Coding Invariance in Factorial Linear Models and a New Tool for Assessing Combinatorial Equivalence of Factorial Designs

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Abstract

This paper provides new insights into coding invariance for linear models with qualitative factors, including a coding invariant way of denoting the model coefficients. On this basis, “interaction contributions” (ICs) are proposed for decomposing generalized word counts for factorial designs into contributions that neither depend on level allocation nor on the coding of factors. Combinatorially equivalent designs yield the same ICs, so that ICs are suitable for classifying factorial designs with qualitative factors. ICs are based on singular value decomposition and have an interpretation in terms of bias contributions of an interaction on the estimation of the overall mean. The paper introduces ICs and their tabulations in interaction contribution frequency tables and illustrates their behavior in various examples. ICs are compared to several other tools for assessing combinatorial equivalence of general factorial designs, and they are found to provide a useful complement to existing methods.

Keywords: experimental design, qualitative factors, combinatorial equivalence, mean aberrations, generalized word length pattern

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* relabellings 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

Abbreviations: IC stands for "Interaction Contribution", *ICFT* for "Interaction Contribution Frequency Table", *DEFT* for "Distance Enumeration Frequency Table",*ODFM* for "Ordered Distance Frequency Matrices", *PFT* for "Projection Frequency Table", *PMFT* for "Power Moment Frequency Table", *MAFT* for "Mean Aberration Frequency Table", *SCFT* for Squared Canonical correlation Frequency Table, and *ARFT* for "Average R^2 Frequency Table".

to non-isomorphic designs. For qualitative factors, on the other hand, each relabelling of factor levels leads to an isomorphic design; this type of isomorphism will be called "combinatorial equivalence" in this paper; the expression "non-isomorphic" is used as a short form for "not combinatorially equivalent", and "equivalence screening" is used as a short form for "checking whether necessary conditions for equivalence are violated". When searching for appropriate designs, designs isomorphic to ones that have already been investigated need not be considered. Therefore, the ability to decide whether or not designs are isomorphic is important for efficiently handling resources. This is not only the case when searching for good or optimal designs, but can also be relevant for basic activities regarding experimental practice, for example when trying to adapt data from an existing experiment to a software tool that provides a factorial structure; the effort of obtaining an appropriate map between two isomorphic designs can be quite large and should only be undertaken if the designs in question are isomorphic.

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 the model matrix of a factorial linear model. In their seminal paper on generalized minimum aberration (GMA), Xu and Wu (2001) introduced the so-called normalized orthogonal coding (see Definition 2 in Section 2), which ensures that all coefficient estimators in a factorial linear model for a full factorial design are uncorrelated and have the same variance. This paper interprets coding invariance as invariance against the choice of a *normalized orthogonal* coding. Throughout the paper, the expression "coding invariant" will always be used in this sense, which comprises both level allocation and effect coding. It will be shown that outer products of effect model matrices are coding invariant in this sense. Furthermore, the paper will provide a coding invariant way of specifying effect coefficient vectors as a linear combination of right singular vectors of the effect model matrix. This allows, for example, to create simulation scenarios involving effect sizes for qualitative factors in a coding invariant way. The results on coding invariance will also serve as the basis for the development of the "interaction contributions" (ICs) that will be introduced in this paper as a tool for assessing combinatorial equivalence.

Clark and Dean (2001) and Katsaounis and Dean (2008) introduced necessary and sufficient conditions for combinatorial equivalence; checking these can be painfully slow, so that various faster tools for equivalence screening have been proposed, and Katsaounis (2012) proposed to use these also for screening designs with qualitative and quantitative factors. Section 2.2 will present a collection of existing tools for equivalence screening, including squared canonical correlation frequency tables ($SCFT$s) by Grömping (2017a) and mean aberration frequency tables ($MAFT$s) by Fontana, Rapallo and Rogantin (2016), among several others. The ICs proposed in this paper focus on general factorial designs with at least some factors at more than two levels (since the toolbox for 2-level designs is already quite powerful); they will have to compete with the existing tools. This article considers screening tools only, and the Examples section contains a non-isomorphic set of designs that cannot be distinguished by any of the screening tools considered here (i.e. none of them provides sufficient conditions for equivalence).

ICs, like several of the other tools for equivalence screening, are based on generalized word counts: 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 $j > 0$, the generalized count A_j of words of length j can be written as a sum of generalized word counts $a_j(S)$ from all sets S of j factors. These $a_j(S)$ are called projected a_j values in this paper, and they will be defined and explained in Section 2.2. 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. The majority of the tools for equivalence screening used in this paper is related to the projected a_j values, with particular focus on projected a_R values; the other tools are based on Hamming distances between design rows (see Section 2.2).

The ICs to be developed in this article provide a new coding invariant decomposition of the projected a_j values. They work for pure or mixed level designs with factors at arbitrary numbers of levels. 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). Like the projected a_j values themselves, ICs have a statistical interpretation in terms of bias contributions of the interaction to estimation of the overall mean. It is proposed to use *ICFT*s for equivalence screening of general factorial designs, and the examples will demonstrate that they complement the existing tools for this purpose. 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.

Section 2 will introduce notation and basic concepts, including a detailed introduction to the existing tools for equivalence screening. Section 3 will provide two fundamental theorems on coding invariance in factorial linear models. Section 4 will introduce the interaction contributions and their properties and will provide the aforementioned two types of *ICFT*s. Section 5 will provide several examples that exemplify the details of ICs as well as their performance in equivalence screening in comparison to other tools. The final section will discuss connections to further related work and reasonable future steps.

2. Notation and basic concepts

We consider factorial designs with n factors in N runs, with s_i levels for the ith factor. The designs are level-balanced, i.e. each factor has each level the same number of times, which implies at least resolution II. Subsets of the factors are denoted by $S \subseteq \{1, \ldots, n\}$, and the cardinality of a set S is denoted by $|S|$. For $j \in \{1, \ldots, n\}$, $\mathcal{S}_j = \{S \subseteq \{1, \ldots, n\} : |S| = j\}$ denotes the set of all j factor sets. The restriction of a design to the factors from a set $S \in \mathcal{S}_j$ is called a j factor projection and is for simplicity identified with the set S.

2.1 Matrix tools and factorial linear models

Before discussing factorial linear models, 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 zeros, respectively, $\mathbf{e}_i$ denotes a unit vector with the value "1" in position i and zeros 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 $\mathbf{B}$, $(\mathbf{A} \odot_r \mathbf{B})(\mathbf{A} \odot_r \mathbf{B})^\top = (\mathbf{A}\mathbf{A}^\top) * (\mathbf{B}\mathbf{B}^\top)$.*

Lemma 1 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 $\mathbf{B}$.

A full factorial linear model for data from a factorial design 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 ($df(S) = \prod_{i \in S}(s_i - 1)$ columns), and $\boldsymbol{\beta}_{\text{effect}}$ the coefficient vector corresponding to the effect indicated in the subscript. Note that $df(S)$ refers to the degrees of freedom (df) 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 factorial design.

Definition 2 provides the normalized orthogonal coding introduced by Xu and Wu (2001), and the subsequent lemma relates main effects model matrices in different normalized orthogonal codings to each other.

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 $\mathbf{X}_i, i \in S$.

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 $\mathbf{AA}^\top$. 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. *$\widetilde{\mathbf{X}} = \mathbf{XQ}$ with an orthogonal matrix $\mathbf{Q} \neq \mathbf{I}$.*

Proof. II implies I: Let $\mathbf{X} = \mathbf{UDV_X}^\top$. Then $\widetilde{\mathbf{X}} = \mathbf{XQ} = \mathbf{UDV}_{\mathbf{X}}^\top\mathbf{Q} = \mathbf{UDV}_{\widetilde{\mathbf{X}}}^\top$, 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 $\mathbf{Q} = \mathbf{V}_{\mathbf{X}}\mathbf{V}_{\widetilde{\mathbf{X}}}^\top$. $\square$

2.2 Tools for equivalence screening

This section briefly explains the existing tools used as competitors for *ICFT*s in this paper. They are based on projected a_j values (Section 2.2.1) or Hamming distances (Section 2.2.2). Some of the tools can also be used as quality criteria (this will be mentioned, if applicable), while others are interesting for equivalence screening only.

2.2.1 Tools based on projected a_j values

It was mentioned in the introduction that the element A_j of the GWLP can be written as the sum over all j factor sets of the projected a_j values, i.e. as $A_j = \sum_{S\in\mathcal{S}_j} a_j(S)$. The following definition provides these projected a_j values in the notation of this paper.

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 definition implies that the projected a_j value is the sum of $df(S)$ squared column means (for complex coding generalized to the sums of squared norms of column means) of the interaction model matrix $\mathbf{X}_{\mathcal{I}(S)}$ in normalized orthogonal coding. This sum is coding invariant, while its summands are not. The $a_j(S)$ and their collection in projection frequency tables (*PFT*s) can be used for equivalence screening (see e.g. Xu et al. 2004, Schoen 2009). In this paper, we will restrict attention to *PFT*s from R factor sets, where R is the resolution of the design. *PFT*s are useful also for ranking designs (large individual a_j values are undesirable).

Fontana et al. (2016) defined "aberrations" as the $df(S)$ summands of $a_j(S)$, if the levels $0, \dots, s_i - 1$ of the ith factor are coded as $\omega^0, \dots, \omega^{s_i-1}$, where ω denotes the s_ith primitive complex root of unity. For a design with s level factors, this coding implies that all columns of $\mathbf{X}_{\mathcal{I}(S)}$ contain elements of $\{\omega^0, \dots, \omega^{s-1}\}$ only. Fontana et al. (2016) attempted to render the aberrations coding invariant by obtaining "mean aberrations", for which - separately for each column of $\mathbf{X}_{\mathcal{I}(S)}$ (corresponding to an interaction df) - the df's summand of $a_j(S)$ is averaged over all permutations of the df's (possible) levels. They made this approach computationally attractive by providing a formula that calculates these mean aberrations without actually conducting the permutations. For factors with up to three levels, the mean aberrations are indeed coding invariant. For $s > 3$, this is no longer the case, as can e.g. be seen by comparing the mean aberrations for Fontana et al.'s 5-level design $\mathcal{F}_2$ in unmodified form and for a version with levels 0 and 1 (coded as ω^0 and ω^1, respectively) for the third factor swapped: the mean aberrations are 60 zeros and four ones for the unmodified design and 48 zeros, eight 0.2 values and eight 0.3 values for the modified design. (4-level examples with such behavior can also be given.) Thus, mean aberration frequency tables (*MAFT*s) are suitable tools for equivalence screening for designs with $s \leq 3$ only. We will consider $MAFT$s of dimension R only, with R the resolution of the entire design. For symmetric designs with s prime, the $df(S)$ mean aberrations for $\mathcal{I}(S)$ sum to $a_j(S)$.

For full resolution sets S, i.e. j factor sets S with resolution j, Grömping and Xu (2014) obtained a different decomposition of $a_j(S)$ into the squared canonical correlations between the main effects model matrix $\mathbf{X}_i$ for $i \in S$ and the interaction model matrix $\mathbf{X}_{\mathcal{I}(S-\{i\})}$; since each element of S can be singled out for the main effects model matrix, there are j decompositions into squared canonical correlations, with a total of $\sum_{i=1}^{j}(s_i-1)$ summands and the total sum $j \cdot a_j(S)$. Grömping (2017a) introduced squared canonical correlation frequency tables ($SCFT$s) and proposed their use both for assessing design quality (large individual values are undesirable, since they imply that there is a coding for which there is a high bias potential from an interaction for individual main effects coefficient estimators) and as a tool for equivalence screening; $SCFT$s are most interesting for R factor projections with R the resolution, but they can also be obtained for higher dimensions (even though they do not necessarily decompose $a_j(S)$ for j factor sets with resolution less than j); like for PFTs and $MAFT$s, we will only consider $SCFT$s from R factor sets. $SCFT$s work for mixed level designs and for arbitrary numbers of levels.

2.2.2 Tools based on Hamming distances

Ma et al. (2001) introduced centered L_2 discrepancies (CD_2 in their notation) for the equivalence screening of 2-level designs and generalized them to the "distance enumerator" B_a for general designs. B_a can be calculated from the Hamming distances between the N rows of a design: the Hamming distance of two vectors $\mathbf{v}_1$ and $\mathbf{v}_2$ of the same length is the count of nonzero elements of $\mathbf{v}_1 - \mathbf{v}_2$. The Hamming distance between two rows of a design d is invariant to column permutations and permutations of factor levels within columns. For any $N \times n$ symmetric s-level design d, an $N \times N$ distance matrix $\mathbf{D}_H(d)$ of the Hamming distances can be created, and two designs d_1 and d_2 are isomorphic, if there is a permutation of the rows of d_2 that leads to identical Hamming distance matrices for all k factor projections of d_1 and the permuted d_2 (Katsaounis and Dean 2008, in extension to Clark and Dean's 2001 result for 2-level designs). As a search for this row permutation can be computationally very intensive, screens based on the frequency distributions of the Hamming distances have been proposed, and B_a is one such screen: with $h_0(d), h_1(d), \ldots, h_n(d)$ denoting the frequencies of elements $0, 1, \ldots, n$ in $\mathbf{D}_H(d)$, $B_a(d) = \sum_{i=0}^{n} h_i(d)a^i/N$; Ma et al. used $B_{4/5}(d)$. For equivalence screening of designs d_1 and d_2, Ma et al. proposed to compare $B_a(d_1)$ and $B_a(d_2)$ for the entire designs, in case of equality for all $n-1$ factor sets and all 1 factors sets, and if necessary for successively larger numbers of projections ($n-2$ factor sets and 2 factors sets, and so forth). Tables of the distance enumerators will be called $DEFT$s in the following.

Xu and Deng (2005) proposed to tabulate power moments of row similarities in the $\binom{n}{t}$ t factor projections, where the power moment is defined as $K_t(d_S) = \sum_{1 \le i < k \le N}(t - \mathbf{D}_H(d_S)_{i,k})^t$ with d_S denoting the design's projection on the t factor set S and $t - \mathbf{D}_H(d_S)_{i,k}$ the number of coincidences between rows i and k of d_S. Tables of the power moments will be called power moment frequency tables ($PMFT$s) in this paper. Katsaounis and Dean (2008) considered *PMFT*s under the name mom^p. Xu and Deng proposed to use *PMFT*s for ranking designs in terms of "moment aberration projection", striving to minimize the frequencies for large values. When comparing resolution R designs, tabulation of the power moments for R factor sets and larger projections are of interest.

Mandal (2015) proposed to use an ordered distance frequency matrix (*ODFM*) for equivalence screening based on his Theorem 2.3; an unordered distance frequency matrix $\mathbf{F}(d)$ can be obtained by replacing each $1 \times n$ row of $\mathbf{D}_H(d)$ with the $1 \times (n+1)$ row of its frequencies for the distance values 0 to n; we denote the ordered version as $\mathbf{F}^*(d)$. Comparing ordered distance frequency matrices avoids the necessity of searching for row permutations. For comparing two designs, Mandal proposed to first compare $\mathbf{F}^*(d_1)$ with $\mathbf{F}^*(d_2)$, and to proceed in case of equality by searching for an $(n-1)$ factor set S_{n-1} such that $\mathbf{F}^*(d_{1;\{1,\dots,n-1\}}) = \mathbf{F}^*(d_{2;S_{n-1}})$, if this can also be found to proceed by searching for an $(n-2)$ factor set S_{n-2} such that $\mathbf{F}^*(d_{1;\{1,\dots,n-2\}}) = \mathbf{F}^*(d_{2;S_{n-2}})$, and so forth, until no adequate subset can be found. For exploiting the full potential of Mandal's Theorem 2.3, it would be necessary to ensure $S_1 \subset \cdots \subset S_{n-2} \subset S_{n-1}$; Mandal's proposed algorithm does not do so. In this paper, for subsets of $q < n$ factors, the method has been implemented by obtaining multisets of the $\binom{n}{q}$ ordered distance frequency matrices for the q dimensional projections of designs d_1 and d_2, and by declaring the designs as non-isomorphic, if their multisets differ. Mandal's approach is more complicated than the other approaches considered in this paper, since its results for a single dimension cannot be presented in a simple table; it seems to be similar to the screening algorithm named "Deseq1" by Dean and Clark (2001) and Katsaounis and Dean (2008).

Ma et al. (2001) conjectured that failure of *DEFT*s to reveal non-isomorphism might be sufficient for proving equivalence; Katsaounis and Dean (2008) proved this to be false for designs with $A_1 > 0$. The Examples section contains several non-isomorphic sets of designs with $A_1 = 0$ that cannot be distinguished by *DEFT*s so that the conjecture seems to be false in general (Examples 4, 5, 7, 8). Mandal (2015) also conjectured that *ODFM*s might be sufficient for proving equivalence; while *ODFM*s are able to ascertain non-isomorphism for some cases for which *DEFT*s and *PMFT*s fail, Examples 4, 5 and 7 of this paper also disprove his conjecture. Xu and Deng (2005) demonstrated that *PMFT*s are stronger than *PFT*s in discriminating designs. For all examples of this paper, *PMFT*s show the same discriminatory behavior as *PFT*s.

The Hamming distance based tools of this section were proposed for pure level designs by their inventors, and their implementation for mixed-level designs has not been attempted, although it is likely straightforward at least for *PMFT*s and *DEFT*s.

2.3 Regularity of designs

There are different types of design regularity. Under the most well-known one, some factors are created using defining relations in the other factors. Kobilinsky, Monod and Bailey (in press) provided a generalized version of this (called "generalized regular"), and Grömping and Bailey (2016) discussed various existing types of regularity and defined three new very general types: geometric regularity, CC regularity and R^2 regularity. CC regularity and R^2 regularity are related to *SCFT*s and may have implications for *ICs*. They are therefore briefly explained here and will be recurred to in the Examples section and in the discussion: a design is called CC regular, if its *SCFT*s in all dimensions contain zeros and ones only; a design is called R^2 regular, if entire factor main effects are either completely confounded or unconfounded with other effects, i.e. if the *average* squared canonical correlations are all zeros or ones in all dimensions for all factor projection combinations; since the average squared canonical correlations can also be considered as average R^2 values from linear models with orthogonal main effects model matrix columns as responses, Grömping 2017a collected them in average R^2 frequency tables (*ARFT*s), and a design is R^2 regular whenever its *ARFT*s in all dimensions contain zeros and ones only. Of course, R^2 regularity implies CC regularity.

3. Coding invariance

This section establishes two general results on coding invariance, which will also 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; this theorem is quite useful for the creation of meaningful and non-redundant simulation scenarios for linear models with qualitative factors.

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 $\mathbf{X}_{\mathcal{I}(S)}^\top\mathbf{X}_{\mathcal{I}(S)}$. □

Note that Srivastava and Raktoe (1976) already found that the eigen values of effect matrix cross products $\mathbf{X}_{\text{eff}}^\top\mathbf{X}_{\text{eff}}$ are invariant to random factor level permutations, where the subscript "eff" denotes an admissible effect according to Srivastava and Raktoe, which could e.g. be $\mathcal{I}(S)$ for an arbitrary choice of $S \subseteq \{1,\ldots,n\}$; this is related to the coding invariance of $\mathbf{D}$ stated in the corollary.

Corollary 2. Let $\mathbf{X}_{\mathcal{I}(S)}$ and $\widetilde{\mathbf{X}}_{\mathcal{I}(S)}$ denote two interaction model matrices for the factors in $S \subseteq \{1, \dots, n\}$ 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* $\mathbf{X}_{eff} = \mathbf{U}\mathbf{D}\mathbf{V}_{\mathbf{X}}^{\top}$ *and the corresponding coefficient vector as* $\boldsymbol{\beta}_{eff}$.
Define $\mathbf{c} = \mathbf{V}_{\mathbf{X}}^{\top}\boldsymbol{\beta}_{eff} \Leftrightarrow \boldsymbol{\beta}_{eff} = \mathbf{V}_{\mathbf{X}}\mathbf{c}$. *Then, the following holds:*

(i) The contribution of effect "eff" to Equation (1) *can be written as* $\mathbf{X}_{eff}\boldsymbol{\beta}_{eff} = \mathbf{U}\mathbf{D}\mathbf{c}$.

(ii) For a different normalized orthogonal coding with the model matrix $\widetilde{\mathbf{X}}_{eff}$ *and the corresponding coefficient vector* $\boldsymbol{\gamma}_{eff}$*, there is an SVD* $\widetilde{\mathbf{X}}_{eff} = \mathbf{U}\mathbf{D}\mathbf{V}_{\widetilde{\mathbf{X}}}^{\top}$ *such that* $\boldsymbol{\gamma}_{eff} = \mathbf{V}_{\widetilde{\mathbf{X}}}\mathbf{c}$ *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 4.2); in those cases, matrix $\mathbf{U}$ and vector $\mathbf{c}$ have to be kept together in suitable pairs.

4. Interaction contributions

This section introduces the ICs as a coding invariant decomposition of $a_j(S)$ and states their relation to the bias of $\bar{Y}$ as an estimator for μ from confounding with the highest order interaction $\mathcal{I}(S)$ (Section 4.1). The case of singular values with multiplicity $r > 1$ will be given special treatment in Section 4.2, since such singular values imply nontrivial non-uniqueness of singular vectors, and thus also of the ICs to be defined in Section 4.1.

4.1. The decomposition

According to Definition 3 and with $\mathbf{X}_{\mathcal{I}(S)} = \mathbf{UDV}^\top$, $a_j(S) = \mathbf{1}_N^\top \mathbf{X}_{\mathcal{I}(S)} \mathbf{X}_{\mathcal{I}(S)}^\top \mathbf{1}_N / N^2 = \bar{\mathbf{u}}\mathbf{D}\mathbf{D}^\top \bar{\mathbf{u}}^\top$, with $\bar{\mathbf{u}}$ the row vector of column averages of $\mathbf{U}$. This quadratic form can be written as a sum and thus provides a decomposition of $a_j(S)$ into $df(S)$ non-negative summands. The following theorem summarizes this representation and provides 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

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

(ii) If all non-zero singular values have multiplicity one, the decomposition (2) is unique.

(iii) 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 (2) 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, 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 (iii), 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 (2) 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 $r_i > 1$, (2) 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 zeros. (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 ICs of Definition 4 are coding invariant, but may be non-unique, if there are non-zero singular values with multiplicity larger than 1. For an interpretation of the ICs, we now point out their relation to the bias of $\bar{Y}$ as an estimator for the overall mean, when omitting the interaction $\mathcal{I}(S)$ from the model in spite of its relevance. Note that Xu and Wu (2001) already pointed out the relation of the generalized word counts A_j to a bias of the overall mean from j-factor interactions. 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

$$E(Y) = \mu + \sum_{i=1}^{R} \mathbf{X}_i \boldsymbol{\beta}_i + \sum_{S \subseteq \{1,\dots,R\}, 2 \le |S| \le R-1} \mathbf{X}_{\mathcal{I}(S)} \boldsymbol{\beta}_{\mathcal{I}(S)} \tag{3}$$

omitting the highest order interaction (for $R = 2$, the third summand in (3) is omitted). The estimator 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 estimator, 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, and $\boldsymbol{\beta} = \mathbf{V}\mathbf{c}$ has length 1 if and only if $\mathbf{c}$ has length 1. The following lemma details the relation of the *IC*s to the bias.

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

(i) Then a coding invariant representation of the bias for the estimation of μ by $\bar{Y} = \mathbf{1}_N^\top \mathbf{Y}/N$ is given as $\bar{\mathbf{u}}\mathbf{D}\mathbf{c} = \sum_{i=1}^{min(N,df(\{1,\dots,R\}))} c_i \zeta_i \bar{u}_i$.

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

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

The ICs are the squared biases if the vector $\mathbf{c}$ is chosen as $\mathbf{e}_i, i = 1,\dots,df(S)$, i.e., if the parameter vector $\boldsymbol{\beta}_{\mathcal{I}(S)}$ is chosen as a right singular vector $\mathbf{v}_i$ of $\mathbf{X}_{\mathcal{I}(S)}$. They are also the summands of the worst case squared bias, as provided in part (ii) of the lemma. When considering arbitrary j factor sets S that have resolution $R < j$, the total bias of $\bar{Y}$ as an estimator for μ may contain other contributors besides the bias contribution of the interaction $\mathcal{I}(S)$.

4.2. Resolving ambiguities

This section presents two different but related ways of obtaining unique summands for ambiguous cases in Equation (2): 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. The following lemma ascertains the existence of rotations that correspond to these allocations.

Lemma 5. *Let $\mathbf{X}_{\mathcal{I}(S)} = \mathbf{UDV}^\top$, ζ a singular value with multiplicity $r > 1$, the $N \times r$ matrix $\mathbf{U}_{sub}$ and the $df(S) \times r$ matrix $\mathbf{V}_{sub}$ the corresponding sub matrices of $\mathbf{U}$ and $\mathbf{V}$, $\bar{\mathbf{u}}_{sub}$ the $1 \times r$ vector of column means of $\mathbf{U}_{sub}$. For an orthogonal $r \times r$ matrix $\mathbf{Q}$, denote $\mathbf{L}_{sub} = \mathbf{U}_{sub}\mathbf{Q}$, $\mathbf{M}_{sub} = \mathbf{V}_{sub}\mathbf{Q}$ and $\bar{\mathbf{l}}_{sub} = \bar{\mathbf{u}}_{sub}\mathbf{Q}$.*

(i) There is a rotation matrix $\mathbf{Q}_c$, such that $\bar{\mathbf{l}}_{sub} = ||\bar{\mathbf{u}}_{sub}||_2\mathbf{e}_1^\top$. The corresponding summands of (2) *are $\zeta^2||\bar{\mathbf{u}}_{sub}||_2^2$ and $r-1$ zeros.*

(ii) There is a rotation matrix $\mathbf{Q}_e$, such that $\bar{\mathbf{l}}_{sub} = ||\bar{\mathbf{u}}_{sub}||_2\mathbf{1_r}^\top/\sqrt{r}$. The corresponding summands of (2) *are all identical to $\zeta^2||\bar{\mathbf{u}}_{sub}||_2^2/r$.*

The proof and technical details regarding the appropriate rotation matrices can be found in Grömping (2017b). The calculation of both rotations is implemented in the R package **DoE.base** (Grömping 2016).

The ICs of Definition 4, with suitable treatment according to Lemma 5 if necessary, lend themselves to tabulation. The resulting interaction contribution frequency tables are now defined.

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 Lemma 5 (if necessary), is called the Interaction Contribution Frequency Table of order j, or $ICFT_j$; it comes in the versions $ICFT_{j,\mathrm{c}}$ and $ICFT_{j,\mathrm{e}}$, with "c" short for concentrated and "e" short for even.

Analogously to PFTs, $SCFT$s and $MAFT$s, we will exclusively consider $ICFT$s of order R, with R the design's resolution. The index for the order is therefore omitted in the following. Contrary to the decomposition results from Grömping and Xu (2014), however, ICs decompose 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

5. Examples

This section gives several examples; some of these use designs provided on the website by Eendebak and Schoen (2010), which were generated by the method described in Schoen, Eendebak and Nguyen (2010). The first three small examples exemplify $ICFT_\mathrm{c}$ and $ICFT_\mathrm{e}$ in substantial detail, comparing

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

	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
SCFT	2	0	3
$ICFT_{\mathrm{c}}$	2	0	1
$ICFT_{\mathrm{e}}$	0	3	0

them to the values of other a_j-based tools for equivalence screening; 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 3 contains a different case. The subsequent examples illustrate the screening performance of $ICFT_{\mathrm{c}}$ and $ICFT_{\mathrm{e}}$ in comparison to the tools presented in Section 2.2. Results from equivalence screening with *DEFT*s, *PMFT*s and *ODFM*s will be reported in the text, because it would be difficult to include them in the tables of the other results. Calculations of *PFT*s, *SCFT*s and *ICFT*s have been done with R package **DoE.base** (Grömping 2016), while *MAFT*s, *DEFT*s, *PMFT*s and *ODFM*s have been calculated with separate R functions; R package **sets** (Meyer and Hornik 2009) was very helpful for the multiset comparisons for *ODFM*s.

Example 1. 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* and *SCFT*. The design consists of a replicated full factorial in the two 2-level factors A and B, which is augmented with a 4-level factor C that takes on the values 0 or 2 for A=B and 1 or 3 for A $\neq$ B. The generalized word count is $A_3 = a_3(\{1, 2, 3\}) = 1$, and the design is CC regular but not R^2 regular, since A and B main effects are completely confounded by the BC or AC interactions, respectively, while only one df of the C main effect (the 0/2 vs 1/3 contrast) is completely confounded by the AB interaction. The calculation of the *ICFT*s is now worked out in detail. 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 $(8, 8, 8)$, 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., $(1/6, 1/2, 1/3)$. Concentrating the entire contribution on the first vector, $ICFT_{\mathrm{c}}$ shows the sum "1" from these as a single entry "1" and two zeros for the remaining contributions, while distributing the contribution evenly, $ICFT_{\mathrm{e}}$ 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 the chosen coding, the largest bias on the intercept resulting from the three factor interaction occurs for coefficient vectors proportional to this $\mathbf{v}_1$.

Example 2: Consider a regular design in 9 runs with three 3-level factors, for which $A_3 = a_3(\{1, 2, 3\}) = 2$. There is only one non-isomorphic design of this type. An interaction model matrix in a specific normalized orthogonal coding can be found in Example 1 of Grömping and Xu (2014). The coding invariant 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 $\zeta_1^2 = 18$, $\zeta_2^2 = \cdots = \zeta_7^2 = 9$, $\zeta_8^2 = 0$,

Table 2: Interaction 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: 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
$SCFT$	0	0	6	0
$ICFT_{\mathrm{c}}$	6	1	0	1
$ICFT_{\mathrm{e}}$	6	1	0	1
$MAFT$	6	0	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 (iii)), and we obtain a unique $ICFT$ that shows one interaction contribution $18/9 = 2$ and seven zeros. For the coding used in Grömping and Xu (2014), 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 this symmetric 3-level design, $MAFT$s are well-defined and coding invariant; they consist of two ones and six zeros; the $SCFT$ solely contains six ones (each main effect df is completely confounded by the interaction of the other two factors).

Example 3: Table 3 shows the three factor design obtained from columns 13 to 15 of the well-known Taguchi 36 run orthogonal array (see NIST / Sematech 2016), together with its metrics; this design has $A_3 = a_3(\{1,2,3\}) = 7/8 = 0.875$ and is isomorphic to one of the 24 non-isomorphic designs to be considered in Example 8. Both $ICFT$s yield the same unequal non-zero subdivision of the a_3 value into ICs ($0.201 + 0.674 = 0.875$): the length 1 parameter vectors that correspond to the larger and smaller positive ICs are $\mathbf{v}_1 = (-0.083, -0.493, -0.493, 0.083, -0.493, 0.083, 0.083, 0.493)^\top$ and $\mathbf{v}_2 = (0.493, -0.083, -0.083, -0.493, -0.083, -0.493, -0.493, 0.083)^\top$, respectively. The entire bias potential of the three-factor interaction from this design is activated for the length 1 parameter vector $\boldsymbol{\beta}_{\mathcal{I}(\{1,2,3\})} = \mathbf{Vc}$ with the $\mathbf{c}$ from Lemma 4 (ii), yielding $(0.164, -0.472, -0.472, -0.164, -0.472, -0.164, -0.164, 0.472)^\top$ (weighted average of $\mathbf{v}_1$ and $\mathbf{v}_2$ 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 plausible. $MAFT$s behave differently, in spite of also decomposing $a_3(\{1,2,3\})$ based on the interaction degrees of freedom. $SCFT$s have a different rationale and are therefore not directly comparable to $ICFT$s and $MAFT$s, although the $SCFT$ entries correspond

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	1/5	1/3	1/2	1
0	0	0	d_1	a_2	0	0	0	0	1
0	1	1		$SCFT$	4	0	0	0	2
1	2	2		$ICFT_{\mathrm{c}}$	8	0	0	0	1
1	3	3		$ICFT_{\mathrm{e}}$	4	5	0	0	0
2	0	0	d_2	a_2	0	0	0	0	1
2	1	3		$SCFT$	2	0	0	4	0
3	2	1		$ICFT_{\mathrm{c}}$	8	0	0	0	1
3	3	2		$ICFT_{\mathrm{e}}$	6	0	3	0	0

to the non-zero $MAFT$ entries for this design.

Example 4: Table 4 shows the two non-isomorphic GMA designs for two 4-level factors in 8 runs; both have $A_2 = a_j(\{1,2\}) = 1$, and the first one is CC regular (but not R^2 regular). The two designs cannot be distinguished by $DEFT$s, $PMFT$s or $ODFM$s. The table shows that they can be distinguished by their $ICFT_{\mathrm{e}}$ but not by their $ICFT_{\mathrm{c}}$. The worst case length 1 parameter vectors are again obtainable as the first right singular vectors (not shown). $SCFT$s can also distinguish these designs, while $MAFT$s are not applicable because of $s > 3$.

Example 5: The two non-isomorphic Latin squares in three 5-level factors are available on teh website by Eendebak and Schoen (2010). These were also considered by Fontana et al. (2016). Both are R^2 regular and have $A_3 = a_3(\{1,2,3\}) = 4$, and they cannot be distinguished by any of the tools for equivalence screening considered in this paper: they have the same distance enumerators (14.824) and power moments (150) and the same ordered distance frequency matrices; both $ICFT$s are unique and identical to each other (63 zeros and one "4" each); both $SCFT$s consist of twelve "1" entries (complete confounding for all main effect degrees of freedom). Table 4 in Fontana et al. suggested that mean aberrations can distinguish these designs; however, since they depend on level allocations (see Section 2.2 above), this conclusion cannot be drawn.

Example 6: Table 5 shows metrics for the three non-isomorphic 18 run orthogonal arrays in seven 3-level factors, which are e.g. obtainable from the Eendebak and Schoen (2010) website; these designs were used by Ma et al. (2001), Schoen (2009), Mandal (2015) and Fontana et al. (2016), among others. All tools for equivalence screening considered here can distinguish these three designs. Table 5 shows that $ICFT_{\mathrm{e}}$s are closely related to $MAFT$s: $MAFT$ entries are identical to those of $ICFT_{\mathrm{e}}$s or split them into halves; however, remember that this is not always the case, as was seen in Example 3. Note that, due to typing errors in the design tables of designs (b) and (d) in Ma et al. (corrections: change element b:(2,7) from 2 to 1, element d:(1,5) from 2 to 3 and element d:(9,6) from 1 to 3), Mandal obtained erroneous results for these designs; with corrected values, $ODFM$s, like $DEFT$s, show no difference between the designs in dimension 7 and correctly identify the non-isomorphic designs when considering 6 factor subsets. $PMFT$s distinguish the designs in dimension 3, as do all a_j-based tools.

Table 5: Metrics for the three non-isomorphic 18 run designs in seven 3-level factors

		0	1/12	1/6	1/4	1/3	1/2	2/3	1	2
d_1	*PFT*	0	0	0	0	0	16	18	0	1
	SCFT	0	0	54	96	0	54	0	6	0
	$ICFT_\mathrm{c}$	227	0	0	0	36	16	0	0	1
	$ICFT_\mathrm{e}$	119	144	0	0	0	16	0	0	1
	MAFT	102	144	0	32	0	0	0	2	0
d_2	*PFT*	0	0	0	0	0	20	12	2	1
	SCFT	2	0	36	120	0	44	0	8	0
	$ICFT_\mathrm{c}$	233	0	0	0	24	20	0	2	1
	$ICFT_\mathrm{e}$	159	96	0	0	0	24	0	0	1
	MAFT	134	96	0	48	0	0	0	2	0
d_3	*PFT*	0	0	0	0	0	28	0	6	1
	SCFT	6	0	0	168	0	24	0	12	0
	$ICFT_\mathrm{c}$	245	0	0	0	0	28	0	6	1
	$ICFT_\mathrm{e}$	239	0	0	0	0	40	0	0	1
	MAFT	198	0	0	80	0	0	0	2	0

For designs with $n > R$ factors, the behavior of PFT_R, $SCFT_R$, $ICFT_R$ 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 non-isomorphic resolution III 3 factor designs only.

Example 7: The ten non-isomorphic GMA 32 run designs in three 4-level factors (from the Eendebak and Schoen 2010 website) have $A_3 = a_3(\{1, 2, 3\}) = 1$; they all have the same $ICFT_\mathrm{c}$ (a single "1" and 26 zeros), while there are six distinct groups of $ICFT_\mathrm{e}$. *SCFT*s discriminate even better into nine distinct groups. *MAFT*s are not applicable, and *DEFT*s, *PMFT*s or *ODFM*s cannot distinguish any of the designs. Table 6 shows the two metrics that can distinguish these designs. Designs d_6 and d_{10} cannot be distinguished, all other designs are distinguishable at least by their *SCFT*.

Example 8: There are 24 non-isomorphic 36 run designs in three 3-level factors, obtained from Pieter Eendebak (personal communication). Example 3 and Tables 7 to 10 provide their a_3 values and *ICFT*s and *MAFT*s. *SCFT*s have not been included in the tables, because they would make them much bigger due to the necessity of including many additional columns. In order to keep table sizes manageable, the designs have been arranged in four groups of similar patterns plus the singleton of Example 3 (isomorphic to design 20 obtained from Pieter Eendebak). The tables display a diversity of relations between $ICFT_\mathrm{c}$, $ICFT_\mathrm{e}$ and *MAFT*s. Regarding equivalence screening, we focus on the three groups of designs that cannot be distinguished by their a_3 values: the three designs d_{14} in Table 8 and d_{10} and d_{18} in Table 9 have $a_3 = 5/12$, the five designs $d_8, d_9, d_{16}, d_{19}, d_{21}$ (all in Table 7) have $a_3 = 1/2$, and the three designs d_7 in Table 8, d_6 in Table 9 and d_{12} in Table 10 have $a_3 = 2/3$. Interestingly, none of these can be distinguished by *DEFT*s or *PMFT*s, while all of them can be distinguished by *ODFM*s. Designs d_6, d_7 and d_{12} can be distinguished by both versions of *ICFT* and by *MAFT*, as well as by *SCFT*; d_{10} and d_{18} from Table 9 cannot be distinguished by any of the metrics in the table but can be distinguished by their *SCFT*s, and these two can be distinguished from d_{14} in Table 8 by all three tabulated metrics

Table 6: Metrics for the ten non-isomorphic GMA 32 run designs in three 4-level factors

SCFT	0	1/4	3/8	1/2	5/8	3/4	1
d_1	6	0	0	0	0	0	3
d_2	3	3	0	0	0	3	0
d_3	4	0	0	4	0	0	1
d_4	2	3	0	3	0	1	0
d_5	1	4	1	2	1	0	0
d_6	3	0	0	6	0	0	0
d_7	2	2	0	5	0	0	0
d_8	1	4	0	4	0	0	0
d_9	0	3	6	0	0	0	0
d_{10}	3	0	0	6	0	0	0

$ICFT_{\mathrm{e}}$	0	1/19	1/15	1/13	1/11	1/9	1/7
d_1	8	19	0	0	0	0	0
d_2	14	0	0	13	0	0	0
d_3	12	0	15	0	0	0	0
d_4	16	0	0	0	11	0	0
d_5	18	0	0	0	0	9	0
d_6	14	0	0	13	0	0	0
d_7	18	0	0	0	0	9	0
d_8	18	0	0	0	0	9	0
d_9	20	0	0	0	0	0	7
d_{10}	14	0	0	13	0	0	0

and by *SCFT*. For the five designs with $a_3 = 1/2$, things are more complicated: d_8 and d_9 cannot be distinguished by the tabulated metrics; *MAFT* groups these two together with d_{16} and distinguishes this triple from the two singletons d_{19} and d_{21}, while $ICFT_{\mathrm{c}}$ groups them together with d_{21} and distinguishes this triple from the two singletons d_{16} and d_{19}. $ICFT_{\mathrm{e}}$ is able to distinguish three singletons from the two indistinguishable designs, i.e. has the best discriminatory power among the three tabulated metrics. *SCFT*s cannot distinguish d_{16} and d_{21} 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, i.e. a combination of these a_3-based metrics can achieve the discriminatory power achieved by *ODFM*s in this example.

6. Discussion

This paper has given two results on coding invariance in factorial linear models: the outer cross product matrices $\mathbf{X}_{\mathcal{I}(S)}\mathbf{X}_{\mathcal{I}(S)}^\top$ are invariant to the choice of normalized orthogonal coding, 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 $\mathbf{X}_{\mathcal{I}(S)}$. This allows to relate different codings to each other, as well as to specify effects, e.g. for simulations, in a very general way. Furthermore, ICs were introduced for a new coding invariant single degree of freedom decomposition of generalized word counts A_j, and their tabulations in *ICFT*s, with the two versions $ICFT_{\mathrm{c}}$ and $ICFT_{\mathrm{e}}$ where necessary,

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

a_3	metric	0	1/32	1/16	3/32	1/8	3/16	1/4	3/8	1/2	9/16	1	9/8	2
d_1	$ICFT_c$	7	.	.	.	.	.	.	.	.	.	.	.	1
2	$ICFT_e$	7	.	.	.	.	.	.	.	.	.	.	.	1
	$MAFT$	6	.	.	.	.	.	.	.	.	.	2	.	.
d_2	$ICFT_c$	6	.	.	.	1	.	.	.	.	.	.	1	.
5/4	$ICFT_e$	6	.	.	.	1	.	.	.	.	.	.	1	.
	$MAFT$	4	.	2	.	.	.	.	.	.	2	.	.	.
d_3	$ICFT_c$	7	.	.	.	.	.	.	.	.	.	1	.	.
1	$ICFT_e$	6	.	.	.	.	.	.	.	2	.	.	.	.
	$MAFT$	4	.	.	.	.	.	4	.	.	.	.	.	.
d_4	$ICFT_c$	6	.	.	.	.	.	1	.	1	.	.	.	.
3/4	$ICFT_e$	5	.	.	.	2	.	.	.	1	.	.	.	.
	$MAFT$	2	.	4	.	.	.	2	.	.	.	.	.	.
d_8	$ICFT_c$	7	.	.	.	.	.	.	.	1	.	.	.	.
1/2	$ICFT_e$	4	.	.	.	4	.	.	.	.	.	.	.	.
	$MAFT$	.	.	8	.	.	.	.	.	.	.	.	.	.
d_9	$ICFT_c$	7	.	.	.	.	.	.	.	1	.	.	.	.
1/2	$ICFT_e$	4	.	.	.	4	.	.	.	.	.	.	.	.
	$MAFT$	.	.	8	.	.	.	.	.	.	.	.	.	.
d_{13}	$ICFT_c$	6	.	.	.	1	.	.	.	1	.	.	.	.
5/8	$ICFT_e$	6	.	.	.	1	.	.	.	1	.	.	.	.
	$MAFT$	4	.	2	.	.	.	2	.	.	.	.	.	.
d_{16}	$ICFT_c$	6	.	.	.	1	.	.	1	.	.	.	.	.
1/2	$ICFT_e$	.	4	.	4	.	.	.	.	.	.	.	.	.
	$MAFT$	.	.	8	.	.	.	.	.	.	.	.	.	.
d_{19}	$ICFT_c$	5	.	.	.	1	2	.	.	.	.	.	.	.
1/2	$ICFT_e$	5	.	.	.	1	2	.	.	.	.	.	.	.
	$MAFT$	4	.	2	.	.	2	.	.	.	.	.	.	.
d_{21}	$ICFT_c$	7	.	.	.	.	.	.	.	1	.	.	.	.
1/2	$ICFT_e$	7	.	.	.	.	.	.	.	1	.	.	.	.
	$MAFT$	6	.	.	.	.	.	2	.	.	.	.	.	.
d_{22}	$ICFT_c$	7	.	.	.	.	.	1	.	.	.	.	.	.
1/4	$ICFT_e$	6	.	.	.	2	.	.	.	.	.	.	.	.
	$MAFT$	4	.	4	.	.	.	.	.	.	.	.	.	.
d_{24}	$ICFT_c$	7	.	.	.	1	.	.	.	.	.	.	.	.
1/8	$ICFT_e$	7	.	.	.	1	.	.	.	.	.	.	.	.
	$MAFT$	6	.	2	.	.	.	.	.	.	.	.	.	.

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

a_3	metric	0	1/48	1/24	1/16	1/12	1/8	1/6	1/4	1/3
d_7	$ICFT_c$	6	.	.	.	.	.	.	.	2
2/3	$ICFT_e$	.	.	.	.	8	.	.	.	.
	$MAFT$	.	.	.	.	8	.	.	.	.
d_{14}	$ICFT_c$	4	.	2	.	.	.	2	.	.
5/12	$ICFT_e$	.	4	.	.	4	.	.	.	.
	$MAFT$	.	4	.	.	4	.	.	.	.
d_{15}	$ICFT_c$	6	.	.	.	.	1	.	1	.
3/8	$ICFT_e$	2	.	3	.	3	.	.	.	.
	$MAFT$	2	.	.	6	.	.	.	.	.
d_{17}	$ICFT_c$	4	.	.	2	2	.	.	.	.
7/24	$ICFT_e$	.	6	.	.	2	.	.	.	.
	$MAFT$	.	6	.	.	2	.	.	.	.
d_{23}	$ICFT_c$	6	.	.	.	2	.	.	.	.
1/6	$ICFT_e$	.	8	.	.	.	.	.	.	.
	$MAFT$	.	8	.	.	.	.	.	.	.

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

a_3	metric	0	1/48	0.023	1/24	0.046	1/16	1/12	7/48	0.269	0.537
d_6	$ICFT_c$	4	.	.	2	1	.	.	.	.	1
2/3	$ICFT_e$	.	4	2	.	.	.	.	.	2	.
	$MAFT$	.	4	.	.	.	.	.	4	.	.
d_{10}	$ICFT_c$	4	.	1	.	.	2	.	.	1	.
5/12	$ICFT_e$	.	6	1	.	.	.	.	.	1	.
	$MAFT$	.	6	.	.	.	.	.	2	.	.
d_{11}	$ICFT_c$	2	.	1	2	.	.	2	.	1	.
13/24	$ICFT_e$	.	4	1	.	.	.	2	.	1	.
	$MAFT$	.	4	.	.	.	.	2	2	.	.
d_{18}	$ICFT_c$	4	.	1	.	.	2	.	.	1	.
5/12	$ICFT_e$	.	6	1	.	.	.	.	.	1	.
	$MAFT$	.	6	.	.	.	.	.	2	.	.

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

a_3	metric	0	1/48	0.023	1/16	0.091	13/48	19/48	23/51	0.768
d_5	$ICFT_c$	4	.	1	2	.	.	.	.	1
11/12	$ICFT_e$	.	6	1	.	.	.	.	.	1
	$MAFT$	.	6	.	.	.	.	2	.	.
d_{12}	$ICFT_c$	4	.	.	2	1	.	.	1	.
2/3	$ICFT_e$	.	6	.	.	1	.	.	1	.
	$MAFT$	.	6	.	.	.	2	.	.	.

were proposed as tools for equivalence screening.

For 2-level factors, *ICFT*s, *SCFT*s and *MAFT*s do not contribute anything over and above *PFT*s or *PMFT*s; for factors at more than 2 levels, they contain far more detail than *PFT*s and are therefore of course more powerful for distinguishing non-isomorphic designs. Where all these are applicable, they have roughly comparable discriminatory power, and seem to be sometimes but not always more powerful than the Hamming distance based methods. $ICFT_\mathrm{e}$ seems to be slightly more powerful than $ICFT_\mathrm{c}$ in distinguishing designs, and *SCFT* was even more powerful in some of the examples (however, see next paragraph). *ICFT* and *SCFT* appear to capture different aspects of the non-isomorphism leading to different detection abilities in some cases (see the five designs with $a_3 = 1/2$ in Example 8). *ICFT*s are therefore a welcome addition to the simpler tools for distinguishing non-isomorphic designs. From the limited experience collected in search for example sets of designs with factors at more than two levels, it seems that the *DEFT*s and *ODFM*s benefit from richer designs and are less powerful with very small designs; nevertheless, *ODFM*s were able to distinguish all non-isomorphic designs in Example 8.

Grömping (2017a) discussed that *SCFT*s have only little discriminatory power for sets of (CC) regular designs, since these have 0/1 *SCFT* entries only. It seems that, for R^2 regular designs, this weakness is shared by all other tools considered in this paper, including *ICFT*s: the R^2 regular designs of Example 5 are indistinguishable, and a further set of R^2 regular designs, the 12 non-isomorphic GMA 36 run designs with three 6-level factors given on the website by Eendebak and Schoen (2010) (not included in this paper), are also indistinguishable by all tools. It is conjectured that both $ICFT_\mathrm{c}$ and $ICFT_\mathrm{e}$ have only integer entries for R^2 regular designs. For designs that are only CC regular but not R^2 regular, $ICFT_\mathrm{c}$ still seems to have integer entries only and is thus quite restricted (see for example the CC regular designs d_1 of Tables 4 and 6), while $ICFT_\mathrm{e}$ may have a potential to distinguish CC regular designs that are indistinguishable by *SCFT*s. This is a topic for further investigation.

*ICFT*s decompose $a_j(S)$ into $df(S)$ contributions that are interpretable in terms of bias risk for $\bar{Y}$ as an estimator for the overall mean. While it is beneficial to have an interpretation for the ICs, the bias of the overall mean estimator is not particularly interesting statistically, since the estimation of the overall mean is usually not among the main purposes of experimental design. Like *ICFT*s, *DEFT*s, *ODFM*s and *MAFT*s are of interest for equivalence screening only, while *SCFT*s, *PFT*s and *PMFT*s provide quality criteria and are thus ranking tools that can also be used for equivalence screening. The *ARFT*s (Grömping 2017a) that were mentioned in Section 2.3 could also be used in this sense for mixed level designs; they enrich the *PFT* entry $a_R(S)$ with information about the numbers of main effect df of the factors in S.

To the author's knowledge, *ICFT*s, *SCFT*s and *MAFT*s (the latter for $s \leq 3$ only) are currently the only coding invariant tools that go beyond entire effects. They decompose the entire effects into individual degrees of freedom, either of the interaction (*ICFT*s and *MAFT*s) or of the main effects of all factors in the factor set (*SCFT*s). With *MAFT*s for $s > 3$, this leads to a dependence on the choice of coding; for $s = 3$, *MAFT*s are useful for equivalence screening because they are powerful and very easy to compute.

$ICFT$s_and $SCFT$s_are more computationally demanding for larger designs especially in case of many factors ($\binom{n}{R}$ sets to be considered). Nevertheless this effort is much smaller than checking for equivalence with the necessary and sufficient criteria by Katsaounis and Dean (2008).

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