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Alexander duality in experimental designs

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Abstract If F is a full factorial design and D is a fraction of F, then for a given monomial ordering, the algebraic method gives a saturated polynomial basis for D which can be used for regression. Consider now an algebraic basis for the complementary fraction of D in F, built under the same monomial ordering. We show that the basis for the complementary fraction is the Alexander dual of the first basis, constructed by shifting monomial exponents. For designs with two levels, the Alexander dual uses the traditional definition for simplicial complexes, while for designs with more than two levels, the dual is constructed with respect to the basis for the design F. This yields various new constructions for designs, where the basis and linear aberration can easily be read from the duality.

Keywords Alexander dual · Factorial design · Linear aberration

1 The algebraic method in experimental design

Pistone and Wynn (1996) first proposed the use of computational commutative algebra approach to analyze full factorial designs and their fractions. This approach allows us

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to identify models for a design and extend the confounding relations which previously were mostly studied for regular fractions.

Algebraic techniques are applicable to any design defined in continuous factors, see the monograph Pistone et al. (2001) and also Riccomagno (2009). The techniques have been extended to a variety of cases, such as the identifiability analysis of mixture experiments in Maruri-Aguilar et al. (2007) and the study of orthogonality when the factorial levels are defined via roots of unity in Pistone and Rogantin (2008). Recently, the concept of minimal "linear aberration" in algebraic models has been studied in Bernstein et al. (2010), together with a description of models in terms of their border complexity measured with Betti numbers, see Maruri-Aguilar et al. (2012).

This paper is concerned with the study of models identified with fractions of factorial designs. The main result is that for a given fraction, Alexander duality, a concept from algebraic topology, relates the algebraic model of the fraction with that for the fraction complement.

A short summary of algebraic method is first presented. In Sect. 1.1 we present results concerning full factorial designs and designs which are special hierarchical subsets of such full grids. In Sect. 1.2 we study Alexander duals of hierarchical sets of monomials, both in the square-free (multilinear) case and as subset of a lattice. Our main result is in Sect. 2, namely that the model for a fraction and the model for the complement of that fraction are related by Alexander duality. We then extend the bounds on minimal aberration in Bernstein et al. (2010) using Alexander duality. In Sect. 3 we present some special cases which still yield Alexander duality but without resorting to operations with ideals. The first case is based on the aliasing table for regular fractions of factorial designs 2^k, while the second case concerns designs obtained by complements and reflections.

We start with a short summary of the algebraic method in experimental design. The reader is referred for further references on polynomial ideals to Cox et al. (2007), and for monomial ideals to Herzog and Hibi (2011) and to Miller and Sturmfels (2005). Consider d indeterminates $x_1, \ldots, x_d$. For a set of non-negative integers $\alpha = (\alpha_1, \ldots, \alpha_d)$ we define a monomial as

$$x^\alpha = x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_d^{\alpha_d}.$$

Any monomial x^α can be represented by its exponent $\alpha = (\alpha_1, \ldots, \alpha_d) \in \mathbb{Z}^d_{\geq 0}$. The total degree of a monomial x^α is $|\alpha| = \sum_{i=1}^d \alpha_i$.

In statistics we are familiar with monomials as linear, quadratic, interaction, and so on: $x_1, x_2^2, x_1x_2, \ldots$, etc. By taking linear combinations of monomials with coefficients in a base field $\mathbf{k}$ we obtain a ring of polynomials, $R := \mathbf{k}[x_1, \ldots, x_d]$. We can write a polynomial in R compactly as

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

where M is a set of distinct multi-exponents. For example, the standard quadratic response surface in two variables is:

$$f(x_1, x_2) = \theta_{00} + \theta_{10}x_1 + \theta_{01}x_2 + \theta_{20}x_1^2 + \theta_{11}x_1x_2 + \theta_{02}x_2^2,$$

and $M = \{(0,0), (1,0), (0,1), (2,0), (1,1), (0,2)\}$.

A design D is considered to be a finite set of n distinct points in $\mathbb{R}^d$. Each point in D is sometimes referred to as treatment combination. We ignore replication, that is, repeated observations at the same design site. In the algebraic method the design is expressed as the solution of a set of equations and thus thought of as a zero-dimensional algebraic variety. The set of all polynomials that vanish on all points of D is the design ideal, $I(D) \subset R$.

We define a monomial term ordering (monomial ordering, for short) which is a total ordering $\prec$ on all monomials satisfying a) $1 \prec x^\alpha$ for all $\alpha \neq 0$, and b) if $x^\alpha \prec x^\beta$ then $x^{\alpha+\gamma} \prec x^{\beta+\gamma}$, for all integer $\gamma \geq 0$. Given a term ordering, there is a unique reduced Gröbner basis (G-basis) for $I(D)$. This reduced Gröbner basis is a finite set of polynomials $\{g_1, \ldots, g_m\} \subset I(D)$ which is a generator of $I(D)$, that is $I(D) = \langle g_1, \ldots, g_m \rangle$. Additionally, the ideal generated by the leading terms of the Gröbner basis equals the ideal of leading terms of $I(D)$, i.e. $\langle LT(g_i) : i = 1, \ldots, m \rangle = \langle LT(f) : f \in I(D) \rangle$. Recall that the leading term $\mathrm{LT}(f)$ of a polynomial f is the largest term with non-zero coefficient under the monomial ordering $\prec$.

The quotient ring

$$\mathbf{k}[x_1, \ldots, x_k]/I(D) \tag{1}$$

can be seen as a vector space spanned by a special set of monomials. This monomial basis can be found using the Gröbner basis of $I(D)$, as the set of all monomials which are not divisible by the leading terms of the G-basis. In terms of exponent vectors, $L = \{\alpha : \alpha < \beta_i \text{ for all } \beta_i \text{ where } \mathrm{LT}(g_i) = x^{\beta_i}\}$; note that the inequality is applied coordinate-wise. We call this set $\{\alpha \in L\}$ the *quotient basis* and note that $|L| = |D|$, see Cox et al. (2007) and Pistone and Wynn (1996).

The set of multi-indices (exponents) in L has the "order ideal" property: $\alpha \in L$ implies $\beta \in L$ for any $0 \leq \beta \leq \alpha$ (coordinatewise). For example, if $x_1^2x_2$ is in the quotient basis so are $1, x_1, x_2, x_1x_2$ and x_1^2. This order ideal property of a model basis is well known in statistical literature, where a linear model that satisfies it is termed a "hierarchical model", see Nelder (1977) and Peixoto (1990). Several free software systems are available for determining quotient bases, such as *Macaulay2* or CoCoA; see Grayson and Stillman (2009) and CoCoATeam (2009).

Any function $y(x) : D \to \mathbb{R}$ has a unique polynomial interpolator over D given by

$$f(x) = \sum_{\alpha \in L} \theta_\alpha x^\alpha \tag{2}$$

such that $y(x) = f(x), \ x \in D$. For a given pair (D, L) the "design matrix" (or X-matrix) is a $n \times n$ matrix with rows indexed by design points and columns indexed by the monomials in L:

$$X = \{x^\alpha\}_{x \in D, \alpha \in L}.$$

The fact that L is a basis for the quotient ring (1) implies that X has full rank n, see Babson et al. (2003). If Y is a column vector that contains values $y(x)$ for $x \in D$, then $X^{-1}Y$ gives the values of coefficients θ_α that guarantee that (2) interpolates values at design points.

A final remark, in this section, is that the algebraic analysis of experimental designs helps considerably to understand aliasing or confounding. An algebraic version of this is that two polynomials $p(x)$, $q(x)$ are aliased if they agree on the design: $p(x) = q(x)$ for all $x \in D$. Equivalently $p(x) - q(x) \in I(D)$, see Pistone and Wynn (1996).

1.1 Full factorial and staircase designs

A full factorial design F in d variables is a product set in which factor x_i takes n_i distinct levels $\{x_{i,0}, \ldots, x_{i,n_i-1}\}$ for $i = 1, \ldots, d$:

$$F = \bigotimes_{i=1}^{d} \{x_{i,0}, \ldots x_{i,n_i-1}\}.$$

Throughout this paper the vector whose entries are the number of levels of each factor will be denoted as $\mathbf{n} := (n_1, \ldots, n_d)$, and the notation $\mathbf{1}$ indicates the vector $(1, \ldots, 1)$. It can easily be established that, under any monomial ordering, the Gröbner basis of $I(F)$ is the set

$$\left\{ \prod_{j=0}^{n_i-1} (x_i - x_{i,j}),\ i = 1, \ldots, d \right\},$$

with leading terms $\{x_i^{n_i}, i = 1, \ldots, d\}$. The unique quotient basis is thus

$$L = \{x^\alpha, 0 \le \alpha \le \mathbf{n} - \mathbf{1}\}, \tag{3}$$

where the inequality is verified for every coordinate.

The property that we obtain a single quotient basis, L, for any monomial ordering is also true of an important class of designs called *echelon* designs in Pistone et al. (2001), which contains the full factorial as a special case. These are designs of staircase shape, such as the example below for $d = 2$:

$$\begin{array}{ccccc}
x_{2,4} & \bullet & & & \\
x_{2,3} & \bullet & \bullet & & \\
x_{2,2} & \bullet & \bullet & & \\
x_{2,1} & \bullet & \bullet & \bullet & \bullet \\
x_{2,0} & \bullet & \bullet & \bullet & \bullet \\
 & x_{1,0} & x_{1,1} & x_{1,2} & x_{1,3}
\end{array}$$

Note that for the design to be of this form we do not require the spacings between points to be equal, as above. These designs are defined formally via a set of "directing" design points:

$$\{x^{(k)} = (x_{1,k_1}, \dots x_{d,k_d}),\ k = 1, \dots, m\},$$

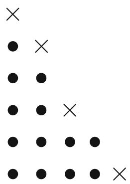
so that

$$D = \{(x_{1,i_1}, \dots, x_{d,i_d}) : (0, \dots, 0) \leq (i_1, \dots, i_d) \leq (i_{k_1}, \dots, i_{k_d}), k = 1, \dots, m\}.$$

For the above design, the directing points have indexes (3, 1), (1, 3) and (0, 4). The G-basis for this design can be found from the staircase, but it is easier to go directly to the quotient basis L. We simply take L to be of the same shape as the design but use the integer grid:

$$L(D) = \{\alpha : (0, \dots, 0) \leq (\alpha_1, \dots, \alpha_d) \leq (i_{k_1}, \dots, i_{k_d}), k = 1, \dots, m\}.$$

Continuing with the above design, the basis $L(D)$ is the set of monomials with exponents $\{(0, 0), (1, 0), (2, 0), (3, 0), (0, 1), (1, 1), (2, 1), (3, 1), (0, 2), (1, 2), (0, 3), (1, 3), (0, 4)\}$. The directing monomials of L are $x_1^3 x_2$, $x_1 x_2^3$, x_2^4 and mirror the role of directing points above. The leading terms of the G-basis are x_1^4, $x_1^2 x_2^2$, $x_1 x_2^4$ and x_2^5. We add the position of the leading terms of the G-basis in the diagram, with crosses.



Note that due to the staircase structure of the design, until this point all the analysis has been performed without knowledge of the actual design levels. Now assume that levels of x_1 in the design are 0, 1, 2, 3 and of x_2 are 0, 1, 2, 3, 4. The G-basis itself is constructed again using the diagram. We simply present the form for this example,

$$\begin{aligned}&\{x_1(x_1 - 1)(x_1 - 2)(x_1 - 3), x_1(x_1 - 1)x_2(x_2 - 1),\\ &x_1 x_2(x_2 - 1)(x_2 - 2)(x_2 - 3),\\ &x_2(x_2 - 1)(x_2 - 2)(x_2 - 3)(x_2 - 4)\}.\end{aligned}$$

1.2 Alexander duality

The Alexander dual of a simplicial complex Δ in a ground set V is the simplicial complex Δ^* constructed by those subsets of V whose complement is not in Δ. Alexander duality plays an important role in simplicial topology, indeed an important homological connection exists between a simplicial complex Δ and its Alexander dual Δ^*. Alexander duality consequently arises when considering the ideals generated by complements of those complexes, see Miller and Sturmfels (2005) and Herzog and Hibi (2011).

In this development we are concerned with the role of Alexander duality for models of fractions of factorial designs. The main interest lies in the relation of the model of a fraction of a design, with the model of the complementary fraction. We first examine the two level case which corresponds precisely to the above definition of Alexander duality, and then examine a generalization of the duality.

1.2.1 Simplicial case: fractions of factorial designs with two levels

If the factors have only two levels in the design, the quotient basis given by L is square-free. That is to say no element of a exponent vector in L is greater than or equal to two, i.e. the model is multilinear. The basis L then naturally forms an (abstract) simplicial complex with vertices indexed by the linear terms $x_1, x_2, \ldots$, edges by interactions $x_i x_j$, and a $k-1$ dimensional simplex indexed by a kth order interaction. Thus the hierarchical property corresponds to the simplicial complex property, i.e. if a simplex is in the complex so are all of its sub-simplexes. We can abuse the notation a little by referring to the simplicial complex as L, and in what follows we will sometimes use $L(D)$ to emphasize the dependence of the simplicial complex (model) on design D.

The *Alexander dual* L^* is obtained from L in the following way. First note that the full factorial two-level design F basis has the basis consisting of all square-free monomials: $L(F) = \{x^\alpha : \alpha \in \bigotimes_{i=1}^d \{0,1\}\}$. Now list all square-free monomials (in the same d factors) not in L, namely $L(F) \setminus L$. Note that this set generates the Stanley–Reisner ideal, associated with L when thought of as simplicial complex. Then take complements of the binary strings in $L(F) \setminus L$. The Alexander dual is

$$L^* = \{\mathbf{1} - \alpha : \alpha \in L(F) \setminus L\}.$$

Example 1 Take L to be the model with directing monomials $x_1x_2x_3$ and x_3x_4, i.e. $L = \{1, x_1, x_2, x_3, x_4, x_1x_2, x_1x_3, x_2x_3, x_3x_4, x_1x_2x_3\}$. The set of monomials in the complement of L is $L(F) \setminus L = \{x_1x_4, x_2x_4, x_1x_2x_4, x_1x_3x_4, x_2x_3x_4, x_1x_2x_3x_4\}$. We now take complements of monomials in $L(F) \setminus L$, for instance the complement of x_1x_4 is x_2x_3, obtained using the complement of exponent vector above $\mathbf{1} - \alpha = (1,1,1,1) - (1,0,0,1) = (0,1,1,0)$. Thus the Alexander dual is $L^* = \{1, x_1, x_2, x_3, x_1x_3, x_2x_3\}$, see Fig. 1.

Alternatively, if L is considered as a simplicial complex, its Stanley–Reisner ideal (see Miller and Sturmfels (2005)) is $I_L = \langle x_1x_4, x_2x_4 \rangle$. Thus L^* has directing monomials x_2x_3 and x_1x_3, obtained as complements of generators of I_L.

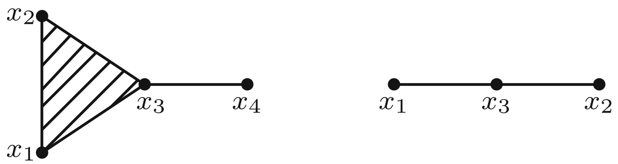


Fig. 1 Simplicial model L (*left*) and its Alexander dual L^* (*right*)

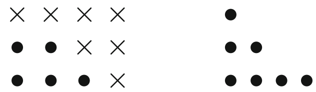


Fig. 2 Model $L(D)$ (*bullets, left panel*) and Alexander dual $L^*(D)$ relative to $L(F)$ with directing exponent $(3, 2)$ (*right panel*)

1.2.2 Designs with more than two levels

The notion of Alexander duality extends to the general case, see Miller and Sturmfels (2005). We take the design D to be embedded in a full factorial grid F, and thus $L(D)$ is a subset of the model for a full factorial $L(F)$. Recall that the model $L(F)$ is defined in (3) by the directing term with exponent vector $\mathbf{n} - \mathbf{1}$ (see notation in Sect. 1.1). The Alexander dual $L^*(D)$ of $L(D)$ is computed *relative to* $L(F)$.

The first step is, as before, to take $L(F) \setminus L(D)$. One can see that this tends to give higher degree monomials, and for non-empty D, the set $L(F) \setminus L(D)$ will never contain the monomial 1. The Alexander dual is based on pivoting downwards from the "corner" point of $L(F)$. We call this operation "flipping":

$$L^*(D) = \{\mathbf{n} - \mathbf{1} - \alpha : \alpha \in L(F) \setminus L(D)\}.$$

Example 2 In the left panel in Fig. 2, bullets represent exponents of $L(D)$ as a subset of the model for a 4×3 full factorial design F with directing exponent $\mathbf{n} - \mathbf{1} = (3, 2)$. The crosses represent term exponents in $L(F) \setminus L(D)$. The Alexander dual $L^*(D)$ is obtained by flipping the crosses to give the right panel in the same figure. In this example, the Alexander dual of $L(D) = \{1, x_1, x_2, x_1^2, x_1x_2\}$ relative to the 4×3 full factorial is $L^*(D) = \{1, x_1, x_2, x_1^2, x_1x_2, x_2^2, x_1^3\}$. For the same design with model $L(D)$, the Alexander dual relative to the 3×2 full factorial is very simple: $L^*(D) = \{1\}$.

2 The main result

Given a design D embedded in a full factorial F, that is to say a fraction of a full factorial, we can consider the complementary design (fraction) $\bar{D} := F \setminus D$. Our main result says that the basis of the complementary design obtained by the algebraic method under a monomial ordering is the Alexander dual (relative to F) of the basis of the original design obtained with the same ordering. Put as succinctly as possible:

$$L^*(D) = L(\bar{D}). \tag{4}$$

Theorem 1 *Let $\prec$ be a fixed monomial ordering. Let F be a full factorial design F with a fraction $D \subset F$. Then the bases of the quotient rings of D and the complementary design $\bar{D} = F \setminus D$, with respect to $\prec$, are Alexander dual, relative to F.*

We start with a lemma.

Lemma 1 *Let $\{g_i\}$ and $\{h_j\}$ be the G-bases for D and $\bar{D}$, respectively, with respect to term ordering $\prec$. Let the leading terms be $LT(g_i) = x^{\alpha^{(i)}}$, $LT(h_j) = x^{\beta^{(j)}}$. Let* *the basis for F be given as in Eq.* (3). *Then for all i, j*

$$\alpha^{(i)} + \beta^{(j)} \in \mathbb{Z}^d_{\geq 0} \setminus L(F).$$

Proof Since the polynomial g_i is zero on D, and h_j is zero on $\bar{D}$, then $g_i h_j$ is zero on $D \cup \bar{D} = F$. It follows that $LT(g_i h_j)$ is in the leading term ideal of F which consists of all monomials x^δ, $\delta \in \mathbb{Z}^d_{\geq 0} \setminus L(F)$. By the properties of monomial orderings,

$$LT(g_i h_j) = LT(g_i) LT(h_j) = x^{\alpha^{(i)} + \beta^{(j)}}.$$

It follows that $\alpha^{(i)} + \beta^{(j)} \in \mathbb{Z}^d_{\geq 0} \setminus L(F)$. □

To prove Theorem 1, we need to establish (4) above, the proof is by contradiction.

Proof Firstly, the cardinalities agree:

$$|L(F)| = |L^*(D)| + |L(D)|.$$

Thus, if we suppose (4) is not true then there is a vector $\gamma \in L(F)$, neither in $(L^*(D))^c$ nor in $L(D)^c$. This follows from the identity

$$|C| = |A| + |B| - |A \cap B| + |A^c \cap B^c|,$$

when $A, B \subseteq C$ and where $C = F,\ A^c = F \backslash A,\ B^c = F \backslash B$, taking $A = L(D)$, $B = L^*(\bar{D})$.

Then $\gamma \notin L(D)$ and (flipping back) $\mathbf{n} - \mathbf{1} - \gamma \notin L(\bar{D})$. But then monomials with exponents γ and $\mathbf{n} - \mathbf{1} - \gamma$ must be in their respective leading term ideals. Thus there exist an $\alpha^{(i)} \leq \gamma$ and a $\beta^{(j)} \leq \mathbf{n} - \mathbf{1} - \gamma$. But then $\alpha^{(i)} + \beta^{(j)} \leq \mathbf{n} - \mathbf{1}$ which is in $L(F)$. So $\alpha^{(i)} + \beta^{(j)} \in L(F)$, contradicting Lemma 1. □

2.1 Algebraic fan, aberration and Alexander dual

Theorem 1 has direct implications for models obtained using algebraic techniques. Recall that the algebraic fan of a design $A(D)$ is the collection of all models obtained by the techniques in Sect. 1 when considering all term orderings

$$A(D) := \{L_\prec(D) : \text{over all term orderings} \prec \text{ in } \mathbf{k}[x_1, \ldots, x_k]\},$$

where we have written $L_\prec(D)$ to emphasize the dependance of basis for the quotient ring (1) on term ordering $\prec$. Mora and Robbiano (1988) showed that this collection of bases is finite. Furthermore each basis is in one-to-one correspondence with a cone in the Gröbner fan and with a vertex of a special polytope called the state polytope, see Bayer and Morrison (1988) and Babson et al. (2003). A number of algorithms and implementations are available to compute $A(D)$, such as the package `Gfan` by Jensen (2011), or the algorithms for universal term orderings Babson et al. (2003).

A corollary of Theorem 1 relates the algebraic fan of a design $A(D)$ to that of its complement, relative to a full factorial design F. Indeed both sets $A(D)$ and $A(F \setminus D)$ have the same cardinality, and models in $A(F \setminus D)$ are the Alexander duals of those in $A(D)$.

Corollary 1 *The bases in the algebraic fan of D are in one-to-one correspondence with bases in the algebraic fan of $F \setminus D$.*

Using model aberration and the state polytopes of $I(D)$ and of $I(F \setminus D)$, we now provide a description of the relation between the two collections of models for D and for $F \setminus D$. For a basis L, define its full state vector as $V(L) := \sum_{\alpha \in L} \alpha$, i.e. the coordinate-wise sum of exponent vectors of monomials in L. As an example, for the models L and L^* of Example 1 we have $V(L) = (4, 4, 5, 2)$ and $V(L^*) = (2, 2, 3, 0)$. The state polytope of a design ideal I is built with the convex hull of all full state vectors in the algebraic fan:

$$\mathcal{S}(I) := \operatorname{conv}\left(\{V(L) : L \in A(D)\}\right) + \mathbb{R}^d_{\geq 0},$$

where the last term above is added with Minkowski summation. Inspecting the vertices of the state polytope index models in the design fan, and their polytopes, we can compare designs in terms of model aberration and minimal linear aberration of designs, see Bernstein et al. (2010).

Alexander duality allows a direct link between the vertexes of the state polytopes for $I(D)$ and for $I(F \setminus D)$. We state this result in the following Lemma. The lemma is based on a direct calculation, noting that

$$V\left(L(F)\right) = V\left(L(D)\right) + V\left(L(F) \setminus L(D)\right).$$

Lemma 2 *Let F be the full factorial design with size $n_1 n_2 \cdots n_d$; let L be the model for a subset D of F, and let L^* be the Alexander dual of L relative to F. Then*

$$V(L^*) = (\mathbf{n} - \mathbf{1}) \frac{|L^*| - |L|}{2} + V(L). \tag{5}$$

The first summand on the right hand side of (5) depends only on the lattice F and on the sizes of fractions $|D| = |L|$ and $|F \setminus D| = |L^*|$. A summary of Corollary 1 and Lemma 2 is that the state polytope of $I(D)$ and that of $I(F \setminus D)$ are related by a shift, given by the first summand in (5).

Corollary 2 *Let F be a full lattice design with an even number of points and let D and $\bar{D} = F \setminus D$ be half fractions of F, i.e. $|\bar{D}| = |D|$. Then the state polytopes for $I(D)$ and for $I(F \setminus D)$ coincide.*

The corollary follows from Lemma 2, noting that fractions D and complement $F \setminus D$ have the same size, then $|L| = |L^*|$ above and thus $V(L^*) = V(L)$. This in turn implies that both state polytopes for $I(D)$ and for $I(F \setminus D)$ are equal as they have the same set of vertices. However, note that two designs having the same state polytope does not imply that models in the algebraic fans are the same, as next example shows.

Example 3 Consider F to be a 4×4 full factorial design with levels 0, 1, 2, 3, and the fraction $D = \{(0, 1), (0, 3), (1, 1), (1, 2), (1, 3), (2, 2), (3, 1), (3, 3)\}$. For the standard term ordering in CoCoA, the model for D is $L = \{1, x_1, x_2, x_1^2, x_1x_2, x_2^2, x_1^2x_2, x_1x_2^2\}$, while its Alexander dual and basis for $F \setminus D$ is $L^* = \{1, x_1, x_2, x_1^2, x_1x_2, x_2^2, x_1^3, x_2^3\}$. We observe $L \neq L^*$, yet $V(L) = V(L^*) = (7, 7)$. For the same design $D \subset F$, and a reverse lexical term ordering, the model for D is $L = \{1, x_1, x_2, x_1^2, x_1x_2, x_2^2, x_1^3, x_1^2x_2\}$, which equals its Alexander dual L^*. In this second case the full state vector is $V(L) = V(L^*) = (9, 5)$.

The aberration of a model L measures the (weighted) degree of L, and is defined in Bernstein et al. (2010) as $A(w, L) := \frac{1}{n} V(L)w^T$, where $w = (w_1, \ldots, w_d)$ is a non-negative weight vector with $\sum_{i=1}^{d} w_i = 1$. The result of Lemma 2 implies a direct relation between aberrations for L and its Alexander dual L^*:

$$A(w, L^*) = b(1 - c) + cA(w, L) \tag{6}$$

with

$$b = \frac{1}{2} w(\mathbf{n} - \mathbf{1})^T$$

and $c = |L|/|L^*|$. In other words, the aberration of Alexander dual L^* consists of a shifting and scaling of the aberration of model L.

We finish by considering the minimal aberration of a design. Recall that the minimal aberration is computed for a fixed weighing vector by minimizing $A(w, L)$ over all models L in the algebraic fan $A(D)$. This minimisation is equivalent to linear minimization over the vertices of the state polytope, i.e. for fixed w, the minimal value of wx^T over $x \in \mathcal{S}(I)$ is attained at a vertex of $\mathcal{S}(I)$. Values of minimal aberration achieve their lowest value over all designs when considering a generic design. A design D is generic when it identifies the set of all corner cut models (of the same size n and dimension d as the design), and recall that a model is a corner cut when its set of exponents can be separated from its complement by a single hyperplane, see Onn and Sturmfels (1999).

If the design D is generic, then the algebraic fan $A(D)$ consists of corner cut models, and bounds on minimal aberration of D are

$$A^+ - 1 \leq \tilde{A}(w, L) \leq A^+ + 1 \tag{7}$$

with $A^+ = (|L|d!w_1 \cdots w_d)^{1/d} \frac{d}{d+1}$ and $\tilde{A}(w, L)$ is the minimum value of $A(w, L)$ computed over all models in $A(D)$, see Bernstein et al. (2010). By the result in (6) above, the bounds in Eq. (7) translate directly into bounds on the minimal aberration of $F \setminus D$, whose fan is the collection of Alexander duals of corner cuts:

$$b(1 - c) + c(A^+ - 1) \leq \tilde{A}(w, L^*) \leq b(1 - c) + c(A^+ + 1). \tag{8}$$

Here $\tilde{A}(w, L^*)$ is the minimum value of aberration over all Alexander duals of corner cuts. In other words, the bound on corner cuts in (7) maps linearly to bounds (8) for

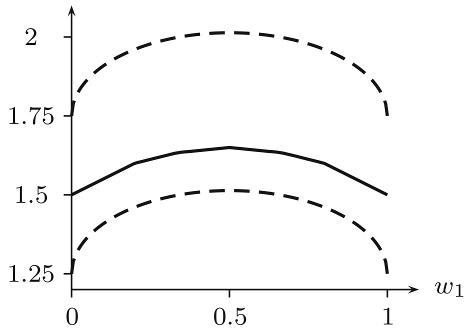


Fig. 3 Minimal linear aberration (*solid*) and bounds (*dashed*) for design $F \setminus D$ of Example 4

complements of corner cuts. Note that if L is corner cut model, its Alexander dual L^* relative to F is not necessarily a corner cut, see Example 4. There are, however, at least two simple cases when the Alexander dual of a corner cut remains so: when F is a 2×2 design and D comprises points in opposite corners of F; and when F is a factorial design of two points and D and $F \setminus D$ have only one point.

Example 4 Consider the design $D = \{(1, 3), (0, 0), (2, 2), (4, 1), (3, 4)\}$ in two factors. The design D is generic and thus its algebraic fan $A(D)$ has six corner cut models with full state vectors $(10, 0)$, $(0, 10)$, $(6, 1)$, $(1, 6)$, $(4, 2)$ and $(2, 4)$. Now consider D as subset of the full 5×5 factorial design F with levels 0, 1, 2, 3 and 4. The algebraic fan of the complement of D in F, namely $A(F \setminus D)$, has six models with full state vectors $(40, 30)$, $(30, 40)$, $(36, 31)$, $(31, 36)$, $(34, 32)$ and $(32, 34)$. As expected, none of the models in $A(F \setminus D)$ are corner cuts, for instance the corner cut model $\{1, x_1, x_2, x_1^2, x_1^3\} \in A(D)$, with full state vector $(6, 1)$ has a non-corner cut Alexander dual consisting of twenty monomials which are directed by $x_1^4x_2^2, x_1^3x_2^3, x_2^4$, and that has full state vector $(36, 31)$.

The state polytopes of $I(F \setminus D)$ and that of $I(D)$ are related by a shift of coordinates, as explained by Eq. (5). The bounds for minimal linear aberration of Eq. (8), are $\frac{5}{4} + \frac{\sqrt{10}}{6}\sqrt{w_1 - w_1^2}$ and $\frac{7}{4} + \frac{\sqrt{10}}{6}\sqrt{w_1 - w_1^2}$, computed with $b = 2$ and $c = \frac{1}{4}$. Figure 3 shows the computed bounds, together with the minimal linear aberration of that family of non-corner cut models in $A(F \setminus D)$.

3 Special constructions

3.1 Regular fractions

There are classes of designs for which the natural models are given by other types of algebraic constructions. Here we show how the Alexander duality applies to classical regular factorial fractions. We confine ourselves here to the 2^k case. The prime power case is similar.

The 2^d full factorial design in the ± 1 coding is $\{-1, 1\}^d$. For any term ordering, the reduced G-basis is: $\{x_1^2 - 1, \ldots, x_d^2 - 1\}$. To obtain a regular 2^{d-k} fraction, we set k algebraically independent square-free "defining" monomials each equal to ± 1, giving the "defining equations". This yields 2^k disjoint fractions (often called blocks) each of size 2^{d-k}. Selecting one of these blocks as the design D above we can compute $L(D)$ which has 2^{d-k} terms.

We now consider as an abelian group under the relations $x_1^2 = 1, \ldots, x_d^2 = 1$. The equations defining the fraction, together with all their pairwise products are the equations that generate the "defining sub-group". The alias classes, that is equivalence classes of monomials congruent under division by $I(D)$ cause the monomials of the full design model to fall in 2^{d-k} classes which provide the rows of the alias table. They are the cosets of the defining subgroup. If we take a single block as our design the rule is we should take at most one monomial term from each row of the alias; two terms from the same row lead to equal columns of the X-matrix (up to sign change). But terms from different rows of the table give orthogonal columns, leading to wide usefulness and efficiency in practice.

As a simple example let $d = 5$ and take the defining relations

$$x_1x_2x_3 - 1 = 0, \quad x_3x_4x_5 - 1 = 0. \tag{9}$$

This gives the $\frac{1}{4}$ fraction:

$$\begin{aligned} D = \{ & (1, 1, 1, 1, 1), (-1, -1, 1, 1, 1), (1, 1, 1, -1, -1), \\ & (-1, 1, -1, -1, 1), (-1, 1, -1, 1, -1), (1, -1, -1, 1, -1), \\ & (1, -1, -1, 1, -1), (-1, -1, 1, -1, -1)\} \end{aligned}$$

Using the algebraic method and the `DegRevLex` monomial ordering (see CoCoATeam 2009), the quotient basis is $L(D) = \{1, x_1, x_2, x_3, x_4, x_5, x_1x_5, x_2x_5\}$. The alias table is built as a table in which the monomials for the defining subgroup appear in the first row; terms in the model $L(D)$ are listed in the first column, and each entry has the complements of model term in the row with respect to the defining monomial in the column. For the current example the relation $x_1x_2x_4x_5 - 1 = 0$ appears as the pairwise product of generators in (9), and thus the table is:

1	$x_1x_2x_3$	$x_3x_4x_5$	$x_1x_2x_4x_5$
x_1	x_2x_3	$x_1x_3x_4x_5$	$x_2x_4x_5$
x_2	x_1x_3	$x_2x_3x_4x_5$	$x_1x_4x_5$
x_3	x_1x_2	x_4x_5	$x_1x_2x_3x_4x_5$
x_4	$x_1x_2x_3x_4$	x_3x_5	$x_1x_2x_5$
x_5	$x_1x_2x_3x_5$	x_3x_4	$x_1x_2x_4$
x_1x_5	$x_2x_3x_5$	$x_1x_3x_4$	x_2x_4
x_2x_5	$x_1x_3x_5$	$x_2x_3x_4$	x_1x_4

For a general two-level design with the ± 1 coding, the flip operation is simply multiplication by the full product $g = \prod_{i=1}^d x_i$ and reduction using $x_i^2 = 1$ for $i = 1, \ldots, d$. For example $x_2x_3x_5 \to x_2x_3x_5 \cdot x_1x_2x_3x_4x_5 = x_1x_4$.

Following this remark we can use Theorem 1 to write down the Alexander dual basis, under the same monomial ordering, for the $\frac{3}{4}$ fraction $F \setminus D$. We express this as a *derived* 8×3 table, constructed from the last three columns of the alias table above by transforming each monomial using the "flip" operation.

x_4x_5	x_1x_2	x_3
$x_1x_4x_5$	x_2	x_1x_3
$x_2x_4x_5$	x_1	x_2x_3
$x_3x_4x_5$	$x_1x_2x_3$	1
x_5	$x_1x_2x_4$	x_3x_4
x_4	$x_1x_2x_5$	x_3x_5
x_1x_4	x_2x_5	$x_1x_3x_5$
x_2x_4	x_1x_5	$x_2x_3x_5$

This represents a hierarchical model with eight three-way interactions as maximal simplices (cliques).

Some of the orthogonality of the original model is preserved. To repeat, for design D, theory says that any monomial term in $L(D)$ in different rows of the alias table gives orthogonal vectors over D. For $F \setminus D$, any term in different rows of the derived matrix (which come from different rows in the original table) leads to orthogonal columns of the X-matrix for $\bar{D}$ and $L(\bar{D}) = L^*$.

Take $\alpha, \beta \in L(\bar{D}) = L^*$, $\alpha \neq \beta$, be in different rows of the derived table. Note that if $g = \prod_{i=1}^d x_i$ then $g^2 = 1$, over the full factorial design F. Then

$$\begin{aligned}
0 = \sum_{x \in \bar{D}} x^\alpha x^\beta &= g^2 \sum_{x \in \bar{D}} x^\alpha x^\beta \\
&= \sum_{x \in \bar{D}} g x^\alpha g x^\beta \\
&= \sum_{x \in F \setminus D} g x^\alpha g x^\beta \\
&= \sum_{x \in F} g x^\alpha g x^\beta - \sum_{x \in D} g x^\alpha g x^\beta \\
&= \sum_{x \in F} x^\alpha x^\beta - \sum_{x \in D} g x^\alpha g x^\beta .
\end{aligned}$$

Since all monomial terms are orthogonal over $L(F)$ the first term on the right hand side is zero. The second term is zero, because the terms gx^α, gx^β are in different rows of the original alias table.

3.2 Self-dual designs

A special type of design is given by certain half fractions of 2^d designs for which the algebraic fan of both fractions coincide.

Definition 1 Let D and $F \setminus D$ be half fractions of a 2^d design. The design D is called self-dual if all the models in its algebraic fan are self-Alexander dual, i.e. $L = L^*$ for every model L in $A(D)$.

The definition above implies that the algebraic fans of D and of $F \setminus D$ are equal. The following theorem follows from close examination of the alias table of regular half fraction design, in which every monomial in the model has only one monomial aliased with it.

Theorem 2 *Let D be a regular* $1/2$ *fraction of factorial design* 2^d*. Then each model L in the algebraic fan* $A(D)$ *equals its Alexander dual* $L^* \in A(F \setminus D)$ *and the algebraic fan* $A(D)$ *equals* $A(F \setminus D)$

Proof We first identify an algebraic model for D. Without lack of generality, consider the fraction with generator $x^\beta - 1 = 0$, for a square-free exponent vector $\beta \neq (0, \dots, 0)$. For every monomial x^α in $L(F)$, pair it with the monomial $x^{\alpha \oplus \beta}$, where $\oplus$ is the bitwise XOR operation performed over elements of exponent vectors. Note that $\beta \neq (0, \dots, 0)$ guarantees that each pair contains different monomials; also that trivially the monomial $x^{\alpha \oplus \beta}$ is always an element of $L(F)$ and thus the pairing is well defined, with every monomial appearing only once in a pair. This action creates 2^{d-1} pairs of aliased monomials. Now set a term order $\prec$, order each pair and list the collection of smallest monomials (per pair). This list is an identifiable algebraic model, and the list of largest monomials gives the second column in the aliasing table, which contains 2^{d-1} rows, one per pair of monomials.

We next show that the models identified are self-Alexander duals. There are two cases. Firstly, if $\beta = \mathbf{1}$ then the operation $\alpha \oplus \beta = \beta \oplus \alpha$ equals $\mathbf{1} \oplus \alpha = \mathbf{1} - \alpha$ and thus each monomial pair has a monomial and its complement x^α and $x^{\mathbf{1} \oplus \alpha}$. The Alexander dual of the model is obtained by taking complement of the largest monomial for each pair, which gives the same model and thus the model is Alexander self-dual.

Secondly, if $\beta \neq \mathbf{1}$ then for a monomial x^{α_1} there exists a monomial x^{α_2} in a different pair, such that $\alpha_2 = \mathbf{1} \oplus \alpha_1$, i.e. x^{α_2} and x^{α_1} are complements of each other. This matching of pairs always exists as all monomials in $L(F)$ are present in the list of pairs. The monomial $x^{\alpha_1 \oplus \beta}$ is complement of $x^{\alpha_2 \oplus \beta} = x^{\mathbf{1} \oplus \alpha_1 \oplus \beta}$. In other words, for a pair of monomials $x^{\alpha_1}, x^{\beta \oplus \alpha_1}$ there is another pair which contains complementary monomials $x^{\mathbf{1} \oplus \alpha_1}, x^{\mathbf{1} \oplus \beta \oplus \alpha_1}$. Note that both x^{α_1} and its complement $x^{\mathbf{1} \oplus \alpha_1}$ cannot be identified simultaneously as this would contradict the term ordering selected $\prec$. By taking complements of the largest monomials, Alexander duality of the model is verified. □

Thus a regular half fraction of 2^d is a self-dual design. For example, consider the half fraction D obtained from the 2^5 design using the generator $x_1 x_2 x_3 x_4 x_5 = 1$. The algebraic fan of D has 81 models and equals the fan of its complementary fraction $F \setminus D$ with generator $x_1 x_2 x_3 x_4 x_5 = -1$. In some cases where the fraction is non-regular, the design is still self-dual, as the next example shows.

Example 5 Consider the design D shown in Table 1 (left side), where symbols $+$ and $-$ stand for 1 and -1, respectively. This is a non-regular half fraction of 2^4, whose algebraic fan $A(D)$ has three models, see Fig. 4. The three models are self-Alexander dual, and thus the design is a self-dual design and $A(D) = A(F \setminus D)$.

However, the equality of algebraic fans does not hold in general for non-regular half fractions of 2^d factorial designs. In this situation the sizes of the fans $A(D)$ and $A(F \setminus D)$ still coincide and the state polytopes of the design and its complementary fraction are still the same object, but models are not necessarily self-Alexander dual.

Table 1 Non-orthogonal half fractions of 2^4 (left) and of 2^5 (right)

x_1	x_2	x_3	x_4
−	−	−	−
−	−	+	−
−	+	−	+
−	+	+	+
+	−	−	−
+	−	+	−
+	+	−	−
+	+	+	+

x_1	x_2	x_3	x_4	x_5
−	−	−	−	+
−	−	+	−	−
−	−	+	−	+
−	−	+	+	−
−	−	+	+	+
−	+	−	−	−
−	+	−	−	+
−	+	−	+	−
−	+	−	+	+
−	+	+	−	−
−	+	+	+	+
+	−	+	+	+
+	−	−	−	+
+	+	−	+	+
+	+	+	+	−
+	+	+	+	+

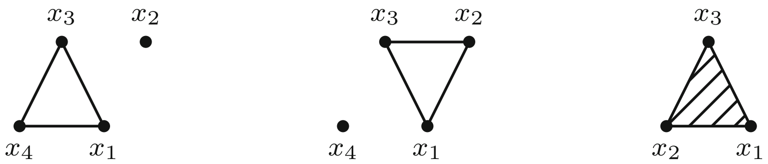


Fig. 4 Self-Alexander dual models of Example 5

Fig. 5 Model L (*left*) and Alexander dual L^* (*right*), see Example 6

Example 6 The set D in Table 1 (right side) forms a sixteen run, non-orthogonal half fraction of a 2^5 design. The algebraic fan $A(D)$ has 15 models, of which 8 are of total degree 26 and 7 of degree 27. The state polytopes of $I(D)$ and of $I(F \setminus D)$ coincide, despite the fact that there are no common models in both fans. In other words, the fan $A(F \setminus D)$ has the same size and distribution of models by degree as thatbreak for D.

Two models $L \in A(D)$ and $L^* \in A(F \setminus D)$ are shown in Fig. 5. Models L and L^* have of total degree 27 and are related by Alexander duality. Lemma 2 is verified as they have the same full state vector $V(L) = (4, 5, 5, 7, 6) = V(L^*)$. However, the models are not equal, and they share only twelve out of their sixteen monomials.

3.3 Complements and reflections

Taking the complement of designs for which we immediately know the basis leads to bases for a whole hierarchy of designs. It is pleasing to explain this with diagrams. To start let us take the complement of a 2^2 full factorial in a symmetrically placed 4^2 full factorial. The diagram showing D and $F \setminus D$ is

$$\begin{array}{cccc} \times & \times & \times & \times \\ \times & \bullet & \bullet & \times \\ \times & \bullet & \bullet & \times \\ \times & \times & \times & \times \end{array}$$

The complement of the full factorial (bullets) is the crosses. The two bases $L(D)$ and $L^*(D)$ are shown below, where we have preserved the bullet and cross notation.

$$\begin{array}{cc} & \\ & \\ \bullet & \bullet \\ \bullet & \bullet \end{array} \qquad \begin{array}{cccc} \times & \times & & \\ \times & \times & & \\ \times & \times & \times & \times \\ \times & \times & \times & \times \end{array}$$

The second diagram gives the basis:

$$L^*(D) = \{1, x_1, x_2, x_1^2, x_1x_2, x_2^2, x_1^3, x_1^2x_2, x_1x_2^2, x_2^3, x_1^3x_2, x_1x_2^3\}.$$

Now take the design of 12 points shown above with crosses and obtain its complement within a 6×6 factorial. Both designs are shown in the next diagram. The 12 points signalled by crosses as before, and its complement shown with diamonds:

$$\begin{array}{cccccc} \diamond & \diamond & \diamond & \diamond & \diamond & \diamond \\ \diamond & \times & \times & \times & \times & \diamond \\ \diamond & \times & \diamond & \diamond & \times & \diamond \\ \diamond & \times & \diamond & \diamond & \times & \diamond \\ \diamond & \times & \times & \times & \times & \diamond \\ \diamond & \diamond & \diamond & \diamond & \diamond & \diamond \end{array}$$

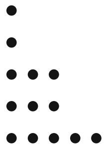
To compute the basis for the design with diamonds, the only action required is to compute the Alexander dual of the model for the design with crosses. The basis has diagram:

$$\begin{array}{cccccc} \diamond & \diamond & & & & \\ \diamond & \diamond & & & & \\ \diamond & \diamond & \diamond & \diamond & & \\ \diamond & \diamond & \diamond & \diamond & & \\ \diamond & \diamond & \diamond & \diamond & \diamond & \diamond \\ \diamond & \diamond & \diamond & \diamond & \diamond & \diamond \end{array}$$

To generate more designs easily, we shall use an extension of the staircase designs using symmetry. Consider the following diamond-shaped pattern.

$$\begin{array}{ccccc} & & \bullet & & \\ & \bullet & \bullet & \bullet & \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet & \\ & & \bullet & & \end{array} \tag{10}$$

We claim that this has basis given by the diagram

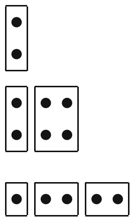


(11)

We have used the following symmetry result.

Theorem 3 *Let D be a design which (i) is invariant under all $\pm$ reflections through the origin in all coordinates (ii) $D_+ = D \cap \mathbb{R}^d_{\geq 0}$ is a staircase design. Then under any monomial order, the basis $L(D)$ is constructed from the (staircase) basis $L(D_+)$ using the following rule. Replace any basis element x^α for which r of the α_j components is non-zero by a block of 2^r monomials with "edges" $\{x^{2\alpha_j}, x^{2\alpha_j+1}\}$ for $\alpha_j \neq 0$.*

This is explained for the diamond (10) by boxing the points in (11):



The proof relies on the explicit construction of the G-basis. For clarity, we highlight below, for the diamond, the correspondence between the position of a leading term on $L(D_+)$ and $L(D)$.

Proof Let $\{x^{\beta^{(k)}}, k = 1, \ldots, m\}$ be the set of leading terms for the design D_+. We first exhibit the leading terms for the design D. They are $\{x^{\tilde{\beta}^{(k)}}, k = 1, \ldots, m\}$, where

$$\tilde{\beta}^{(k)}_j = \begin{cases} 2\beta^{(k)}_j - 1 & \text{if } \beta^{(k)}_j > 0 \\ 0 & \text{otherwise} \end{cases}$$

For D_+ the Gröbner basis is $\{g_k(x), k = 1, \ldots, m\}$, where $g_k(x)$ has an explicit formula, well known from the staircase property, $g_k(x) = \prod_{i=1}^d \prod_{j=0}^{\beta^{(k)}_j - 1} (x_i - j)$. In the diagram below, for the monomial marked with a star, $x_1^2 x_2$ is the leading term of $x_1(x_1 - 1)x_2$.

Every element of the Gröbner basis for D_+ gives us exactly one element for the Gröbner basis for D which is obtained by adding the sign changes. They are $\tilde{g}_k(x) = \prod_{i=1}^d \left(x_i \prod_{j=1}^{\beta^{(k)}_j - 1} (x_i \pm j) \right)$, where $(x_i \pm j) = (x_i - j)(x_i + j)$. The element of the Gröbner basis in the above example is $x_1(x_1 - 1)(x_1 + 1)x_2$ whose corresponding leading term for D is $x_1^3 x_2$.

We claim that the zero set of $\{\tilde{g}_k(x), k = 1, \ldots, m\}$ is the design D. This claim is verified by intersecting the zero set of all the $\tilde{g}_k(x)$, see Miller and Sturmfels (2005, Section 18.2). The fact that this set is a Gröbner basis is standard and follows from the position of the exponents in the staircase structure $L(D)$, and indeed it is also a universal Gröbner basis which establishes the result for any term ordering. □

$$
\begin{array}{lll}
 & & \qquad \bullet \\
 & & \qquad \bullet \\
\bullet & & \qquad \bullet\ \bullet\ \bullet \\
\bullet\ \bullet\ \times & & \qquad \bullet\ \bullet\ \bullet\ \times \\
\bullet\ \bullet\ \bullet & & \qquad \bullet\ \bullet\ \bullet\ \bullet\ \bullet
\end{array}
$$

The full Gröbner basis for the diamond shape in (10) is

$$
\begin{aligned}
&\{x_2(x_2+1)(x_2-1)(x_2+2)(x_2-2), x_1x_2(x_2+1)(x_2-1), \\
&x_1(x_1+1)(x_1-1)x_2, x_1(x_1+1)(x_1-1)(x_1+2)(x_1-2)\}.
\end{aligned}
$$

Using symmetry and complements we can produce a large variety of designs and read off the basis directly. As a final example consider the 7^2 tableau below in which the dot design is based on a double use of the reflection.

$$
\begin{array}{ccccccc}
\times & \bullet & \times & \times & \times & \bullet & \times \\
\bullet & \bullet & \bullet & \times & \bullet & \bullet & \bullet \\
\times & \bullet & \times & \times & \times & \bullet & \times \\
\times & \times & \times & \times & \times & \times & \times \\
\times & \bullet & \times & \times & \times & \bullet & \times \\
\bullet & \bullet & \bullet & \times & \bullet & \bullet & \bullet \\
\times & \bullet & \times & \times & \times & \bullet & \times
\end{array}
$$

Using Theorem 3, the respective bases are given by the following patterns;

$$
\begin{array}{lll}
 & & \times \\
\bullet\ \bullet & & \times \\
\bullet\ \bullet & & \times\ \times\ \times\ \times\ \times \\
\bullet\ \bullet & & \times\ \times\ \times\ \times\ \times \\
\bullet\ \bullet & & \times\ \times\ \times\ \times\ \times \\
\bullet\ \bullet\ \bullet\ \bullet\ \bullet\ \bullet & & \times\ \times\ \times\ \times\ \times \\
\bullet\ \bullet\ \bullet\ \bullet\ \bullet\ \bullet & & \times\ \times\ \times\ \times\ \times\ \times\ \times
\end{array}
$$

3.4 Combining interpolators over fractions

In experimental design, it is often of interest to combine information coming from different experiments. In the following example we describe a technique to combine interpolators, where the emphasis is on combining information and still achieving interpolation. This technique is a variation of the general interpolation technique described by Becker and Weispfenning (1991).

Theorem 4 *Let F be a full factorial design, and let D and $\bar{D}$ be complementary fractions of F. For a fixed term ordering, let y_F, y_D and $y_{\bar{D}}$ be the exact interpolators of data with respect to their basis $L(F), L(D)$ and $L(\bar{D})$. Then y_f =*

$NF\left(y_D 1_D + y_{\bar{D}}(1 - 1_D), I(F)\right)$, where 1_D and $1_{\bar{D}}$ are the polynomial indicator functions of D and $\bar{D}$ over F, and $NF(f, I)$ is the normal form of the polynomial F with respect to the ideal I.

Proof The polynomial indicators of the design fraction D and of its complement $\bar{D} := F \setminus D$ are linear combinations of monomials in $L(F)$, defined as $1_D(x) = \begin{cases} 1 \text{ if } x \in D \\ 0 \text{ if } x \in \bar{D} \end{cases}$ and $1_{\bar{D}}(x) = (1 - 1_D(x))$. The interpolating polynomial functions y_D and $y_{\bar{D}}$, when multiplied by indicators yield $1_D(x) y_D(x) = \begin{cases} y_F(x) & \text{if } x \in D \\ 0 & \text{if } x \in \bar{D} \end{cases}$ and $1_{\bar{D}}(x) y_{\bar{D}}(x) = \begin{cases} 0 & \text{if } x \in D \\ y_F(x) & \text{if } x \in \bar{D} \end{cases}$ and thus $y_D 1_D + y_{\bar{D}}(1 - 1_D)$ equals y_F over all points in F. However, this sum $y_D 1_D + y_{\bar{D}}(1 - 1_D)$ contains terms of high degree and does not coincide with y_F outside points in F. By taking its normal form we achieve the desired result. The uniqueness of the normal form guarantees the equality with y_F. □

Example 7 The numbers 12, 10, 6, 16, 18, 20, 24, 14 are synthetic response values for a full factorial experiment F in three factors x_1, x_2, x_3, each with two levels ± 1. The response values above are presented in Yates' order, see Box et al. (2005).

Set D to be the regular 2^{3-1} fraction of F with generator $x_1 x_2 x_3 = 1$ and set $\bar{D}$ to be the complementary fraction of D so that $D \cup \bar{D} = F$. For the standard term ordering in CoCoA, the basis for D is $L(D) = \{1, x_1, x_2, x_3\}$. By Theorem 2, bases $L(D)$ and $L(\bar{D})$ are mutual Alexander duals and so $L(\bar{D}) = L(D)$. Using the above data, the interpolator for response values over D is $y_D = 18 + 2x_2 + 4x_3$, and the corresponding interpolator over $\bar{D}$ is $y_{\bar{D}} = 12 - 2x_2 + 4x_3$.

We now combine interpolators over the fractions to obtain a global interpolator. To achieve this, we use indicator functions $1_D = (1 - x_1 x_2 x_3)/2$ and $1_{\bar{D}} = 1 - 1_D$ so that

$$y_D 1_D + y_{\bar{D}}(1 - 1_D) = 15 + 4x_3 - 3x_1 x_2 x_3 - 2x_1 x_2^2 x_3, \tag{12}$$

which although interpolating the data, contains higher order terms. A reduction of (12) computing the normal form (see Cox et al. 2007) with respect to the ideal of the full design F gives the interpolator

$$y_F = 15 + 4x_3 - 2x_1 x_3 - 3x_1 x_2 x_3.$$

This reduced polynomial still interpolates the given response values over the full design F, and coincides with the interpolating polynomial using all of the design and data.

The results above concern interpolation. Using Alexander duality ideas to attain relationships between testing, residuals etc. over D and $\bar{D}$ is under development.

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