}_{\mathcal{I}(\{1,\ldots,R\})}\boldsymbol{\beta}_{\mathcal{I}(\{1,\ldots,R\})}/N = \bar{\mathbf{u}}\mathbf{Dc} = \sum_{i=1}^{min(N,df(\{1,\ldots,R\}))} c_i\zeta_i\bar{u}_i$.
Part (ii) follows from Corollary 1 and Theorem 2. For Part (iii), note that the worst case absolute bias for a length 1 $\mathbf{c}$ (representing a length 1 $\boldsymbol{\beta}_{\mathcal{I}(\{1,\ldots,R\})}$) is the singular value of the row vector $\bar{\mathbf{u}}\mathbf{D}$, attained for $\mathbf{c}$ equal to the right singular vector of $\bar{\mathbf{u}}\mathbf{D}$. ☐

Remark. Part (iii) of Lemma 4 provides the vector $\mathbf{c}$ for the coding invariant representation of the worst-case $\boldsymbol{\beta}_{\mathcal{I}(\{1,\ldots,R\})}$ and expresses the worst-case squared bias of $\bar{Y}$ as an estimate for μ in terms of $\mathbf{c}$. Since we already saw that that worst case squared bias equals $a_R(\{1,\ldots,R\})$, part (iii) of Lemma 4 also provides a decomposition of $a_R(\{1,\ldots,R\})$ into the $df(\{1,\ldots,R\})$ coding invariant summands $\zeta_i^2\bar{u}_i^2$, $i = 1,\ldots,df(\{1,\ldots,R\})$. The same decomposition will be obtained below with a related but different reasoning, and the coefficient vectors for which the squared bias equals a particular summand will be given.

According to Lemma 4 (i), the squared bias of $\bar{Y}$ as an estimator for μ can be written as

$$\boldsymbol{\beta}_{\mathcal{I}(\{1,\ldots,R\})}^\top \mathbf{X}_{\mathcal{I}(\{1,\ldots,R\})}^\top \mathbf{1}_N\mathbf{1}_N^\top \mathbf{X}_{\mathcal{I}(\{1,\ldots,R\})}\boldsymbol{\beta}_{\mathcal{I}(\{1,\ldots,R\})}/N^2 = \left(\sum_{i=1}^{min(N,df(\{1,\ldots,R\}))} c_i\zeta_i\bar{u}_i\right)^2. \tag{3}$$

Considering a length 1 $\mathbf{c}$ (corresponding to a length 1 $\boldsymbol{\beta}$), the simplest such choices are $\mathbf{c} = \mathbf{e}_i$, $i = 1,\ldots,df(S)$, for which (3) becomes $(\zeta_i\bar{u}_i)^2$ and $\boldsymbol{\beta}_{\mathcal{I}(\{1,\ldots,R\})}$ equals the ith right singular vector $\mathbf{v}_i$ of $\mathbf{X}_{\mathcal{I}(\{1,\ldots,R\})}$ (depending on the choice of normalized orthogonal coding). The $(\zeta_i\bar{u}_i)^2$ are exactly the summands of the worst case squared bias given in Lemma 4 (iii). The next section states all results on the coding invariant decomposition of $a_j(S)$ for j factor sets S; the generalization from R factor sets of resolution R is a switch from considering the total bias of $\bar{Y}$ as an estimate for μ, which solely consists of the contribution by the interaction $\mathcal{I}(\{1,\ldots,R\})$ to the bias contribution of the interaction $\mathcal{I}(S)$ as one of possibly several bias contributions in a j-factor set S of resolution $R \leq j$.

5. Coding invariant decomposition of $a_j(S)$ and its relation to the bias

This section assembles results on the coding invariant decomposition of $a_j(S)$ and its relation to the bias of $\bar{Y}$ as an estimator for μ from confounding with the highest order interaction $\mathcal{I}(S)$ (Section 5.1). The case of singular values with multiplicity $r > 1$ will be given special treatment in Section 5.2, since such singular values imply nontrivial non-uniqueness of singular vectors, and thus also of the "interaction contributions" to be defined in Section 5.1.

5.1. The decomposition

According to Definition 3, $a_j(S) = \mathbf{1}_N^\top \mathbf{X}_{\mathcal{I}(S)} \mathbf{X}_{\mathcal{I}(S)}^\top \mathbf{1}_N / N^2 = \bar{\mathbf{u}}\mathbf{D}\mathbf{D}^\top \bar{\mathbf{u}}^\top$, with $\bar{\mathbf{u}}$ the row vector of column averages of $\mathbf{U}$. This is an alternative route to the decomposition that was already provided in Lemma 4 (iii). The next theorem summarizes this representation, the relation of the summands to the bias, and the conditions under which the decomposition is unique.

Theorem 3. *Let $\zeta_i = \zeta_i(\mathbf{X}_{\mathcal{I}(S)})$ denote the ith singular value of the matrix $\mathbf{X}_{\mathcal{I}(S)}$, $\bar{u}_i$ the column average of the corresponding ith left singular vector.*

(i) Then the projected $a_j(S)$ value can be decomposed as

$$a_j(S) = \sum_{i=1}^{min(N,df(S))} \zeta_i^2 \bar{u}_i^2. \tag{4}$$

(ii) The summand $\zeta_i^2 \bar{u}_i^2$ of (4) is the contribution of the interaction $\mathcal{I}(S)$ to the squared bias of $\bar{Y}$ as an estimator for μ in case $\boldsymbol{\beta}_{\mathcal{I}(S)} = \mathbf{v}_i$.

(iii) If all non-zero singular values have multiplicity one, the decomposition (4) is unique.

(iv) Assuming there is at least one non-zero singular value ζ_i with multiplicity $r_i > 1$ and corresponding $N \times r_i$ matrix $\mathbf{U}_{sub,i}$ of left singular vectors, the decomposition (4) is unique if and only if $\mathbf{1}_N^\top \mathbf{U}_{sub,i} = \mathbf{0}_{r_i}^\top$ for all such pairs ζ_i and $\mathbf{U}_{sub,i}$.

Proof. Part (i) directly follows from Definition 3 (see above). For part (ii), note that $\mathbf{c} = \mathbf{e}_i$ implies $\boldsymbol{\beta}_{\mathcal{I}(S)} = \mathbf{V}_\mathbf{X}\mathbf{e}_i = \mathbf{v}_i$; the assertion follows from Equation (3). For part (iii), note that, if all non-zero singular values are unique, all corresponding columns of the matrix $\mathbf{U}$ are unique up to sign changes; sign changes do not affect the squared column averages.

Regarding part (iv), a non-zero singular value ζ_i with multiplicity $r_i > 1$ has a corresponding $N \times r_i$ matrix $\mathbf{U}_{\text{sub},i}$ of left singular vectors whose columns are non-unique, as they can be rotated or reflected in arbitrary ways. However, if $\mathbf{1}_N^\top \mathbf{U}_{\text{sub},i} = \mathbf{0}_{r_i}^\top$, the same is also true for all rotated versions $\mathbf{L}_{\text{sub},i} = \mathbf{U}_{\text{sub},i}\mathbf{Q}$, i.e. $\mathbf{1}_N^\top \mathbf{L}_{\text{sub},i} = \mathbf{1}_N^\top \mathbf{0}_{r_i}^\top$. Thus, all the corresponding summands in (4) are zero, regardless of the choice of columns. If this is the case for all matrices of left-singular vectors corresponding to non-zero singular values with multiplicity $r_i > 1$, (4) yields a unique decomposition. Otherwise, the decomposition will change, depending on the arbitrary choice of left singular vectors. □

Definition 4 (interaction contributions)**.** (i) For a set $S \in \mathcal{S}_j$, the terms $\zeta_i^2 \bar{u}_i^2, i = 1, \ldots, df(S)$, are called the interaction contributions for the set. For $N < df(S)$, the last $df(S) - N$ interaction contributions are defined as zeroes. (ii) For an entire design in $n \geq j$ factors, the interaction contributions of all j factor sets $S \in \mathcal{S}_j$ are called the interaction contributions of order j.

The interaction contributions of Definition 4 are coding invariant, but may be non-unique, if there are non-zero singular values with multiplicity larger than 1.

5.2. Resolving ambiguities

In the following, two different but related ways of obtaining unique summands for ambiguous cases in Equation (4) are presented: a concentrated allocation (indexed with "c") concentrates the entire sum of all ambiguous summands from a particular singular value ζ with multiplicity r in a single summand and leaves $r-1$ zero summands; an even allocation (indexed with "e") distributes the sum evenly over r summands. Initially, a remark collects the known facts about rotations of singular spaces for this context.

Remark (rotations). Let ζ be a singular value with multiplicity r for matrix $\mathbf{X}_{\mathcal{I}(S)}$, denoting the $N \times r$ matrix $\mathbf{U}_{\text{sub}}$ and the $df(S) \times r$ matrix $\mathbf{V}_{\text{sub}}$ as the corresponding columns of matrices $\mathbf{U}$ and $\mathbf{V}$. Consider an arbitrary orthogonal $r \times r$ matrix $\mathbf{Q}$ with $\mathbf{L}_{\text{sub}} = \mathbf{U}_{\text{sub}}\mathbf{Q}$ and $\mathbf{M}_{\text{sub}} = \mathbf{V}_{\text{sub}}\mathbf{Q}$, and define $\bar{\mathbf{u}} = \mathbf{1}_N^\top \mathbf{U}/N$ and $\bar{\mathbf{l}} = \mathbf{1}_N^\top \mathbf{L}/N$, with $\bar{\mathbf{u}}_{\text{sub}}$ and $\bar{\mathbf{l}}_{\text{sub}}$ denoting the $1 \times r$ sub vectors corresponding to the singular space of ζ.

(i) $\bar{\mathbf{l}}_{\text{sub}} = \bar{\mathbf{u}}_{\text{sub}}\mathbf{Q}$.
(ii) $\bar{\mathbf{l}}_{\text{sub}} = \mathbf{0}_r$ if and only if $\bar{\mathbf{u}}_{\text{sub}} = \mathbf{0}_r$.
(iii) For $\bar{\mathbf{u}}_{\text{sub}} \neq \mathbf{0}_r$, the total contribution $\zeta^2 \sum_{i=1}^r \bar{l}_{\text{sub},i}^2 = \zeta^2 \bar{\mathbf{l}}_{\text{sub}}^\top \bar{\mathbf{l}}_{\text{sub}} = \zeta^2 \bar{\mathbf{u}}_{\text{sub}}^\top \bar{\mathbf{u}}_{\text{sub}}$ to (4) is unaffected by the choice of $\mathbf{Q}$, while the individual summands can (strongly) depend on $\mathbf{Q}$.
(iv) $\mathbf{X}_{\mathcal{I}(S),\text{sub}} = \zeta \mathbf{U}_{\text{sub}} \mathbf{V}_{\text{sub}}^\top = \zeta \mathbf{L}_{\text{sub}} \mathbf{M}_{\text{sub}}^\top$ is the $N \times df(S)$ summand of $\mathbf{X}_{\mathcal{I}(S)}$ that corresponds to the singular space for ζ; it is invariant to the chosen rotation $\mathbf{Q}$.
(v) The group's contribution to $\mathbf{X}_{\mathcal{I}(S)}\boldsymbol{\beta}_{\mathcal{I}(S)} = \mathbf{UDc_U} = \mathbf{LDc_L}$ can be written as $\mathbf{X}_{\mathcal{I}(S),\text{sub}}\boldsymbol{\beta}_{\mathcal{I}(S)} = \zeta \mathbf{U}_{\text{sub}} \mathbf{c}_{\mathbf{U},\text{sub}} = \zeta \mathbf{L}_{\text{sub}} \mathbf{c}_{\mathbf{L},\text{sub}}$, where $\mathbf{c}_{\mathbf{U},\text{sub}}$ and $\mathbf{c}_{\mathbf{L},\text{sub}}$ denote the suitable $r \times 1$ sub vectors of the rotation dependent vectors $\mathbf{c_U}$ and $\mathbf{c_L}$, respectively.

The following two remarks provide the details for the concentrated or even ICs, respectively.

Remark (the concentrated rotation). Let ζ be a singular value with multiplicity r for matrix $\mathbf{X}_{\mathcal{I}(S)}$, applying all notations as given in the remark on rotations.

(i) $\mathbf{Q}$ can be chosen such that $\bar{\mathbf{l}}_{\text{sub}} = ||\bar{\mathbf{u}}_{\text{sub}}||_2 \mathbf{e}_1^\top$; this is called the concentrated rotation. It can be obtained as $\mathbf{Q}_{\text{c}} = \mathbf{H}^\top$ with $\mathbf{H}$ the Householder transformation matrix that changes the direction of $\bar{\mathbf{u}}_{\text{sub}}$ to collinearity with $\mathbf{e}_1$.
The corresponding summands of (4) are $\zeta^2 ||\bar{\mathbf{u}}_{\text{sub}}||_2^2$ and $r-1$ zeroes.
(ii) For the coefficient vector $\boldsymbol{\beta}_{\mathcal{I}(S)}$, the bias contribution from the group is
$\mathbf{1}_N^\top \mathbf{X}_{\mathcal{I}(S),\text{sub}} \boldsymbol{\beta}_{\mathcal{I}(S)}/N = \zeta \bar{\mathbf{l}}_{\text{sub}} \mathbf{M}_{\text{sub}}^\top \boldsymbol{\beta}_{\mathcal{I}(S)} = \zeta ||\bar{\mathbf{u}}_{\text{sub}}||_2 \mathbf{m}_{\text{sub},1}^\top \boldsymbol{\beta}_{\mathcal{I}(S)}$, where $\mathbf{m}_{\text{sub},1}$ is the first right singular vector in terms of the concentrated rotation for the group (i.e. the first column of $\mathbf{M}_{\text{sub}} = \mathbf{V}_{\text{sub}}\mathbf{H}^\top$). It simplifies to $\zeta ||\bar{\mathbf{u}}_{\text{sub}}||_2 c_{\mathbf{L},\text{sub},1} = \zeta |\bar{l}_{\text{sub},1}| c_{\mathbf{L},\text{sub},1}$.
(iii) Among length 1 vectors $\boldsymbol{\beta}_{\mathcal{I}(S)}$, $\boldsymbol{\beta}_{\mathcal{I}(S)} = \pm \mathbf{m}_{\text{sub},1}$ maximizes the squared bias contribution of the group, and the maximum is $\zeta^2 ||\bar{\mathbf{u}}_{\text{sub}}||_2^2 = \zeta^2 \bar{l}_{\text{sub},1}^2$. The corresponding vector $\mathbf{c_L}$ is the vector $\pm \mathbf{e}_i$ with i the position of the first element of $\mathbf{c}_{\mathbf{L},\text{sub}}$.

The even rotation does the opposite of the concentrated rotation: instead of concentrating the entire contribution on one degree of freedom, it allocates it as evenly as possible. The rotation matrix $\mathbf{Q}_{\text{e}}$ for achieving the even allocation can be obtained by making use of a rectangular r-simplex, which is the generalization of a tri-rectangular tetrahedron to r dimensions: the r "legs" (=edges neighboring the apex) all meet at right angles at the apex; for the special r-simplex used for the even case, the apex is the origin $\mathbf{0}_r$, and all legs have length 1, which implies that the base of the r-simplex is a regular $r-1$-simplex, e.g., an equilateral triangle in case $r = 3$. The altitude of such a rectangular r-simplex has the same angle $acos(1/\sqrt{r})$ to all legs and has length $1/\sqrt{r}$, and the average of all legs equals the altitude; a prototype of such an r-simplex has the vertices $\mathbf{0}_r$, $\mathbf{e}_1$, ..., $\mathbf{e}_r$, where the unit vectors are in r-dimensional space (the base of this

r-simplex is called the "standard simplex" in dimension $r-1$). The following remark will be based on a matrix $\mathbf{R}$ whose columns consist of the r vertices (except for the apex $\mathbf{0}_r$) of a rectangular r-simplex oriented such that the altitude is collinear to $\mathbf{e}_1$; these vertices also define the r legs of length 1, and they yield an orthogonal matrix. The base point of the altitude of this simplex is $\mathbf{e}_1/\sqrt{r}$ (implying that this is also the average of the columns of $\mathbf{R}$), and the simplex is then rotated such that the altitude becomes collinear with the vector $\bar{\mathbf{u}}$. Note that there are infinitely many possible matrices $\mathbf{R}$ belonging to a rectangular r-simplex with length 1 legs, apex $\mathbf{0}_r$ and altitude collinear to $\mathbf{e}_1$, because there are infinitely many possible rotations. This implies that – though the even interaction contributions are unique – the corresponding pairs of singular vectors are not.

Remark (the even rotation). Let ζ be a singular value with multiplicity r for matrix $\mathbf{X}_{\mathcal{I}(S)}$, applying all notations as given in the remark on rotations.

(i) $\mathbf{Q}$ can be chosen such that $\bar{\mathbf{l}}_{\text{sub}} = ||\bar{\mathbf{u}}_{\text{sub}}||_2 \mathbf{1_r}^\top/\sqrt{r}$; this is called the even rotation. It can be obtained as $\mathbf{Q}_{\text{e}} = \mathbf{H}^\top\mathbf{R}$, where $\mathbf{H}^\top$ is the inverse of the Householder transformation matrix that changes the direction of $\bar{\mathbf{u}}_{\text{sub}}$ to collinearity with $\mathbf{e}_1$ (see remark on the concentrated rotation) and $\mathbf{R}$ is an orthogonal matrix composed of the length 1 legs of a rectangular r-simplex with apex $\mathbf{0}_r$ and altitude collinear to $\mathbf{e}_1$. This achieves an equal angle of $\bar{\mathbf{u}}_{\text{sub}}^\top$ to all columns of $\mathbf{Q}_{\text{e}}$, and an equal angle of $\mathbf{1}_N$ to all columns of $\mathbf{L}_{\text{sub}} = \mathbf{U}_{\text{sub}}\mathbf{Q}_{\text{e}}$.

(ii) For the coefficient vector $\boldsymbol{\beta}_{\mathcal{I}(S)}$, the bias contribution of the group in terms of the even rotation is $\mathbf{1}_N^\top\mathbf{X}_{\mathcal{I}(S),\text{sub}}\boldsymbol{\beta}_{\mathcal{I}(S)}/N = \zeta\bar{\mathbf{l}}_{\text{sub}}\mathbf{M}_{\text{sub}}^\top\boldsymbol{\beta}_{\mathcal{I}(S)} = \zeta||\bar{\mathbf{u}}_{\text{sub}}||_2\mathbf{1}_N\mathbf{M}_{\text{sub}}^\top\boldsymbol{\beta}_{\mathcal{I}(S)}/\sqrt{r}$. It simplifies to $\zeta\bar{\mathbf{l}}_{\text{sub}}\mathbf{c}_{\mathbf{L},\text{sub}}$.

(iii) Each length 1 vector $\boldsymbol{\beta}_{\mathcal{I}(S)} = \pm\mathbf{m}_{\text{sub},i}$, $i = 1, \ldots, r$, has the same squared bias contribution $||\bar{\mathbf{u}}_{\text{sub}}||_2^2/r$; the vectors $\mathbf{c}$ corresponding to these contributions are suitably chosen unit vectors.

(iv) The normalized average of the r vectors from (iii), i.e., any vector $\boldsymbol{\beta}_{\mathcal{I}(S)} = \mathbf{M}_{\text{sub}}\text{diag}_r(\pm 1)\mathbf{1}_r/\sqrt{r}$, maximizes the squared bias contribution of the group among all length 1 vectors, where $\text{diag}_r(\pm 1)$ denotes an r-dimensional diagonal matrix whose diagonal elements are arbitrary combinations of "$+1$" or "-1" values. The maximum is (of course) identical to that given for the concentrated case ($\zeta^2||\bar{\mathbf{u}}_{\text{sub}}||_2^2$). The maximizing length 1 vector $\mathbf{c}_{\mathbf{L}}$ has zeroes everywhere, except for $\mathbf{c}_{\mathbf{L},\text{sub}} = \mathbf{1}_r^\top/\sqrt{r}$.

The final remark of this section discusses the relation between the two cases.

Remark (relation between concentrated and even rotations). Let ζ be a singular value with multiplicity r for matrix $\mathbf{X}_{\mathcal{I}(S)}$, applying all notations as given in the remark on rotations, and add suffixes "c" and "e" for the concentrated and even case, respectively.

(i) The group's normalized average right singular vector $\mathbf{M}_{\text{sub.e}}\mathbf{1}_r/\sqrt{r}$ of the even rotation (see part (iv) of the remark on the even rotation, where all permissible sign changes were included through the diagonal matrix) coincides with the group's first right singular vector $\mathbf{m}_{\text{sub,c,1}}$ of the concentrated rotation.

(ii) Part (i) of this remark holds for all corresponding pairs of $\mathbf{M}_{\text{sub.e}}$ and $\mathbf{m}_{\text{sub,c,1}}$. Note in particular that non-identity diagonal matrices in part (iv) of the remark on the even rotation correspond to a modified $\mathbf{M}_{\text{sub,e}}$ with an identity matrix instead, implying modified $\mathbf{L}_{\text{sub,e}}$, $\mathbf{M}_{\text{sub,c}}$ and $\mathbf{L}_{\text{sub,c}}$, and the identical maximum $\zeta^2||\bar{\mathbf{u}}||_2^2$.

Proof. Let $\mathbf{H}$ denote the Householder transformation introduced for the concentrated rotation, $\mathbf{R}$ a matrix derived from a rectangular r-simplex as introduced for the even case. Then, according to the previous remarks, $\mathbf{L}_{\text{sub,c}} = \mathbf{U}\mathbf{H}^\top$ and $\mathbf{L}_{\text{sub,e}} = \mathbf{U}\mathbf{H}^\top\mathbf{R} = \mathbf{L}_{\text{sub,c}}\mathbf{R}$ as well as $\mathbf{M}_{\text{sub,c}} = \mathbf{V}\mathbf{H}^\top$ and $\mathbf{M}_{\text{sub,e}} = \mathbf{V}\mathbf{H}^\top\mathbf{R} = \mathbf{M}_{\text{sub,c}}\mathbf{R}$. Furthermore, the coincidences $\mathbf{L}_{\text{sub,e}}\mathbf{1}_r/\sqrt{r} = \mathbf{l}_{\text{sub,c,1}}$ and $\mathbf{M}_{\text{sub,e}}\mathbf{1}_r/\sqrt{r} = \mathbf{m}_{\text{sub,c,1}}$ result from $\mathbf{l}_{\text{sub,c,1}} = \mathbf{L}_{\text{sub,c}}\mathbf{e}_1$ and $\mathbf{m}_{\text{sub,c,1}} = \mathbf{M}_{\text{sub,c}}\mathbf{e}_1$, together with the fact that $\mathbf{R}\mathbf{1}_r/\sqrt{r}$ is $\sqrt{r}$ times the average of the legs of the r-simplex that defined $\mathbf{R}$; this average is the altitude $\mathbf{e}_1/\sqrt{r}$. ☐

Table 1: Example design in two 2-level factors and one 4-level factor, with ICFTs.

	1	2	3	4	5	6	7	8
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

	0	1/3	1
concentrated	2	0	1
even	0	3	0

5.3. Interaction contribution frequency tables

The interaction contributions of Definition 4 lend themselves to tabulation and can be used for assessing how the bias depends on the vector of interaction coefficients as well as for distinguishing non-isomorphic designs with the same projected a_j values. It will be most interesting to consider such tables for projected a_R values, with R the resolution of the design. Contrary to the decomposition results from Grömping and Xu (2014), however, this decomposition works for projected a_j values with arbitrary j; the statistical interpretation as a bias contribution works as well, if it is acknowledged that this is not the only contribution towards the bias of $\bar{Y}$ for μ.

Definition 5 (interaction contribution frequency tables)**.** The table of the $(\zeta_i \bar{u}_i)^2$ obtained from all sets $S \in \mathcal{S}_j$, with uniqueness enforced as indicated in Section 5.2 (if necessary), is called the Interaction Contribution Frequency Table of order j, or $ICFT_{\mathrm{j}}$; it comes in the versions $ICFT_{j,\mathrm{c}}$ and $ICFT_{j,\mathrm{e}}$, with “c” short for concentrated and “e” short for even.

6. Examples

This section gives several examples. Where possible (i.e., for symmetric designs), $MAFT$s by Fontana et al. (2016) are calculated in addition to $ICFT_{\mathrm{c}}$ and $ICFT_{\mathrm{e}}$. In most cases, PFT_R are given as well, with R the resolution (for an R factor set, PFT_R reduces to an indicator for a_R). For some smaller designs, the worst case interaction parameter vectors according to Lemma 4 are also given; these are sometimes but not always simply the first right singular vectors of the concentrated rotation; Example 5 contains a different case. Some of the designs are at least “generalized regular” or “Abelian group regular” (see Kobilinski, Monod and Bailey in press; Grömping and Bailey 2016). They are simply called “regular” in the sequel. Calculations of PFTs and $ICFT$s have been done with R package DoE.base (Grömping 2016), while $MAFT$s have been calculated with separate R functions.

The first worked example uses the design given in Table 2 of Grömping and Xu (2014), which is given in Table 1 for convenience, together with both types of $ICFT$.

Example 1. $A_3 = a_3(\{1,2,3\}) = 1$ for the regular design of Table 1: the AB interaction is completely confounded with the 0/2 vs 1/3 contrast of factor C. This implies the $ICFT$s as shown in the table. Factors A and B are coded as -1/+1 (unique normalized orthogonal coding), factor C is coded with normalized Helmert coding. With $S = \{1,2,3\}$, the coding-dependent 8×3 matrix $\mathbf{X}_{\mathcal{I}(S)}$ and its coding invariant 8×8 cross product $\mathbf{X}_{\mathcal{I}(S)}\mathbf{X}_{\mathcal{I}(S)}^\top$ are given in Table 2. The three non-zero eigen values of $\mathbf{X}_{\mathcal{I}(S)}\mathbf{X}_{\mathcal{I}(S)}^\top$, equal to the non-zero squared singular values of $\mathbf{X}_{\mathcal{I}(S)}$, are equal to $(8,8,8)$, i.e. there are three non-unique pairs of singular vectors. With the SVD algorithm used in R for Windows, the initial squared column means of the matrix $\mathbf{U}$ are $(1/48, 1/16, 1/24)$; the contributions to $a_3(S)$ are thus 8 times these values, i.e., $(1/6, 1/2, 1/3)$.

Table 2: Model matrix and coding invariant outer product for the design of Table 1.

A1:B1:C1	A1:B1:C2	A1:B1:C3	1	2	3	4	5	6	7	8
-1.414214	-0.8164966	-0.5773503	3	-1	1	1	1	1	-1	3
0.000000	1.6329932	-0.5773503	-1	3	1	1	1	1	3	-1
-1.414214	0.8164966	0.5773503	1	1	3	-1	-1	3	1	1
0.000000	0.0000000	-1.7320508	1	1	-1	3	3	-1	1	1
0.000000	0.0000000	-1.7320508	1	1	-1	3	3	-1	1	1
-1.414214	0.8164966	0.5773503	1	1	3	-1	-1	3	1	1
0.000000	1.6329932	-0.5773503	-1	3	1	1	1	1	3	-1
-1.414214	-0.8164966	-0.5773503	3	-1	1	1	1	1	-1	3

Table 3: Coding invariant outer product for regular 9 run design in three 3-level factors.

1	2	3	4	5	6	7	8	9
8	2	2	2	-1	2	2	2	-1
2	8	2	2	2	-1	-1	2	2
2	2	8	-1	2	2	2	-1	2
2	2	-1	8	2	2	2	-1	2
-1	2	2	2	8	2	2	2	-1
2	-1	2	2	2	8	-1	2	2
2	-1	2	2	2	-1	8	2	2
2	2	-1	-1	2	2	2	8	2
-1	2	2	2	-1	2	2	2	8

Concentrating the entire contribution on the first vector, $ICFT_{3,\mathrm{c}}$ shows the sum "1" from these as a single entry "1" and two zeroes for the remaining contributions, while distributing the contribution evenly, $ICFT_{3,\mathrm{e}}$ shows three 1/3 values instead. The right singular vector related to the only non-zero singular value in the concentrated case is $\mathbf{v}_1 = \left(-\sqrt{1/2}, \sqrt{1/6}, -\sqrt{1/3}\right)^\top$, i.e. with this coding, the largest bias on the intercept resulting from the three factor interaction occurs for coefficient vectors proportional to this $\mathbf{v}_1$. The even vectors are non-unique, but their normalized average coincides with the above $\mathbf{v}_1$.

Example 2: Consider a regular design in 9 runs with three 3-level factors and an interaction model matrix as given in Example 1 of Grömping and Xu (2014), for which $A_3 = a_3(\{1,2,3\}) = 2$. With $S = \{1,2,3\}$, the coding invariant cross product $\mathbf{X}_{\mathcal{I}(S)}\mathbf{X}_{\mathcal{I}(S)}^\top$ is given in Table 3. The eigen values of $\mathbf{X}_{\mathcal{I}(S)}\mathbf{X}_{\mathcal{I}(S)}^\top$, equal to the first 8 squared singular values of $\mathbf{X}_{\mathcal{I}(S)}$, are $\zeta_1^2 = 18$, $\zeta_2^2 = \cdots = \zeta_7^2 = 9$, $\zeta_8^2 = 0$, i.e. there are two unique and six non-unique pairs of singular vectors. In this case, $\bar{\mathbf{u}} = (1/3, 0, 0, 0, 0, 0, 0, 0)$. Thus, the non-uniqueness of the second to seventh pairs of singular vectors is irrelevant (see Theorem 3 (iv)), and we obtain a unique $ICFT_3$ that shows one interaction contribution $18/9 = 2$ and seven zeroes. The right singular vector corresponding to the non-zero contribution is $(-0.433, -0.25, -0.25, 0.433, 0.25, -0.433, -0.433, -0.25)^\top$ (rounded to three digits), i.e. the most harmful coefficient vectors in terms of bias for the intercept are proportional to this vector for the coding used. For this symmetric 3-level design, the mean aberrations by Fontana et al. (2016) are well-defined and coding invariant; they consist of two ones and six zeroes.

Example 3: Table 4 shows the two non-isomorphic GMA designs for two 4-level factors in 8 runs; both have A_2=1, and the first one is regular. The table shows that they can be distinguished by their $ICFT_{2,\mathrm{e}}$ but not by their $ICFT_{2,\mathrm{c}}$. The worst case length 1 parameter vectors are again obtainable as the first right singular

Table 4: Two resolution II designs in two 4-level factors (d_1=(A,B1) and d_2=(A,B2)), with metrics.

A	B1	B2			0	1/12	1/6	1/5	1/3	1
0	0	0	d_1	$ICFT_{\mathrm{c}}$	8	0	0	0	0	1
0	1	1		$ICFT_{\mathrm{e}}$	4	0	0	5	0	0
1	2	2		$MAFT_{\mathrm{orig.}}$	7	0	0	0	2	0
1	3	3		$MAFT_{\mathrm{swapped}}$	5	0	4	0	0	0
2	0	0	d_2	$ICFT_{\mathrm{c}}$	8	0	0	0	0	1
2	1	3		$ICFT_{\mathrm{e}}$	6	0	0	0	3	0
3	2	1		$MAFT_{\mathrm{orig.}}$	3	4	2	0	0	0
3	3	2		$MAFT_{\mathrm{swapped}}$	7	0	0	0	2	0

Table 5: Metrics for L18, entire design (left) and symmetric portion (right).

	0	1/6	1/2	2/3	1	2
PFT	12	0	28	9	6	1
$ICFT_{\mathrm{c}}$	320	0	28	9	6	1
$ICFT_{\mathrm{e}}$	287	36	40	0	0	1

	0	1/4	1/2	1	2
PFT	0	0	28	6	1
$ICFT_{\mathrm{c}}$	245	0	28	6	1
$ICFT_{\mathrm{e}}$	239	0	40	0	1
$MAFT$	198	80	0	2	0

vectors (not shown). The mean aberrations depend on the level allocation: the table shows the *MAFT*s for the printed designs and for a version with levels 1 and 2 in factor A swapped. Also note that the mean aberrations do not sum to the overall A_2 in this case (their sum is only 2/3 for both designs with both level allocations); it was already mentioned by Fontana et al. (2016) that mean aberrations are only guaranteed to sum to the generalized word count if the number of factor levels is a prime.

Example 3 underlines the fact that *MAFT*s for designs with factors at more than three levels depend on the level coding, which was already mentioned in the introduction for one of the 5-level designs investigated by Fontana et al. For both of these 5-level designs, $ICFT_{3,\mathrm{e}}$ and $ICFT_{3,\mathrm{c}}$ coincide with each other, and the two unique *ICFT*s are also identical (63 zeroes and one “4” each).

Example 4: Table 5 shows metrics for the classical L18, which is a mixed level design, and for its symmetric portion of seven 3-level factors. For the entire design, there is no *MAFT*, since *MAFT*s have so far not been defined for mixed-level designs. Note that the concentrated *ICFT* in this case yields exactly one non-zero IC from each projection, i.e. the non-zero entries of $ICFT_{3,\mathrm{c}}$ coincide with those of PFT_3. When changing from concentrated to even *ICFT*, the “1” entries are from a group of two identical singular values, so that they turn into two “1/2” entries each, while the “2/3” are from a group of four identical singular values and thus turn into four “1/6” entries each. The entry “2” corresponds to a unique singular value and thus remains intact. For the symmetric portion, a_3 values are “1/2”, “1” or “2” (the “2/3” came from mixed level projections). The *MAFT* reflects that mean aberrations split the a_3 values into even smaller portions than the even *ICFT*: the entries that were not split by *ICFT* (“1/2” and “2” entries) are split into two halves each, the “1” entries that were split into two halves by $ICFT_{\mathrm{e}}$ are split into four “1/4” entries each by mean aberrations.

For designs with $n > R$ factors, the behavior of PFT_R, $ICFT_R$ and $MAFT_R$ is entirely driven by the behaviors of the $\binom{n}{R}$ R factor sets. For the last two examples, we therefore consider a_3 values, *ICFT*s and *MAFT*s for 3 factor sets only; furthermore, we only consider pure-level designs with 3-level factors, for which both *ICFT*s and *MAFT*s can be calculated and are coding invariant. Example 5 considers a particular 36 run

Table 6: Columns 13 to 15 from the 36 run Taguchi orthogonal array (cell entries are levels of factor C).

A\B	0	1	2
0	0,0,0,1	0,2,2,2	1,1,1,2
1	0,2,2,2	1,1,1,2	0,0,0,1
2	1,1,1,2	0,0,0,1	0,2,2,2

	0	0.201	7/16	0.674	7/8
a_3	0	0	0	0	1
$ICFT_\mathrm{c}$	6	1	0	1	0
$ICFT_\mathrm{e}$	6	1	0	1	0
$MAFT$	6	0	2	0	0

design with three 3-level factors, for which the concentrated and even *ICFT* coincide but involve more than one singular vector. This example is interesting both for *ICFT* itself and for comparing *ICFT* with *MAFT*; Example 6 considers all non-isomorphic 36 run designs with three 3-level factors.

Example 5: Table 6 shows columns 13 to 15 of the well-known Taguchi 36 run orthogonal array (see NIST / Sematech 2016), together with its metrics; this design has $a_3 = 7/8 = 0.875$ and is isomorphic to one of the non-isomorphic 24 designs to be considered in the next example. Both *ICFT*s yield the same unequal non-zero subdivision of the a_3 value into ICs ($0.201 + 0.674 = 0.875$), while the mean aberrations subdivide 7/8 into two equal non-zero portions. Such comparisons between *ICFT*s and *MAFT*s may eventually help understand the difference between the methods. Let us consider more detail for the *ICFT* of this design: the length 1 parameter vectors that correspond to the individual bias contributions of the larger and smaller positive ICs are $(-0.083, -0.493, -0.493, 0.083, -0.493, 0.083, 0.083, 0.493)^\top$ and $(0.493, -0.083, -0.083, -0.493, -0.083, -0.493, -0.493, 0.083)^\top$, respectively. The entire bias potential of the three-factor interaction from this design is activated for the length 1 parameter vector $\boldsymbol{\beta}_{\mathcal{I}(\{1,\dots,3\})} = \mathbf{Vc}$ with the $\mathbf{c}$ from Lemma 4 (iii), yielding $(0.164, -0.472, -0.472, -0.164, -0.472, -0.164, -0.164, 0.472)^\top$ (weighted average of the previous two vectors with unequal weights). As the design appears to be quite imbalanced (it consists of one Latin square replicated three times combined with another Latin square replicated once), the imbalanced behavior of *ICFT* appears adequate. It is conjectured that average aberration, by averaging over permutations of the levels of interaction columns, removes some of the imbalance, while *ICFT* keeps it intact, leading to an unequal subdivision of the a_3 value. The exact nature of this behavior remains to be studied.

Example 6: There are 24 non-isomorphic 36 run designs in three 3-level factors, obtained from Pieter Eendebak. Tables 6 to 10 provide their a_3 values and *ICFT* and *MAFT* and their ranks in terms of a_3; the designs have been arranged in four groups of similar patterns plus the singleton of Table 6 (isomorphic to the design tabulated by Pieter Eendebak, rank 20 in terms of a_3). There are instances of coincidence between concentrated and even ICs, and instances where even ICs are halves, thirds or quarters of concentrated ICs, and there are many instances for which mean aberrations coincide with even ICs or are halves of even ICs, but also instances for which mean aberrations provide entirely different splits of the a_3 value from even ICs (see also Example 5).

The 24 designs contain three groups that cannot be distinguished by their a_3 values: three times $a_3 = 5/12$ (one in Table 8 and two in Table 9), five times $a_3 = 1/2$ (all in Table 7) and three times $a_3 = 2/3$ (one each in Tables 8, 9 and 10). The latter can be distinguished by both versions of *ICFT* and by *MAFT*, the designs with $a_3 = 5/12$ from Table 9 cannot be distinguished by any of the metrics, while they can be distinguished from the one in Table 8 by both versions of *ICFT* and by *MAFT*. For the five arrays with $a_3 = 1/2$, things are more complicated: numbering the designs from 1 to 5 in the order of appearance in Table 7, designs 1 and 5 cannot be distinguished by any of the metrics; *MAFT* groups these two together with design 2 and distinguishes this triple from the two singletons 3 and 4, while $ICFT_\mathrm{c}$ groups them together with design 4

Table 7: Metrics for non-isomorphic 36 run 3^3 designs, Part I (denominators 2^a, $a \in \mathbb{N}_0$).

rank	metric	0	1/32	1/16	3/32	1/8	3/16	1/4	3/8	1/2	9/16	5/8	3/4	1	9/8	5/4	2
24	a_3	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1
24	$ICFT_c$	7	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1
24	$ICFT_e$	7	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1
24	$MAFT$	6	.	.	.	.	.	.	.	.	.	.	.	2	.	.	.
23	a_3	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	.
23	$ICFT_c$	6	.	.	.	1	.	.	.	.	.	.	.	.	1	.	.
23	$ICFT_e$	6	.	.	.	1	.	.	.	.	.	.	.	.	1	.	.
23	$MAFT$	4	.	2	.	.	.	.	.	.	2	.	.	.	.	.	.
22	a_3	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.
22	$ICFT_c$	7	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.
22	$ICFT_e$	6	.	.	.	.	.	.	.	2	.	.	.	.	.	.	.
22	$MAFT$	4	.	.	.	.	.	4	.	.	.	.	.	.	.	.	.
19	a_3	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.	.
19	$ICFT_c$	6	.	.	.	.	.	1	.	1	.	.	.	.	.	.	.
19	$ICFT_e$	5	.	.	.	2	.	.	.	1	.	.	.	.	.	.	.
19	$MAFT$	2	.	4	.	.	.	2	.	.	.	.	.	.	.	.	.
15	a_3	.	.	.	.	.	.	.	.	.	.	1	.	.	.	.	.
15	$ICFT_c$	6	.	.	.	1	.	.	.	1	.	.	.	.	.	.	.
15	$ICFT_e$	6	.	.	.	1	.	.	.	1	.	.	.	.	.	.	.
15	$MAFT$	4	.	2	.	.	.	2	.	.	.	.	.	.	.	.	.
9	a_3	.	.	.	.	.	.	.	.	1	.	.	.	.	.	.	.
9	$ICFT_c$	7	.	.	.	.	.	.	.	1	.	.	.	.	.	.	.
9	$ICFT_e$	4	.	.	.	4	.	.	.	.	.	.	.	.	.	.	.
9	$MAFT$	.	.	8	.	.	.	.	.	.	.	.	.	.	.	.	.
9	a_3	.	.	.	.	.	.	.	.	1	.	.	.	.	.	.	.
9	$ICFT_c$	6	.	.	.	1	.	.	1	.	.	.	.	.	.	.	.
9	$ICFT_e$	.	4	.	4	.	.	.	.	.	.	.	.	.	.	.	.
9	$MAFT$	.	.	8	.	.	.	.	.	.	.	.	.	.	.	.	.
9	a_3	.	.	.	.	.	.	.	.	1	.	.	.	.	.	.	.
9	$ICFT_c$	5	.	.	.	1	2	.	.	.	.	.	.	.	.	.	.
9	$ICFT_e$	5	.	.	.	1	2	.	.	.	.	.	.	.	.	.	.
9	$MAFT$	4	.	2	.	.	2	.	.	.	.	.	.	.	.	.	.
9	a_3	.	.	.	.	.	.	.	.	1	.	.	.	.	.	.	.
9	$ICFT_c$	7	.	.	.	.	.	.	.	1	.	.	.	.	.	.	.
9	$ICFT_e$	7	.	.	.	.	.	.	.	1	.	.	.	.	.	.	.
9	$MAFT$	6	.	.	.	.	.	2	.	.	.	.	.	.	.	.	.
9	a_3	.	.	.	.	.	.	.	.	1	.	.	.	.	.	.	.
9	$ICFT_c$	7	.	.	.	.	.	.	.	1	.	.	.	.	.	.	.
9	$ICFT_e$	4	.	.	.	4	.	.	.	.	.	.	.	.	.	.	.
9	$MAFT$	.	.	8	.	.	.	.	.	.	.	.	.	.	.	.	.
3	a_3	.	.	.	.	.	.	1	.	.	.	.	.	.	.	.	.
3	$ICFT_c$	7	.	.	.	.	.	1	.	.	.	.	.	.	.	.	.
3	$ICFT_e$	6	.	.	.	2	.	.	.	.	.	.	.	.	.	.	.
3	$MAFT$	4	.	4	.	.	.	.	.	.	.	.	.	.	.	.	.
1	a_3	.	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.
1	$ICFT_c$	7	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.
1	$ICFT_e$	7	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.
1	$MAFT$	6	.	2	.	.	.	.	.	.	.	.	.	.	.	.	.

Table 8: Metrics for non-isomorphic 36 run 3^3 designs, Part I (denominators $2^a 3^b$, $a, b \in \mathbb{N}_0$).

rank	metric	0	1/48	1/24	1/16	1/12	1/8	1/6	1/4	7/24	1/3	3/8	5/12	2/3
16	a_3	.	.	.	.	.	.	.	.	.	.	.	.	1
16	$ICFT_{\mathrm{c}}$	6	.	.	.	.	.	.	.	.	2	.	.	.
16	$ICFT_{\mathrm{e}}$	.	.	.	.	8	.	.	.	.	.	.	.	.
16	$MAFT$	.	.	.	.	8	.	.	.	.	.	.	.	.
6	a_3	.	.	.	.	.	.	.	.	.	.	.	1	.
6	$ICFT_{\mathrm{c}}$	4	.	2	.	.	.	2	.	.	.	.	.	.
6	$ICFT_{\mathrm{e}}$	.	4	.	.	4	.	.	.	.	.	.	.	.
6	$MAFT$	.	4	.	.	4	.	.	.	.	.	.	.	.
5	a_3	.	.	.	.	.	.	.	.	.	.	1	.	.
5	$ICFT_{\mathrm{c}}$	6	.	.	.	.	1	.	1	.	.	.	.	.
5	$ICFT_{\mathrm{e}}$	2	.	3	.	3	.	.	.	.	.	.	.	.
5	$MAFT$	2	.	.	6	.	.	.	.	.	.	.	.	.
4	a_3	.	.	.	.	.	.	.	.	1	.	.	.	.
4	$ICFT_{\mathrm{c}}$	4	.	.	2	2	.	.	.	.	.	.	.	.
4	$ICFT_{\mathrm{e}}$	.	6	.	.	2	.	.	.	.	.	.	.	.
4	$MAFT$	.	6	.	.	2	.	.	.	.	.	.	.	.
2	a_3	.	.	.	.	.	.	1	.	.	.	.	.	.
2	$ICFT_{\mathrm{c}}$	6	.	.	.	2	.	.	.	.	.	.	.	.
2	$ICFT_{\mathrm{e}}$	.	8	.	.	.	.	.	.	.	.	.	.	.
2	$MAFT$	.	8	.	.	.	.	.	.	.	.	.	.	.

Table 9: Metrics for non-isomorphic 36 run 3^3 designs, Part III.

rank	metric	0	1/48	0.023	1/24	0.046	1/16	1/12	7/48	0.269	5/12	0.537	13/24	2/3
16	a_3	.	.	.	.	.	.	.	.	.	.	.	.	1
16	$ICFT_{\mathrm{c}}$	4	.	.	2	1	.	.	.	.	.	1	.	.
16	$ICFT_{\mathrm{e}}$	.	4	2	.	.	.	.	.	2	.	.	.	.
16	$MAFT$	.	4	.	.	.	.	.	4	.	.	.	.	.
14	a_3	.	.	.	.	.	.	.	.	.	.	.	1	.
14	$ICFT_{\mathrm{c}}$	2	.	1	2	.	.	2	.	1	.	.	.	.
14	$ICFT_{\mathrm{e}}$	.	4	1	.	.	.	2	.	1	.	.	.	.
14	$MAFT$	.	4	.	.	.	.	2	2	.	.	.	.	.
6	a_3	.	.	.	.	.	.	.	.	.	1	.	.	.
6	$ICFT_{\mathrm{c}}$	4	.	1	.	.	2	.	.	1	.	.	.	.
6	$ICFT_{\mathrm{e}}$	.	6	1	.	.	.	.	.	1	.	.	.	.
6	$MAFT$	.	6	.	.	.	.	.	2	.	.	.	.	.
6	a_3	.	.	.	.	.	.	.	.	.	1	.	.	.
6	$ICFT_{\mathrm{c}}$	4	.	1	.	.	2	.	.	1	.	.	.	.
6	$ICFT_{\mathrm{e}}$	.	6	1	.	.	.	.	.	1	.	.	.	.
6	$MAFT$	.	6	.	.	.	.	.	2	.	.	.	.	.

Table 10: Metrics for non-isomorphic 36 run 3^3 designs, Part IV.

rank	metric	0	1/48	0.023	1/16	0.091	13/48	19/48	23/51	2/3	0.768	11/12
21	a_3	.	.	.	.	.	.	.	.	.	.	1
21	$ICFT_\mathrm{c}$	4	.	1	2	.	.	.	.	.	1	.
21	$ICFT_\mathrm{e}$	.	6	1	.	.	.	.	.	.	1	.
21	$MAFT$	.	6	.	.	.	.	2	.	.	.	.
16	a_3	.	.	.	.	.	.	.	.	1	.	.
16	$ICFT_\mathrm{c}$	4	.	.	2	1	.	.	1	.	.	.
16	$ICFT_\mathrm{e}$	.	6	.	.	1	.	.	1	.	.	.
16	$MAFT$	.	6	.	.	.	2	.	.	.	.	.

and distinguishes this triple from the two singletons 2 and 3. $ICFT_\mathrm{e}$ is able to distinguish three singletons from the two indistinguishable designs, i.e. has the best discriminatory power among the three approaches. As a matter of interest, note that the *SCFT* introduced by Grömping (in press) based on Grömping and Xu (2014) cannot distinguish designs 2 and 4 but can distinguish these two from three singletons; thus, with any of the *ICFT*s or *MAFT*s in combination with *SCFT*s, non-isomorphism of all five designs can be established. *SCFT*s can also distinguish the two designs with $a_3 = 5/12$ from Table 9.

7. Discussion

This paper has introduced interaction contributions and the related *ICFT*s for a new coding invariant single degree of freedom decomposition of generalized word counts A_j according to Xu and Wu (2001). *ICFT*s can be used for ascertaining absence of combinatorial equivalence. Two auxiliary results are of interest in their own right: under normalized orthogonal coding, the outer cross product matrices $\mathbf{X}_{\mathcal{I}(S)}\mathbf{X}_{\mathcal{I}(S)}^\top$ are coding invariant, and the vector $\boldsymbol{\beta}_{\mathcal{I}(S)}$ of model coefficients can be expressed in a coding invariant way in terms of the vector $\mathbf{c}$ of linear combination coefficients for the right singular vectors of the matrix $\mathbf{X}_{\mathcal{I}(S)}$.

*ICFT*s decompose $a_j(S)$ from a j factor set S into $df(S)$ contributions (with $df(S)$ the degrees of freedom for the j factor interaction $\mathcal{I}(S)$ in a full factorial design); for symmetric designs, the *MAFT*s by Fontana et al. are another method of decomposing $a_j(S)$ into $df(S)$ contributions. However, while *ICFT*s are coding invariant, regardless of the situation, *MAFT*s are coding invariant for designs with factors at two or three levels only. Where applicable and coding invariant, *MAFT*s and *ICFT*s have the potential to distinguish non-isomorphic designs, for which projected a_j values are the same. *ICFT*s, while being applicable and coding invariant in far more situations than *MAFT*s, have far worse computing times than *MAFT*s, at least in the author's implementation. It is thus worthwhile to investigate how *MAFT*s are related to *ICFT*s, hoping that this leads to an easily calculable coding invariant metric for (not necessarily symmetric) designs with factors at more than three levels.

As was already mentioned, the *SCFT*s introduced by Grömping (in press) based on Grömping and Xu (2014) also support distinguishing combinatorially non-equivalent j-factor designs with identical a_j values: they decompose projected a_R values (R the resolution) based on the relation of main effects to $R-1$ factor interactions and are interpretable in terms of bias risks for main effect estimates. Besides for non-isomorphism detection, they are therefore also interesting for the assessment of design quality, since main effect estimation is often of interest; *ICFT*s and *MAFT*s are not so interesting as quality criteria, since the estimation of the overall mean is usually not among the main purposes of experimental design. In terms of distinguishing non-isomorphic R-factor designs with identical a_R values, $SCFT$s have good discriminatory abilities in some classes of designs, as was already discussed in Grömping (in press) and in the example section, where it was also observed that $SCFT$s complemented $ICFT$s or $MAFT$s regarding the distinction of non-equivalent 36 run designs for three 3-level factors. There are, however, also cases for which neither $ICFT$s nor $SCFT$s are able to distinguish non-isomorphic designs, for example the 12 non-isomorphic GMA 36 run designs with three 6-level factors given on the website by Eendebak and Schoen (2010) (generated by the method described in Schoen et al. 2010), for which all designs have the same $ICFT$ and $SCFT$ (and $MAFT$ is not meaningful because of the coding dependence for factors with more than three levels).

Grömping (in press) discussed that $SCFT$s have only little discriminatory power for sets of regular designs, since these have 0/1 squared canonical correlations only. It seems that this weakness is partly shared by $ICFT$s: the 12 indistinguishable GMA 36 run designs are all regular under all three definitions introduced by Grömping and Bailey (2016) (geometric regularity, CC regularity and R^2 regularity); the latter two of these definitions refer to $SCFT$s and Average R^2 frequency tables ($ARFT$s, see Grömping in press), respectively. So far, a compelling general relation of ICs to design regularity has not been established; however, it is conceivable that CC regular designs (which have 0/1 $SCFT$ entries only) always have only integers among the concentrated ICs (e.g. the regular design of Table 4), and it is conjectured that R^2 regular designs (i.e. those which have 0/1 $ARFT$ entries only) have integer entries only in both $ICFT_{\text{c}}$ and $ICFT_{\text{e}}$ (as is e.g. the case for the twelve GMA 36 run designs in three 6-level factors, for the two 5-level Latin squares studied by Fontana, Rapallo and Rogantin (2016), and also for the only regular GMA 32 run design in three 4-level factors). This is another topic for further investigation.

For the cases for which $MAFT$s are uniquely defined, the even $ICFT$s seem to be closer to the $MAFT$s than the concentrated $ICFT$s (in case the two are different); the examples have shown that $MAFT$s tend to subdivide the a_R values as fine or finer than $ICFT$s; Example 5 has created the suspicion that the averaging over level orderings undertaken for the calculation of $MAFT$s might mask some imbalance in designs; this observation should be explored further. Ideally, a better understanding of the relation between $ICFT$s and $MAFT$s may contribute to developing a coding invariant tabulation that makes use of insights behind the calculation of $MAFT$s for fast calculation but also respects the entire imbalance available in a design and is truly coding invariant for factors with more than three levels. Such a metric could become a very useful tool in checking combinatorial equivalence of factorial designs.

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