

# Minimal average degree aberration and the state polytope for experimental designs

Yael Berstein <sup>a</sup>, Hugo Maruri-Aguilar <sup>b,\*</sup>, Shmuel Onn <sup>a</sup>,  
Eva Riccomagno <sup>c</sup>, Henry Wynn <sup>b</sup>

<sup>a</sup>*Technion, Israel Institute of Technology, Haifa 32000, Israel*

<sup>b</sup>*Department of Statistics, London School of Economics, London WC2A 2AE, UK*

<sup>c</sup>*Dipartimento di Matematica, Università di Genova, Genova 16146, Italy*

---

## Abstract

For a particular experimental design, there is interest in finding which polynomial models can be identified in the usual regression set up. The algebraic methods based on Gröbner bases, developed by G Pistone, H P Wynn, E Riccomagno and co-authors, provide a systematic way of doing this. The algebraic method does not in general produce all estimable models but it can be shown that it yields models which have minimal average degree in a well-defined sense and in both a weighted and unweighted version. This provides an alternative measure to that based on “aberration” and moreover is applicable to any experimental design. Bounds are derived for the criteria and a simple algorithm given.

*Key words:* Linear aberration, design ideal, factorial design, Latin Hypercube sampling, corner cut, state polytope.

---

## 1 Introduction

It is of considerable value to represent an experimental design as the solution of a set of polynomial equations. In the terminology of algebraic geometry a design is a zero dimensional variety and the corresponding ideal comprising all polynomials which are zero on every design point is called an “ideal of points”. Issues to do with identifiability of polynomial regression models, or

---

\* Corresponding author.

*Email address:* H.Maruri-Aguilar@lse.ac.uk (Hugo Maruri-Aguilar).

interpolators, can be translated into problems about such varieties and ideals, see [25].

The purpose of this paper is to introduce the notion of linear aberration of a polynomial model for an experimental design. The definition of it is given below to help the motivation.

Let  $\alpha = (\alpha_1, \dots, \alpha_d)$  be a nonnegative  $d$ -dimensional integer multi-index. A monomial in the indeterminates  $x_1, \dots, x_d$  is the power product  $x^\alpha = x_1^{\alpha_1} \cdots x_d^{\alpha_d}$ . A *model basis* is a collection of distinct monomials  $\{x^\alpha, \alpha \in L\}$ , where  $L$  is a finite set of multi-indices. By combining linearly monomials in  $L$  we form polynomials:

$$\eta_L(x) = \sum_{\alpha \in L} \theta_\alpha x^\alpha,$$

where  $\theta_\alpha$  are real coefficients. The polynomial  $\eta_L(x)$  is a candidate for interpolation or statistical modelling.

This paper is concerned with the following concept.

**Definition 1** *Let  $L$  be a model basis and let  $w = (w_1, \dots, w_d)$  be a collection of non-negative weights with  $\sum_{i=1}^d w_i = 1$ . We define the weighted linear aberration of  $L$  as*

$$A(w, L) = \frac{1}{n} \sum_{(\alpha_1, \dots, \alpha_d) \in L} \sum_{i=1}^d w_i \alpha_i, \quad (1)$$

where  $n$  is the number of elements in  $L$ .

We shall often refer to the linear aberration of Equation (1) simply as aberration. We are interested in studying aberration for models identifiable by an experimental design. We are also interested in comparing models and designs of the same size  $n$  with this concept.

**Definition 2** *An experimental design  $D$ , of sample size  $n = |D|$ , is a set of points in  $\mathbb{R}^d$ .*

We say that a model basis  $L$  with cardinality  $|L| = n$  is identifiable by  $D$  if the design model matrix  $X = [x^\alpha]_{x \in D, \alpha \in L}$  is invertible.

We use the name aberration to acknowledge the work on “minimum aberration” for regular fractional factorial designs of Wu and others, see [13] and [29]. We do not make a direct mathematical comparison with that work but simply point to a common motivation. For a given experimental design the ability to identify models,  $\eta_L$ , with low linear aberration is advantageous. The weight vector  $w = (w_1, \dots, w_d)$  creates a simple way of preferring one factor over another, which extends readily to the selection of the elements in  $L$ . One advantage of the method of this paper is being applicable to an arbitrary design.

In Section 2 we review the basic ideas on algebraic identifiability. The search for identifiable models is driven by a divisibility condition, which makes the search problem tractable. We then introduce the *state polytope*, whose vertices correspond to the models identified using the algebra. In Section 3 we study aberration. The basic ideas on aberration are closely linked with the algebraic work on corner cut models and state polytopes by Onn and Sturmfels in [22]. We are specially interested in obtaining minimal values for aberration for which we establish upper and lower bounds. An approximate approach to minimal aberration is discussed. In Section 4 we discuss various examples. In Section 5 we discuss possible extensions of the theory and, by example, a connection with the notion of aberration by Wu and others is discussed.

## 2 The G-basis method and the state polytope

The aberration  $A(w, L)$  has remarkable connections with the algebraic method in experimental design introduced by Pistone and Wynn [26] and outlined in the monograph [25] and joint work of Onn and Sturmfels. In this Section we present the basic ideas on identifiability using algebraic techniques.

Let the set of all monomials in  $d$  indeterminates be  $T^d = \{x^\alpha, \alpha \in \mathbb{Z}_{\geq 0}^d\}$ , where  $\mathbb{Z}_{\geq 0}$  is the set of non-negative integers and  $\mathbb{Z}_{\geq 0}^d$  is the set of all vectors in  $d$  dimensions and with entries in  $\mathbb{Z}_{\geq 0}$ . A polynomial is a finite linear combination of monomials in  $T^d$  with real coefficients. The set of all polynomials is denoted as  $\mathbb{R}[x_1, \dots, x_d]$ . It has the structure of a ring with the usual operations of sum and product of polynomials.

A term ordering  $\succ$  on  $\mathbb{R}[x_1, \dots, x_d]$  is a total ordering on  $T^d$  such that i)  $x^\alpha \succ 1$  for all  $x^\alpha \in T^d$ ,  $\alpha \neq (0, \dots, 0)$  and ii) for all  $x^\alpha, x^\beta, x^\gamma \in T^d$  if  $x^\alpha \succ x^\beta$  then  $x^\alpha x^\gamma \succ x^\beta x^\gamma$ . The leading term of a polynomial is the largest term with non-zero coefficient with respect to  $\succ$ . For a polynomial  $f \in \mathbb{R}[x_1, \dots, x_d]$ , we write its leading term as  $\text{LT}_\succ(f)$ .

A partial order on  $T^d$  is defined by a vector  $w \in \mathbb{R}_{\geq 0}^d$  as  $x^\alpha \succeq_w x^\beta$  if  $w^T \alpha \geq w^T \beta$ , where  $x^\alpha, x^\beta \in T^d$  and  $w^T$  is the transposed vector of  $w$ . Under some conditions on  $w$  (see [1, 10]) this defines a term order. Given a term order  $\succ$ , there are  $w$  such that  $x^\alpha \succ x^\beta$  if and only if  $x^\alpha \succeq_w x^\beta$ .

A design  $D$ , considered as a zero-dimensional variety gives rise to a *design ideal*,  $I(D)$  which is the set of all polynomials which have zeros at all the points of  $D$ . We have that  $I(D) \subset \mathbb{R}[x_1, \dots, x_d]$ . The polynomial ideal  $I$  is generated by the set of polynomials  $G = \{g_1, \dots, g_s\}$  if  $I = \{\sum_{i=1}^s f_i g_i : f_i \in \mathbb{R}[x_1, \dots, x_d]\}$  and we write  $I = \langle g_1, \dots, g_s \rangle$ .

An important set of generators for the design ideal is the Gröbner basis. Gröbner bases were introduced by Buchberger in [5] and they have become a powerful computational tool in many fields [10, 11]. A Gröbner basis of  $I(D)$  with respect to a term order  $\succ$  is a finite subset  $G_\succ(D) \subset I(D)$  such that  $\langle \text{LT}_\succ(g) : g \in G_\succ(D) \rangle = \langle \text{LT}_\succ(f) : f \in I(D) \rangle$ . The computation of Gröbner bases is implemented in standard computer programs such as CoCoA, Singular or Maple, see [8, 15, 19].

Two polynomials  $f$  and  $g$  in  $\mathbb{R}[x_1, \dots, x_d]$  are equivalent with respect to  $I(D)$  if the following conditions hold:

- i)  $f - g \in I(D)$
- ii)  $f(d) = g(d)$  for all  $d \in D$

Given a term ordering  $\succ$ , the quotient ring  $\mathbb{R}[x_1, \dots, x_d]/I(D)$  has a unique  $\mathbb{R}$ -vector space basis given by the monomials in  $T^d$  that cannot be divided by the leading terms of the polynomials in  $G_\succ(D)$  for  $I(D)$ . The monomial basis so obtained, or equivalently, the set of its exponents  $L = L(D, \succ)$ , has a *staircase* (also *echelon*, *order ideal*) property: for  $\alpha \in L$ , if  $\beta \leq \alpha$  componentwise, then  $\beta \in L$ . Equivalently we say that for any  $x^\alpha \in L$ , if  $x^\beta$  divides  $x^\alpha$  then  $x^\beta \in L$ . We call bases which have a staircase structure *staircase models*. The dimension of  $\mathbb{R}[x_1, \dots, x_d]/I(D)$  as  $\mathbb{R}$ -vector space is  $n$  [26], i.e. the number of points in  $D$  and of multi-indices in  $L$  is  $n$ .

For a given basis of the quotient ring and a set of real values (data)  $Y_x, x \in D$ , there exists a unique interpolator  $\eta_L(x)$  such that  $Y_x = \eta_L(x)$ ,  $x \in D$ . Other non-saturated statistical sub-models can be constructed from subsets of  $L$ , see [16, 23].

**Definition 3** *The algebraic fan of  $D$  is  $\mathcal{L}_a(D) = \{L(D, \succ), \text{ where } \succ \text{ is a term ordering in } \mathbb{R}[x_1, \dots, x_d]\}$ . This is the collection of staircases  $L(D, \succ)$  arising from a fixed design  $D$  by varying all monomial orderings.*

The algebraic fan of a design was proposed in [6] while the algebraic fan of an ideal is introduced in [20]. Babson *et al.* in [1] proposed a polynomial time algorithm to compute  $\mathcal{L}_a(D)$ . They compute an efficient set of weight vectors and perform a change of basis which stems from the so-called FGLM algorithm, see [12]. In Section 3.1 an algorithm is presented to identify a model in the algebraic fan using a weight vector.

It is important to note that not all staircase models identified by  $D$  are in  $\mathcal{L}_a(D)$ . We denote the set of all identifiable staircase models for a design  $D$  as  $\mathcal{L}_s(D)$ . In fact the algebraic fan is small relative to  $\mathcal{L}_s(D)$ , that is  $\mathcal{L}_a(D) \subseteq \mathcal{L}_s(D)$ , see Chapter 6 in [17] and Section 4 in [24].

We now establish the link between the algebraic fan of a design and the state

polytope of the design ideal. For a model basis  $L$  define

$$\bar{\alpha}_L = \sum_{(\alpha_1, \dots, \alpha_d) \in L} \alpha_i \in \mathbb{Z}_{\geq 0}^d.$$

This vector appears in the definition of  $A(w, L)$  and we can write  $A(w, L) = (w^T \bar{\alpha}_L)/n$ . The set all such vectors over  $\mathcal{L}_a(D)$  gives the state polytope.

**Definition 4** *The state polytope  $S(D)$  of a design  $D$ , or equivalently of the design ideal  $I(D)$  is the convex hull*

$$S(D) := \text{conv}(\{\bar{\alpha}_L : L \text{ is a staircase in } \mathcal{L}_a(D)\}).$$

The following theorem summarizes the connection between the state polytope and the set of models  $\mathcal{L}_a(D)$ , i.e. the relation between a design and its algebraic fan.

**Theorem 1** (*Sturmfels, 1995*) *Let  $D$  be a design and let  $S(D)$  be its state polytope. Then the set of vertices of the state polytope of  $D$  is in one to one correspondence with the algebraic fan of  $D$ .*

The state polytope does not only contain information concerning models in the algebraic fan of a design, but it also provides information about the term ordering vectors needed to construct it. We recall that a  $d$ -dimensional polytope is a bounded subset of  $\mathbb{R}^d$ , which corresponds to the solutions of a system of linear inequalities. The *normal cone* of a face of a polytope is the relatively open cone of those vectors in  $\mathbb{R}^d$  uniquely minimised over the face of the polytope. The *normal fan* of a polytope is the collection of all the normal cones of the polytope.

Two ordering vectors  $w$  and  $w'$  are equivalent (modulo  $I(D)$ ) if  $L(D, \succ_w) = L(D, \succ_{w'})$ . The normal fan of the state polytope partitions  $\mathbb{R}_{\geq 0}^d$  into equivalence classes of ordering vectors, see [1, 14, 27]. Indeed every vertex of  $S(D)$  corresponds to a model in  $\mathcal{L}_a(D)$ . Moreover, the interior of the normal cone of a vertex in  $S(D)$  contains those vectors  $w$  which correspond to the same equivalence class.

We motivate Theorem 2 below with a simple example. The black dots in Figure 1 give a 5 point design in 2 dimensions,  $D$ . They also give the set of exponents  $L$  obtained for any term ordering, indeed the size of the algebraic fan of  $D$  is one. The crosses represent the exponents of the leading terms of the Gröbner basis:  $(2, 0)$ ,  $(1, 2)$ ,  $(0, 3)$ . The line separates the model exponents,  $L$ , from these leading terms. This is an example of a *corner cut* model. Note that equivalently the line separates  $L$  from its complement in  $\mathbb{Z}_{\geq 0}^2$ .

**Definition 5** *A model  $L$ , of size  $|L| = n$ , is said to be a corner cut model if*

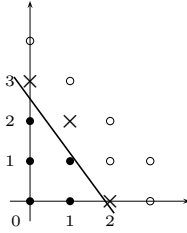


Fig. 1. Corner cut and separating hyperplane.

there is a  $(d - 1)$  dimensional hyperplane separating  $L$  from its complement  $\mathbb{Z}_{\geq 0}^d \setminus L$ .

Not all staircases are corner cuts, for example  $L = \{(0, 0), (1, 0), (0, 1), (1, 1)\}$  is a staircase that cannot be separated by a hyperplane from its complement in  $\mathbb{Z}_{\geq 0}^2$ .

The set of exponents of a corner cut model is referred to as a corner cut staircase or simply, as a corner cut. Corner cuts were introduced by Onn and Sturmfels in [22]. A generating function for the number of bidimensional corner cuts is given in [9], while the order of the cardinality of the set of corner cuts is proven bounded by  $(n \log n)^{d-1}$  in [28]. A special class of designs is composed with those designs that identify all corner cut models of a given size.

**Definition 6** A design  $D \subset \mathbb{R}^d$  comprised of  $n$  distinct points is said to be generic if all corner cut models of size  $n = |D|$  are identifiable.

A special polytope is constructed with the exponents for corner cut models. It will be used to compute the algebraic fan of generic designs.

**Definition 7** The corner cut polytope is  $CC(n, d) := \text{conv}(\{\bar{\alpha}_L : L \text{ is a corner cut staircase in } d \text{ dimensions and of size } n\})$ .

For a discussion on the properties of bidimensional corner cut polytopes see [21]. The algebraic fan of generic designs corresponds to the set of corner cut models, as stated in the following theorem.

**Theorem 2** (Onn and Sturmfels, 1999) Let  $D \subset \mathbb{R}^d$  be a generic design with  $n$  points. Then

- i)  $S(D) = CC(n, d)$  and
- ii) the algebraic fan of  $D$  is the set of corner cut models in  $d$  dimensions and with  $n$  elements.

We remark that the corner cut polytope is an invariant object for the class of all the ideals generated by generic designs with the same sample size  $n$  and number of factors  $d$  and all generic designs have the same state polytope.

### 3 Minimal linear aberration

An important feature of the state polytope is that its vertices are automatically “lower” vertices in the sense of convexity. State polytopes relate directly to models with minimal linear aberration. In Section 3.1 an algorithm to compute a models of minimal aberration is presented.

**Theorem 3** *Given a design  $D \subset \mathbb{R}^d$  with  $n$  distinct points and a weight vector  $w \in \mathbb{R}_{>0}^d$ , there is a least one vertex  $\alpha^* \in S(D)$  which minimises  $A(w, L)$  over all identifiable staircase models  $\mathcal{L}_s(D)$ , that is*

$$\frac{1}{n}(w^T \alpha^*) = A(w, L^*) = \min_{L \in \mathcal{L}_s(D)} A(w, L)$$

for all  $L^*$  such that  $\bar{\alpha}_{L^*} = \alpha^*$ . Moreover, given a vertex of  $S(D)$ , there is at least one  $w^* \in \mathbb{R}_{>0}^d$  such that this vertex (model) minimizes  $A(w, L)$ , that is,

$$A(w^*, \bar{L}) = \min_{w \in \mathbb{R}_{>0}^d} A(w, L)$$

for  $\bar{L}$  such that  $\bar{\alpha}_{\bar{L}} = \bar{\alpha}_L$ .

**Proof.** First, for given  $w$  we minimise  $w^T \bar{\alpha}_L$  for  $L \in \mathcal{L}_a(D)$ , which is a finite set, see [20]. The  $\bar{\alpha}_L$  for  $L \in \mathcal{L}_a(D)$  are vertices of  $S(D)$  by definition. Furthermore, because we restrict  $L$  to the algebraic fan of  $D$  there cannot be three aligned  $\bar{\alpha}_L$  in  $S(D)$ , see [27]. For the second claim, it is sufficient to take a vector  $w_L$  in the interior of a normal cone for  $\bar{\alpha}_L$ . By definition,  $A(w, L)$  is minimised for vectors on the interior of the normal cone. ■

Theorem 4 follows directly from Theorem 3.

**Theorem 4** *For every weight vector  $w$  there is a design  $D \subset \mathbb{R}^d$  which minimizes  $A(w, L)$ , among all designs with sample size  $n$  and identifiable staircases.*

This is stated compactly as:

$$A^*(w, n) = \min_{D: |D|=n} \min_{L \in \mathcal{L}_a(D)} A(w, L)$$

is achieved for a generic design. That is, if a design is generic then automatically its algebraic fan contains models of minimal aberration.

#### 3.1 Computation of the minimal aberration model

The model minimizing linear aberration can be found by the *greedy algorithm*. Let  $D$  be a design; let  $w$  be a fixed weight vector in  $\mathbb{R}_{>0}^d$  and let  $\Gamma$  be the

following set of potential exponents

$$\Gamma := \left\{ \alpha = (\alpha_1, \dots, \alpha_d) \in \mathbb{N}^d : \prod_{i=1}^d (\alpha_i + 1) \leq n \right\}.$$

The set  $\Gamma$  contains all staircase models with  $n$  terms, see [1]. Now define the *weight* of  $\alpha \in \Gamma$  to be  $\omega(\alpha) := \frac{1}{n} \sum_{i=1}^d w_i \alpha_i = (w^T \alpha)/n$ . Order the vectors in  $\Gamma$  by their weight  $\omega(\cdot)$  in increasing order, that is, index them as  $\alpha^1, \dots, \alpha^{|\Gamma|}$  such that  $\omega(\alpha^1) \leq \dots \leq \omega(\alpha^{|\Gamma|})$ , where  $|\Gamma|$  is the cardinality of  $\Gamma$ . Then the set  $L \subseteq \Gamma$  with the first  $n$  terms of  $\Gamma$  which are identifiable by  $D$  has minimum aberration.

The model basis  $L$  is constructed by the following procedure: initialize  $L := \emptyset$ ; while  $|L| < n$ , find  $\alpha^i$  of smallest index with respect to  $\omega(\cdot)$  such that the column vectors  $d^\alpha$ ,  $\alpha \in L \cup \{\alpha^i\}$ ,  $d \in D$ , are linearly independent; update  $L := L \cup \{\alpha^i\}$  and repeat until  $|L| = n$ . We have the following theorem.

**Theorem 5** *Let  $D \subset \mathbb{R}^d$  be a design; let  $w$  be a fixed weight vector with positive entries and let  $L$  be the model basis constructed by the greedy algorithm. Then  $L$  belongs to the algebraic fan of the design.*

**Example 1** Consider the design  $D = \{(0, 0), (1, 0), (0, 1), (-1, 1)\}$  and the weight vector  $w = (4, 1)$ . The set of potential exponents,  $\Gamma$  contains 8 elements, which are sorted out using the weight function  $\omega(\cdot)$  as

$$\begin{array}{l} \Gamma = \{ (0, 0), (0, 1), (0, 2), (0, 3), (1, 0), (1, 1), (2, 0), (3, 0) \} \\ n\omega(\cdot) = \quad 0 \quad 1 \quad 2 \quad 3 \quad 4 \quad 5 \quad 8 \quad 12 \end{array}$$

The first 4 elements in  $\Gamma$  such that their design columns are linearly independent are  $L = \{(0, 0), (0, 1), (1, 0), (0, 1)\}$ . Thus the set  $L$  of minimal linear aberration corresponds to the model with terms  $\{1, x_1, x_2, x_1x_2\}$ .

### 3.2 Examples

We can compare different designs using aberration as long as they have the same number of factors  $d$  and the number of points  $n$ . For a design  $D$ , the state polyhedron of  $D$  is obtained by (Minkowski) addition of  $\mathbb{R}_{\geq 0}^d$  to the state polytope  $S(D)$  [1]. The state polyhedron yields the same information as the state polytope. Indeed the normal fan of the (negative) state polyhedron yields automatically the first orthant [14].

**Example 2** Consider a central composite design (CCD, see [4]) with two factors, one observation at the origin and axial distance  $\alpha = \sqrt{2}$ . The CCD



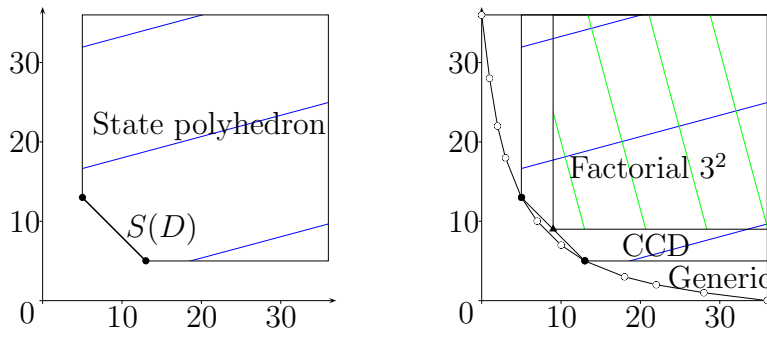


Fig. 2. The left graph depicts  $S(D)$  and the state polyhedron for the CCD of Example 2. The right graph shows state polyhedrons for the three designs of Example 2. The empty dots correspond to vertexes/models identified by the generic design only, while the triangle is for the sole model in the algebraic fan of the  $3^2$  design.

has 9 runs and its algebraic fan contains exactly two models, namely

$$\{1, x_1, x_1^2, x_1^3, x_1^4, x_2, x_1x_2, x_1^2x_2, x_2^2\} \quad (2)$$

together with the model obtained by permuting the roles of  $x_1$  and  $x_2$ . Let  $L_1$  be the set of exponents of the model support in Equation (2). Clearly,  $\bar{\alpha}_{L_1} = (13, 5)$  and the state polytope for the design ideal of the CCD is  $\text{conv}(\{(13, 5), (5, 13)\})$ , see left graph of Figure 2. Now consider a generic design with the same number of runs as the CCD. In [9, 22] it is shown that there are 12 corner cut models for  $d = 2$  and  $n = 9$ . By Theorem 2, the algebraic fan of the generic design contains all the 12 corner cut models, including those in the algebraic fan of the CCD. We consider also a full factorial design  $3^2$ , which identifies only the model with support  $\{1, x_1, x_1^2\} \otimes \{1, x_2, x_2^2\}$ , where  $\otimes$  is the Kronecker product. Its state polytope is the point  $(9, 9)$ . In the right graph of Figure 2 we depict the state polyhedrons for the three designs and in Figure 3 we plot  $\min_{L \in \mathcal{L}_a(D)} A(w, L)$  for  $w = (w_1, w_2) \in [0, 1]^2$  and  $w_1 + w_2 = 1$ . For the CCD this is

$$\begin{cases} ((w_1, 1 - w_1)(13, 5)^T) / 9 = (8w_1 + 5) / 9 & \text{if } w_1 \leq 1/2 \\ ((w_1, 1 - w_1)(5, 13)^T) / 9 = (-8w_1 + 13) / 9 & \text{if } w_1 > 1/2 \end{cases}$$

For the generic design the aberration curve is a piecewise linear function with 12 segments. Finally, the aberration for the design  $3^2$  is constant for all weights. As expected, the aberration takes its minimum value for the generic design, over all possible weights.

**Example 3** Consider the design  $D = \{(0, 0), (1, 1), (2, 2), (3, 4), (5, 7), (11, 13), (\alpha, \beta)\}$ , where  $(\alpha, \beta) \approx (1.82997, 1.82448)$  is the only real solution of a system of polynomial equations, see [22, Page 47]. The algebraic fan of the above design has ten models and its state polytope is

$$\text{conv}(\{(21, 0), (15, 1), (11, 2), (9, 3), (6, 5), (5, 6), (3, 9), (2, 11), (1, 15), (0, 21)\}).$$

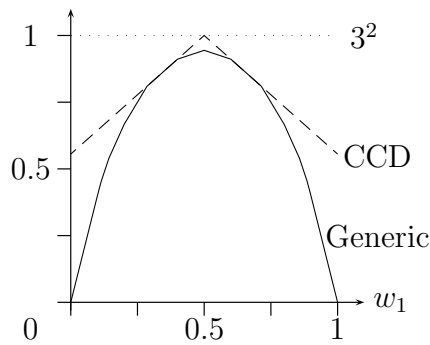


Fig. 3. Minimal aberration for three designs in two factors and nine runs, see Example 2.

Now consider a generic design  $G$  with the same number of runs and factors. The algebraic fan of  $G$  is the set of corner cut models which for 7 points in 2 dimensions has 8 elements [9, 22] and thus its state polytope is the corner cut polytope:

$$CC(7, 2) = \text{conv}(\{(21, 0), (15, 1), (11, 2), (7, 4), (4, 7), (2, 11), (1, 15), (0, 21)\}).$$

In Figure 4 we graph the aberration for both designs as a function of  $w_1$ . Although the size of the algebraic fan of  $D$  is bigger than that for a generic design, the weighted aberration takes minimal value for the generic design for all possible weight vectors  $(w_1, 1 - w_1)$ .

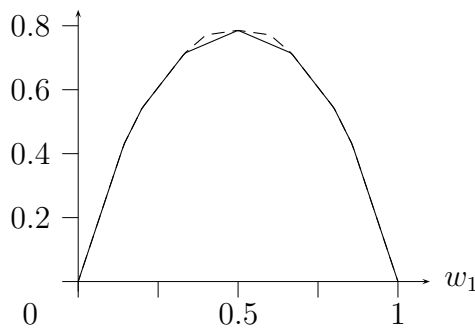


Fig. 4. Minimal aberration for  $G$  (solid line) and  $D$  (dashed line), see Example 3.

### 3.3 Bounds for the aberration

Although the minimal value of the aberration  $A^*(w, n)$ , depends on the weight vector  $w = (w_1, \dots, w_d)$ , we can carry out a special normalisation which leads to bounds for the minimal aberration. These bounds depend only on a simple function of the weights, surprisingly the geometric mean. Our construction is based upon the expected value of auxiliary random variables which are suitably constructed.

For the rest of this Section let  $D \subset \mathbb{R}^d$  be a generic design with  $n$  points. Let

$w$  be a fixed weight vector with positive elements and let  $L$  be the corner cut model identified by  $w$ . We recall that  $|L| = n$ .

For an integer multindex  $\alpha$  define its *upper cell* as the unit cube with lower vertex at  $\alpha$

$$\bar{c}(\alpha) = \{v \in \mathbb{R}^d : \alpha_i \leq v_i \leq \alpha_i + 1\}$$

and similarly the *lower cell* of  $\alpha$  is

$$\underline{c}(\alpha) = \{v \in \mathbb{R}^d : \alpha_i - 1 \leq v_i \leq \alpha_i\}$$

Define:

$$\underline{Q} = \cup_{\alpha \in L} \underline{c}(\alpha), \quad \bar{Q} = \cup_{\alpha \in L} \bar{c}(\alpha).$$

See Figure 5 for a depiction of lower and upper cells with  $L$  a corner cut.

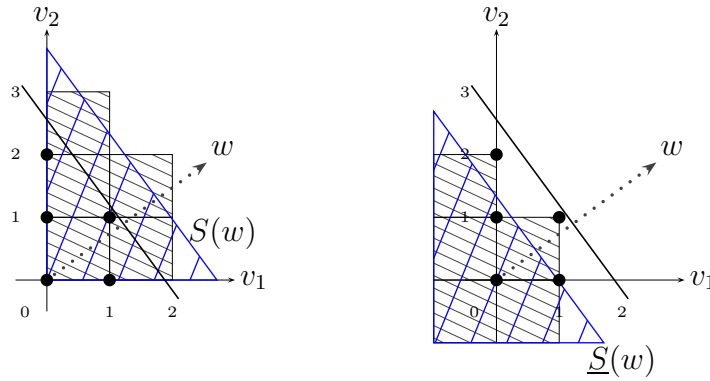


Fig. 5. Bidimensional corner cut together with upper (left diagram) and lower cells (right diagram)  $\bar{Q}$  and  $\underline{Q}$ . In both diagrams the vector  $w$ , a separating hyperplane and equivalent simplices  $S(w)$  and  $\underline{S}(w)$  were added.

Clearly, the volume of  $\bar{Q}$  and of  $\underline{Q}$  equals  $n$ , that is the cardinality of  $L$ . We now create a simplex  $S(w) \subset \mathbb{R}^d$  which is directed by the vector  $w$  and has volume  $n$ . We call this simplex and the subset of the first orthant below it the *equivalent simplex*, which is formally  $S(w) = \{v \in \mathbb{R}_{\geq 0}^d : \sum_{i=1}^d v_i w_i \leq c\}$ . The volume of  $S(w)$  is determined up to the constant  $c > 0$ . We find the value of this constant by setting the total volume of the equivalent simplex equal to  $n$ :

$$n = \frac{c^d}{d! \prod_{i=1}^d w_i},$$

giving

$$c = (nd!)^{\frac{1}{d}} g(w), \tag{3}$$

where

$$g(w) = \left( \prod_{i=1}^d w_i \right)^{\frac{1}{d}}$$

is the geometric mean of the components of the weight vector  $w$ . We call  $H(w)$  the hyperplane which limits the equivalent simplex, that is  $H(w) = \{v \in \mathbb{R}_{\geq 0}^d : \sum_{i=1}^d v_i w_i = c\}$ .

The expected value of a random variable with uniform support over  $S(w)$  will be used now to compute bounds for aberration. We can compute a notional value of  $A$ , the linear aberration for a distribution  $D$  as the expectation  $A(w, S(w)) = E(\sum w_i X_i)$  for the random vector  $(X_1, \dots, X_d)$  with uniform distribution over  $S(w)$ . Thus for the equivalent simplex we have that

$$A(w, S(w)) = \frac{1}{n} \frac{d}{(d+1)!} \frac{c^{d+1}}{\prod_{i=1}^d w_i} = (nd!)^{\frac{1}{d}} \frac{d}{d+1} g(w), \quad (4)$$

after substituting Equation (3) in  $A(w, S(w))$

We observe that the region  $\underline{Q}$  is obtained from  $\overline{Q}$  by a negative shift  $(-1, \dots, -1)$ . As before, we consider a random vector with joint uniform distribution over  $\underline{Q}$ . We then use the expected value of  $\sum w_i X_i$  as the aberration  $A(w, \underline{Q})$ . Analogously we define  $A(w, \overline{Q})$  and we have

$$A(w, \underline{Q}) = A(w, \overline{Q}) - 1$$

Similarly we can create a region  $\underline{S}(w)$  by the same downward shift, and we have

$$A(w, \underline{S}(w)) = A(w, S(w)) - 1.$$

As  $D$  is generic and thus  $L$  is a corner cut there exist cutting hyperplanes separating  $L$  from its complement in  $\mathbb{Z}_{\geq 0}^d$ . Moreover if  $w$  is in the interior of the normal cone of the corner cut polytope, then we can select a cutting hyperplane  $H$  which is orthogonal to  $w$  and thus parallel to  $H(w)$  [22].

**Example 4** Consider a generic design with  $d = 2, n = 3$  and  $L = \{(0, 0), (1, 0), (2, 0)\}$ . The weight vector  $w = (1, 2)$  is not in the interior of a normal cone of the corner cut polytope  $CC(2, 3)$ . Indeed the weight vector is on the boundary of the normal cone separating  $L$  from the corner cut model  $\{(0, 0), (1, 0), (0, 1)\}$ . The hyperplanes perpendicular to  $w$  are  $2x_1 - x_2 = c$  and none of them is a cutting hyperplane for  $L$ .

By a simple argument the simplex  $S_H$  with faces  $x_i = 0$ ,  $(i = 1, \dots, d)$  and  $H$  lies wholly within the upper quadrant region  $\overline{Q}$  because otherwise, the cutting hyperplane hypothesis for  $H$  would be violated and thus  $S_H$  has volume less than  $n$ . Recall that the equivalent simplex  $S(w)$  has volume  $n$ .

There is one additional argument that leads to our first inequality. Since the region  $\overline{Q}$  and the equivalent simplex  $S(w)$  have the same volume  $n$ , it must be that  $\overline{Q}$  protrudes beyond  $S(w)$ . Equivalently we may move mass from  $\overline{Q}$ , that is, beyond  $H(w)$ , inside  $S(w)$ . As this mass occurs orthogonally to  $w$ , we

claim that this movement diminishes the aberration, thus

$$A(w, S(w)) \leq A(w, \overline{Q}).$$

This property is also inherited by the downward shifted version, and we have  $A(w, \underline{S}(w)) \leq A(w, \underline{Q})$ . The same orthogonality argument shows the middle inequality in the following sequence:

$$A(w, \underline{S}(w)) \leq A(w, \underline{Q}) \leq A(w, S(w)) \leq A(w, \overline{Q}).$$

By Theorem 4, as the design is generic and  $L$  is the model identified by  $w$ , clearly we have

$$A(w, \underline{Q}) \leq A^*(w, n) \leq A(w, \overline{Q}).$$

Analogous argument and construction as above shows that  $A(w, \overline{Q}) \leq A(w, S(w)) + 1$ .

**Theorem 6** *Let  $D \subset \mathbb{R}^d$  be a generic design with  $n$  points; let  $w \in \mathbb{R}^d$  be a vector of positive weights. Then the minimal aberration  $A^*(w, n)$  satisfies the bounds*

$$A(w, S(w)) - 1 \leq A^*(w, n) \leq A(w, S(w)) + 1, \quad (5)$$

where  $A(w, S(w))$  is computed in Equation (4).

There are various kinds of asymptotic that this formula leads to. From the inequality between geometric and arithmetic mean we have  $g(w) \leq \frac{1}{d}$ . This suggests the condition:

$$g(w) \xrightarrow{d \rightarrow \infty} \frac{c}{d}$$

for some constant  $0 \leq c \leq 1$ . Now for  $w_i = \frac{1+\delta_i}{d}$ , with  $\sum \delta_i = 0$ , and assuming convergence of  $\sum \delta_i^2$  and  $n = k^d$ , we use Stirling's approximation to obtain

$$A^*(w, n) \xrightarrow{d \rightarrow \infty} \frac{kc}{e}.$$

**Example 5** For small  $d$  and  $n$  the bounds of Equation (5) are rather coarse. Figure 6 shows the bounds  $A(w, S(w)) \pm 1$  of Theorem 6 together with the minimal aberration  $A^*(w, n)$ , plotted as function of  $w_1$  for  $d = 2$  and  $n = 4$ . Notice that, as function of  $w$ , the minimal aberration  $A^*(w, n)$  is a piece-wise linear graph (this is a general fact, consequence of Definition 1), each segment corresponding to a different vertex (different corner cut) of the corner cut polytope. Figures 7 and 8 give the bounds and minimal aberration for  $n = 20$  and  $n = 100$ . In Figures 6, 7 and 8 we also added a curve for the approximate aberration which is presented in Theorem 7 below.

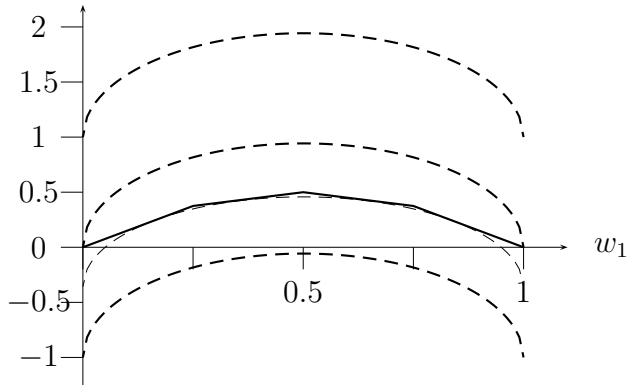


Fig. 6. Minimal aberration  $A^*(w, n)$  (solid line) for a generic design with  $d = 2$ ,  $n = 4$ ; bounds  $A(w, S(w))$  and  $A(w, S(w)) \pm 1$  of Theorem 6 (dashed lines). We also show approximate aberration  $\tilde{A}$  using Theorem 7 (thin dashed line).

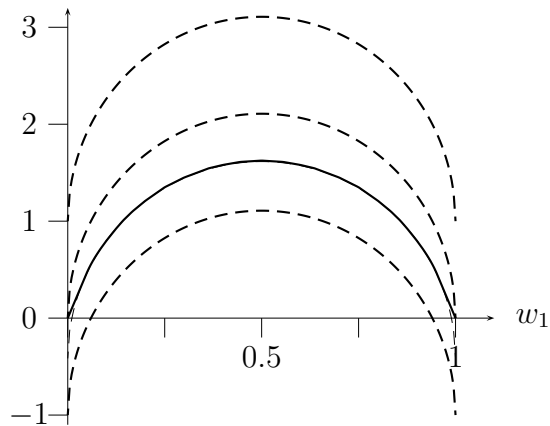


Fig. 7. Minimal aberration  $A^*(w, n)$  (solid line) for a generic design with  $d = 2$ ,  $n = 20$ ; bounds  $A(w, S(w))$  and  $A(w, S(w)) \pm 1$  and (dashed lines) of Theorem 6. The figure also shows approximate aberration  $\tilde{A}$  of Theorem 7 (thin dashed line) which almost overlaps the solid line.

### 3.4 Approximated state polytope for generic designs

Note that as  $w$  changes the hyperplanes  $H(w)$  are tangent to the surface defined by

$$\prod_{i=1}^d x_i = c^d = nd! \left(\frac{1}{d}\right)^d$$

and the (normalised) centroids of the equivalent simplices lie on the surface defined by

$$\prod_{i=1}^d x_i = b^+ = n \left(\frac{1}{d+1}\right)^d d! \quad (6)$$

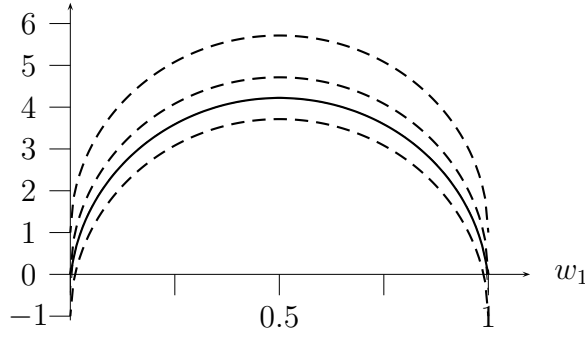


Fig. 8. Minimal aberration  $A^*(w, n)$  (solid line) for a generic design with  $d = 2$ ,  $n = 100$ ; bounds  $A(w, S(w))$  and  $A(w, S(s)) \pm 1$  (dashed lines). The approximate aberration  $\tilde{A}$  of Equation (8) (thin dashed line) is also plotted, but is undistinguishable from the minimal aberration.

We can solve an equivalent optimisation problem to the computations of  $A(w, S(w))$  in terms of the tangent surfaces: for all centroids lying above or on the surface of Equation (6), the minimum value of  $A(w, S(w))$  is achieved at the centroid of the tangent.

In the above argument, we are essentially using the surface in Equation (6) to approximate the lower border of the state polytope for a generic design, i.e. the lower border of the corner cut polytope. In order to improve the bounds given in Theorem 6, it seems natural simply to take a surface defined by

$$\prod_{i=1}^d (x_i + a) = b \quad (7)$$

with fixed  $a, b$ . In Theorem 6, we have  $a = \pm 1$  and  $b = b^+$  in Equation (6). In Appendix B we discuss an approach to select the values  $a, b$  to obtain a good approximation of the corner cut polytope.

The following theorem estimates minimal aberration for generic designs using the approximation of Equation (7). The proof is based on simple ideas of constrained optimization, see Appendix A.

**Theorem 7** *Let  $w = (w_1, \dots, w_d)$  be a fixed positive weight vector; let  $D \subset \mathbb{R}^d$  be a generic design with  $n$  points. Let the state polytope of  $I(D)$  be approximated by Equation (7). Then the value*

$$\tilde{A}(w) = db^{1/d}g(w) - a \sum_{i=1}^d w_i \quad (8)$$

*is an approximation of  $A^*(w, n)$ .*

We recall that  $g(w)$  is the geometrical mean of the components in  $w$ . Figures 6,

7 and 8 give examples ( $d = 2$  factors,  $n = 4, 20, 100$ ) of the minimal aberration  $\tilde{A}(w)$  in Theorem 7. The values  $a, b$  for each case were selected using the technique in Appendix B.

## 4 Examples

In this section we discuss through extended examples other possible uses of the ideas on generic designs and aberration. In Section 4.1 we explore and conjecture the existence of generic designs over Latin hypercubes for all factors and sample sizes. In Section 4.2 we compare fractional factorial designs through their state polytopes.

### 4.1 Latin hypercube design

Latin hypercube designs (LH) were first proposed in [18] in the context of computer experiments. Latin hypercubes are designs with reasonable space filling properties and good projections in lower dimensions.

Theorem 4 relates minimal aberration to generic designs, i.e. if the design is generic, then it identifies models of lower weighted degree (and minimal aberration) for any weight vector  $w$ . In what follows we study LH using Definition 6 of generic designs.

The construction of a Latin hypercube design can be summarised as follows.

- (1) Divide the range of each factor into  $n$  equal segments.
- (2) Select a value in each segment using a random uniform distribution, or any other continuous distribution.
- (3) Randomly permute the list for each factor.

By Theorem 30 in [25], a Latin hypercube design constructed as above is generic with probability one.

We now consider a special type of LH designs. This type is constructed by selecting a fixed value in every segment in Step 2. For instance, we could select the minimum, maximum or the midpoint value for every segment.

There are a few obvious cases of LH designs which are not generic, for example when the points of the design lie on a line. We have performed exhaustive search for a few cases of LH in two dimensions. Our search points out to the existence of generic LH for different values of  $d, n$ . In fact for the values we tried the proportion of generic LH tends clearly to one. See Figures 9 and



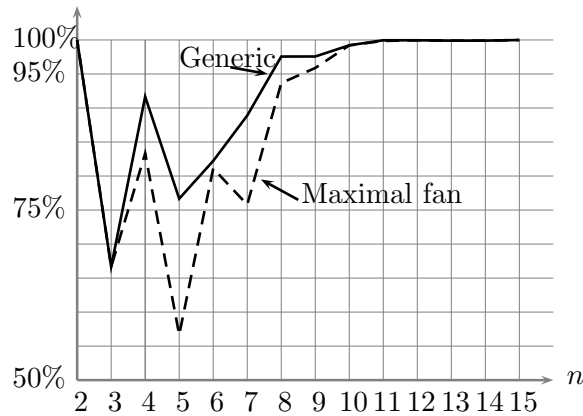


Fig. 9. Percentage of generic LHS designs for  $d = 2$  and  $n \leq 15$ .

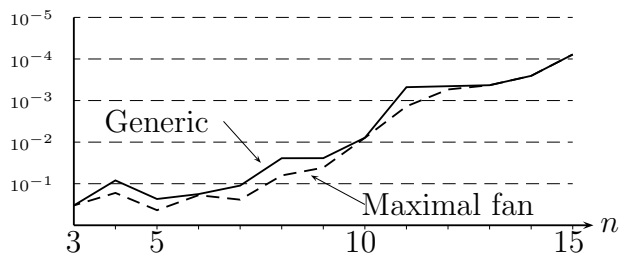


Fig. 10. Minus logarithm of the percentage of non generic LHS designs for  $d = 2$  and  $n \leq 15$ .

10 for a depiction of the results, where we additionally plot the proportion of *maximal fan* designs among LH, i.e. LH designs that identify all possible staircase models for given  $d, n$ . We have the following conjecture for the existence of generic LHS for any value of  $d, n$ .

**Conjecture 8** *For every  $d \geq 2$  and  $n \geq 2$  there exists at least one generic LH design, constructed by setting a fixed value for every one of the  $n$  segments in the above procedure.*

Experimentally we observed that when the sample size is  $n = \binom{k+1}{d}$  for  $k \geq 1$ , the genericity of a LH design is closely linked to the identification of a model of total degree  $k - 1$ . For example for  $k = 4, d = 2, n = 10$  there are  $10!$  LH of which 99% are generic. Of the remaining 1% which are not generic only 6 designs (up to reflection and rotation), which are given in Figure 11, identify the cubic model with exponent set

$$L = \{(0, 0), (1, 0), (0, 1), (2, 0), (1, 1), (0, 2), (3, 0), (2, 1), (1, 2), (0, 3)\}.$$

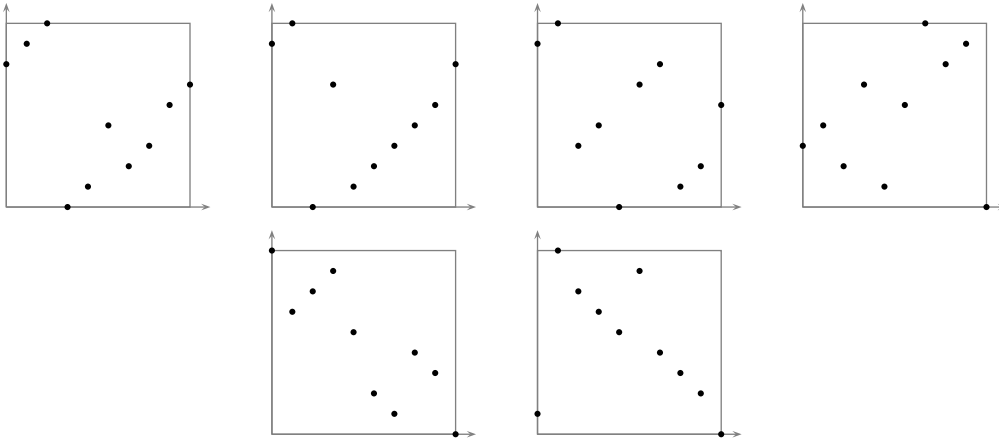


Fig. 11. LH on  $[0, 1]^2$  for  $d = 2, n = 10$  which are not generic and identify  $L$ .

#### 4.2 Orthogonal fractions

In this Section we consider some of the techniques of this paper for the class of fractional factorial designs with two levels. We first explore the relation between state polyhedron and then later propose a tool to compare the identification capability of designs.

In Examples 2 and 3 we observed that in general, nesting of state polyhedrons for two designs does not imply any easy relation between the algebraic fan of the designs. If instead we restrict to the family of designs with two levels then there is a clear relation between such nesting and algebraic fans. We have the following Lemma from Chapter 6 in [17].

**Lemma 9** *Let  $F_1$  and  $F_2$  be two fractional factorial designs with two levels and let  $S_1$  and  $S_2$  be their corresponding state polyhedrons of  $I(F_1), I(F_2)$ . Then the nesting of state polyhedrons  $S_1 \subset S_2$  implies nesting of algebraic fans  $\mathcal{L}_a(F_1) \subset \mathcal{L}_a(F_2)$ .*

The following example is based upon Lemma 9 and presents an interesting relation between resolution and identifiability. That is, bigger resolution points to more models in the algebraic fan.

**Example 6** Let  $F_1$  and  $F_2$  be the  $2_{IV}^{4-1}$  and  $2_{III}^{4-1}$  fractional factorial designs with eight runs in four factors and respective generators  $x_1x_2x_3x_4 - 1 = 0$  and  $x_1x_2x_3 - 1 = 0$ . The subindices III, IV refer to the *resolution* of the fraction, see [2, 3]. Their corresponding state polyhedrons are nested, i.e.  $S(F_2) \subset S(F_1)$  and by direct computation we confirm that the algebraic fans are also nested. The algebraic fan  $\mathcal{L}_a(F_2)$  has four models, while  $\mathcal{L}_a(F_1)$  includes 12 elements.

However, exploiting this nesting of fans to compare designs using *aberration* might need additional considerations.

**Example 7** Let  $F_1, F_2$  be the fractions  $2_{IV}^{7-2}$  given by generators  $x_6 - x_1x_2x_3 = 0, x_7 - x_2x_3x_4 = 0$  and  $x_6 - x_1x_2x_3x_4 = 0, x_7 - x_1x_2x_3x_5 = 0$  respectively. Although both fractions have the same resolution, the fraction  $F_2$  corresponds to a *minimum aberration design* using the definition of [13]. The state polyhedron  $S(F_1)$  has 133 vertices while  $S(F_2)$  has 1708. There is no nesting of the state polyhedrons and  $\mathcal{L}_a(F_1) \cap \mathcal{L}_a(F_2) \neq \emptyset$ .

A proposal to compare two designs  $D_1, D_2$  of the same size through their state polytopes is to map the vertices of the state polytopes  $S(D_1), S(D_2)$  with a function  $f : \mathbb{R}^d \rightarrow \mathbb{R}$ . In this way the state polytopes of  $D_1$  and  $D_2$  are compared by the univariate projections of their vertices. We propose a weighted sum of the vertex coordinates

$$f(v_1, \dots, v_d) = \sum_{i=1}^d w_i v_i, \quad (9)$$

with positive weights  $w_i > 0$ . We use  $w_i = 1$  for  $i = 1, \dots, d$  and thus Equation (9) allows for direct comparison of designs based on the distribution of total degrees for models in the algebraic fan.

**Example 8** (Continuation of Example 7) We transform the vertices of the state polytopes for  $F_1$  and  $F_2$  using Equation (9). In Table 1 in Appendix C we summarize the results for each fraction as the distribution of absolute and relative frequencies. Clearly, the fraction  $F_2$  with minimum aberration for generators identifies models with a smaller total degree than that for  $F_1$  and in that sense it has smaller linear aberration. See Figure 12 for a histogram of the relative frequencies for  $F_1$  and  $F_2$ .

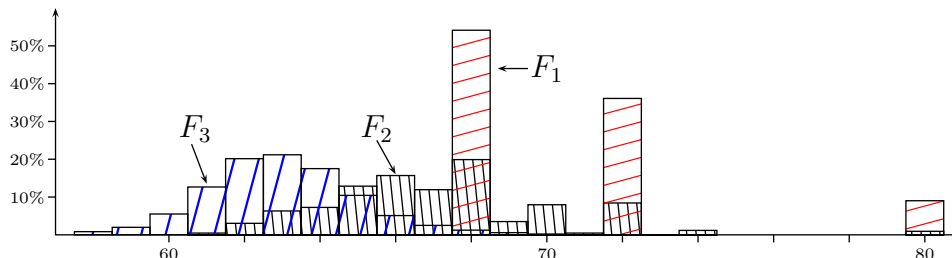


Fig. 12. Histograms of relative frequencies for fractions  $F_1$  and  $F_2$ , see Example 8. We added  $F_3$  of Example 9.

## 5 Discussion

### 5.1 Generalised concave aberration

This paper is partly concerned with a problem of linear programming, i.e. optimising a linear function  $f : \mathbb{R}^d \rightarrow \mathbb{R}$  over a convex polytope. We now dis-

cuss extensions of our work using other types of aberration. When we consider concave aberration criteria, some of our results still hold.

Consider any concave function  $f : \mathbb{R}^d \rightarrow \mathbb{R}$ . Now, given a model  $L$ , define its aberration by

$$A(f, L) := f \left( \sum_{\alpha \in L} \alpha_1, \dots, \sum_{\alpha \in L} \alpha_d \right).$$

The linear aberration of Definition 1 is the special case where  $f$  is the following linear (hence concave) function,

$$f : \mathbb{R}^d \longrightarrow \mathbb{R}$$

$$x = (x_1, \dots, x_d) \mapsto \frac{1}{n} \sum_{i=1}^d w_i x_i.$$

Since we only appealed to convexity, Theorem 3 is valid when we replace  $A(w, L)$  by the more general form  $A(f, L)$ . That is to say, the set of lower vertices of the state polytope (corresponding to models in the algebraic fan) contains the solution to minimising any concave aberration function. This will be exploited in further research. A further development is to consider aberration  $A(w, S(w))$  with respect to other distributions rather than the uniform.

## 5.2 Connection with aberration of Wu and others

In the statistical literature, the word aberration has been used to refer to properties of the generators for fractional factorial designs, see [7, 13, 29]. Another topic of future research is to link minimal aberration of Definition 1 with the traditional measure based on generators for a fractional factorial design.

We conjecture that among the class of orthogonal fractions of  $2^d$  designs there is some kind of correspondence between the minimal linear aberration of this paper and minimum generator aberration of Wu and others. If we select non-orthogonal fractions, the situation is more complex, as the next example shows.

**Example 9** Let  $F_3$  be the non-orthogonal fraction with size  $n = 32$  of a  $2^7$  design given in Table 2 of Appendix D. We also consider the designs  $F_1$  and  $F_2$  of Examples 7 and 8. The three designs have the same size, but the design  $F_3$  cannot be compared with  $F_1$  or  $F_2$  in traditional terms as it is not even orthogonal. However, we can compare the designs based in the distribution of degrees in their algebraic fans.

An interpolation as presented in Appendix B suggests that the minimum degree of models identified by a generic design with  $n = 32, d = 7$  is  $53.5 \approx 54$ . This number is a lower bound for the total degree of models identified by designs  $F_1, F_2$  and  $F_3$ . In other words, the set of total degrees for models in algebraic fan of  $F_1, F_2$  and  $F_3$  is lower bounded by 54, e.g.  $54 \leq \min(\{\sum_{i=1}^d \bar{\alpha}_L : L \in \mathcal{L}_a(F_i)\})$  for  $i = 1, 2, 3$ .

Initial results show that

- i) the size of  $\mathcal{L}_a(F_3)$  is much longer (it has around  $6 \times 10^5$  models) than that for designs  $F_1$  and  $F_2$ , see Table 1 in Appendix B;
- ii) the algebraic fans of  $F_1$  and  $F_2$  are not contained in the algebraic fan of  $F_3$ , and
- iii) the design  $F_3$  identifies model of lower degree than  $F_1$  or  $F_2$  (indeed of total degree 58), and the bound 54 is verified.

It is clear that  $F_3$  has smaller minimal linear aberration than  $F_1$  and  $F_2$ , see Figure 12. We also note that the histogram for  $F_3$  presents more symmetry than that for  $F_1$  and  $F_2$ .

## Appendix A: Proof of Theorem 7

**Proof.** The proof is basically the minimisation over the first orthant of  $\sum_{i=1}^d w_i x_i$  subject to the constraint  $\prod_{i=1}^d (x_i + a) = b$ . The problem is solved by a change of coordinates to  $x'_i = x_i + a$  for  $i = 1, \dots, d$ . We minimise  $\sum_{i=1}^d w_i x'_i$  subject to  $\prod_{i=1}^d x'_i - b = 0$ . Using standard optimization tools, we form the Lagrange multiplier

$$L(x', \lambda) = \sum_{i=1}^d w_i x'_i - \lambda \left( \prod_{i=1}^d x'_i - b \right)$$

and then solve the system of equations  $\nabla L(x', \lambda) = 0, \frac{\partial L(x, \lambda)}{\partial \lambda} = 0$ . The solution vector is  $x^{*'} = (x_1^{*'}, \dots, x_d^{*'})$  where

$$x_i^{*'} = b^{1/d} \frac{\prod_{i=1}^d w_i^{1/d}}{w_i}. \quad (10)$$

The convexity of the functions  $\sum_{i=1}^d w_i x_i$  and  $\prod_{i=1}^d x_i = b$  over the first orthant guarantees that  $x^{*'}$  is indeed the minimum. The aberration for this minimal point is

$$\sum_{i=1}^d w_i x_i^* = db^{1/d} g(w).$$

Finally we note that  $x_i^* = x_i^{*' } - a$  and compute the aberration using  $x_i^*$ , achieving the approximate aberration  $\tilde{A}$  of Equation (8). ■

We remark that for a fixed  $w$ ,  $x_i^*$  serves as an approximation to the centroid of the corresponding corner cut model and therefore  $\tilde{A}$  is an approximation to  $A^*(w, n)$ . Although the approximate aberration  $\tilde{A}$  does not depend on the actual corner cut identified by  $L$ , the minimal aberration  $A^*(w, n)$  does depend on it. If  $L$  is the corner cut directed by  $w$ , the practical validity of the approximate aberration  $\tilde{A}$  relies on  $x_i^*$  being close enough to  $\frac{1}{n} \sum_{\alpha \in L} \alpha_i$ . This closeness depends ultimately on  $a, b$ . See Appendix 5.2 for a proposal to compute  $a, b$ .

## Appendix B: Computing values $a, b$ for the approximate corner cut polytope

In Section 3.4 we proposed the continuous function of Equation (7) to approximate the corner cut polytope (which is piecewise linear surface). In this section we discuss on the selection of the values  $a, b$  so that the approximation is good enough. In general, the values  $a, b$  will depend on the number of dimensions  $d$  and number of points in the design  $n$ . However, for fixed  $d$ , the approximation will be coarse for small values of  $n$ .

For our approximation we use the following properties of the corner cut polytope, which have been studied as well in [21] and [22].

**Lemma 10** *The corner cut polytope satisfies the following properties.*

- i) *The intersection of the corner cut polytope with the axes occurs at the point  $\binom{n}{2}$ .*
- ii) *When for  $k \geq 1$ , the sample size  $n$  satisfies*

$$n = \binom{k + d - 1}{d} \tag{11}$$

*then the corner cut polytope is pointed.*

**Proof.**

- i) The intersection is the the sum of exponents for any marginal model of the form  $\{1, x_i, x_i^2, \dots, x_i^{n-1}\}$ . Therefore the intersection must occur at  $\sum_{i=0}^{n-1} i = \binom{n}{2}$ .
- ii) The corner cut polytope is pointed when the sample size is the same as the size of a model of total degree  $k - 1$ , that is, there are  $\binom{d+1-j}{j}$  terms of degree  $j$  in the model where  $j = 0, \dots, k - 1$ . Therefore the sample size must be  $n = \sum_{j=0}^{k-1} \binom{d+1-j}{j} = \binom{k+d-1}{d}$ .

■

**Remark 11** When Equation (11) is satisfied, the tip of the pointed corner cut polytope has coordinates  $\alpha_L = \left( \binom{k+d-1}{d+1}, \dots, \binom{k+d-1}{d+1} \right)$ .

We propose to force Equation (7) to satisfy the condition of Item 1 in Lemma 10 and pass through the tip point  $\alpha_L$  for the model of total degree  $k - 1$ . To summarize, when sample size satisfies Equation (11) then  $a, b$  must satisfy the following equations:

$$b = a^{d-1} \left( \frac{n-1}{2} + a \right) \text{ and } b = (c+a)^d,$$

where  $c = \frac{1}{n} \binom{k+d-1}{d+1}$  is the scaled tip of the corner cut polytope. When design size,  $n$ , is not of the form  $n = \binom{k+d-1}{d}$  for some  $k \geq 1$ , we propose to interpolate the value for  $c$ , the scaled tip of the polytope, that is to solve Equation (11) for  $k$  and interpolate the corresponding tip with  $\frac{1}{n} \binom{k+d-1}{d+1}$ .

For two dimensions ( $d = 2$ ) by interpolation and solving the two conditions above we obtain the following formulæ for  $a, b$  in terms of  $n$ :

$$a = \frac{5 - 3\sqrt{1 + 8n} + 4n}{3(3 - 2\sqrt{1 + 8n} + 3n)}, \quad b = a \left( \frac{n-1}{2} + a \right).$$

See Figure 13 for a depiction of the corner cut polytope and the approximate curve for  $d = 2, n = 7$ . This interpolation is difficult for  $d > 2$  and we have to rely on approximations. The following formulæ are rough approximations for  $a, b$  obtained by truncation of the binomial expansions

$$a \approx \left( \frac{2d!n}{(d+1)^d(n-1)} \right)^{\frac{1}{d-1}}, \quad b = a^{d-1} \left( \frac{n-1}{2} + a \right) \approx \frac{d!n}{(d+1)^d}.$$

## Acknowledgments

The research of Shmuel Onn and Henry Wynn was partially supported by the Joan and Reginald Coleman-Cohen Exchange Program during a stay of Henry Wynn at the Technion. Yael Berstein was supported by an Irwin and Joan Jacobs Scholarship and by a scholarship from the Graduate School of the Technion. Shmuel Onn was also supported by the ISF: Israel Science Foundation. Henry Wynn and Hugo Maruri-Aguilar were also supported by the Research Councils UK (RCUK) Basic Technology grant ‘‘Managing Uncertainty in Complex Models’’.

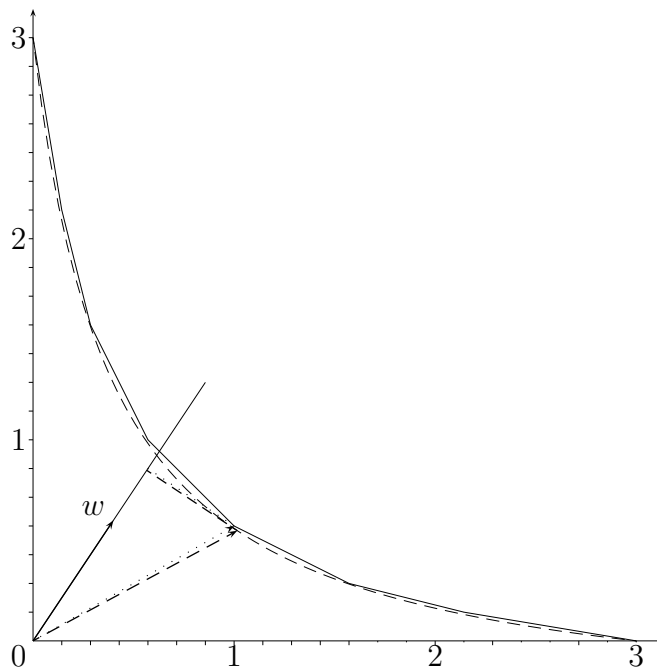


Fig. 13. Minimal aberration using the corner cut polytope. The corner cut polytope is the piecewise linear solid curve, while the approximation is the dashed curve. The minimal aberration is the projection over the direction of  $w$  of the vertex (using dotted line), and an approximate value uses Equation (7) (dashed line).

## References

- [1] E. Babson, S. Onn, and R. Thomas. The Hilbert zonotope and a polynomial time algorithm for universal Gröbner bases. *Adv. Appl. Math.*, 30(3):529–544, 2003.
- [2] G.E.P. Box and J.S. Hunter. The  $2^{k-p}$  fractional factorial designs. I. *Techno.*, 3:311–351, 1961.
- [3] G.E.P. Box and J.S. Hunter. The  $2^{k-p}$  fractional factorial designs. II. *Techno.*, 3:449–458, 1961.
- [4] G.E.P. Box and K.B. Wilson. On the experimental attainment of optimum conditions. *J. Roy. Statist. Soc. Ser. B*, 13(1):1–45, 1951.
- [5] B. Buchberger. *On finding a vector space basis of the residue class ring modulo a zero dimensional polynomial ideal (in German)*. Ph.D. thesis, Department of Mathematics, University of Innsbruck, 1966.
- [6] M. Caboara, G. Pistone, E. Riccomagno, and H.P. Wynn. The fan of an experimental design. SCU Research Report 33, Department of Statistics, University of Warwick, May 1997.
- [7] H. Chen and A. S. Hedayat. Some recent advances in minimum aberration designs. In *New developments and applications in experimental design (Seattle, WA, 1997)*, volume 34 of *IMS Lecture Notes Monogr. Ser.*, pages 186–198. Inst. Math. Statist., Hayward, CA, 1998.
- [8] CoCoATeam. CoCoA: a system for doing Computations in Commutative



Total degree	AF $F_1$	AF $F_2$	AF $F_3$	RF $F_1$	RF $F_2$	RF $F_3$
58	-	-	2290	-	-	0.84
59	-	-	5437	-	-	1.99
60	-	-	15036	-	-	5.51
61	-	8	34574	-	0.47	12.66
62	-	52	55025	-	3.04	20.15
63	-	108	57848	-	6.32	21.18
64	-	124	47851	-	7.26	17.52
65	-	220	28511	-	12.88	10.44
66	-	268	13928	-	15.7	5.1
67	-	204	6837	-	11.94	2.5
68	72	340	3378	54.14	19.91	1.24
69	-	60	1596	-	3.51	0.58
70	-	136	567	-	7.96	0.21
71	-	8	140	-	0.47	0.05
72	48	144	33	36.09	8.43	0.01
73	-	-	12	-	-	0.00
74	-	20	5	-	1.17	0.00
80	12	16	-	9.02	0.94	0.00
83	-	-	1	-	-	0.00
85	-	-	1	-	-	0.00
119	1	-	-	0.75	-	-
Total	133	1708	273071	100.00	100.00	100.00

Table 1

Absolute (AF) and relative (RF) frequencies of total degrees for models identified by fractions  $F_1$  and  $F_2$  of Example 8 and  $F_3$  of Example 9. The symbol - represents zero.

Algebra. Available at <http://cocoa.dima.unige.it>.

- [9] S. Corteel, G. Rémond, G. Schaeffer, and H. Thomas. The number of plane corner cuts. *Adv. Appl. Math.*, 23(1):49–53, 1999.
- [10] D. Cox, J. Little, and D. O’Shea. *Ideals, Varieties, and Algorithms*. Springer-Verlag, New York, 1997. Second Edition.
- [11] D.A. Cox, J. Little, and D. O’Shea. *Using algebraic geometry*, volume 185 of *Graduate Texts in Mathematics*. Springer, New York, second edition, 2005.
- [12] J.C. Faugère, P. Gianni, D. Lazard, and T. Mora. Efficient computation of zero-dimensional Gröbner bases by change of ordering. *J. Symb. Comp.*, 16(4):329–344, 1993.
- [13] A. Fries and W.G. Hunter. Minimum aberration  $2^{k-p}$  designs. *Techno.*, 22(4):601–608, 1980.
- [14] K. Fukuda, A.N. Jensen, and R. Thomas. Computing Gröbner fans, 2005. Preprint submitted to Mathematics of Computation.
- [15] G.M. Greuel, G. Pfister, and H. Schönemann. SINGULAR 3.0. A Computer Algebra System for Polynomial Computations, Centre for Computer Algebra, University of Kaiserslautern, 2005. <http://www.singular.uni-kl.de>.
- [16] T. Holliday, G. Pistone, E. Riccomagno, and H.P. Wynn. The application of computational algebraic geometry to the analysis of designed experiments: a case study. *Comput. Statist.*, 14(2):213–231, 1999.
- [17] H. Maruri-Aguilar. *Algebraic statistics in experimental design*. Ph.D.

$x_1$	$x_2$	$x_3$	$x_4$	$x_5$	$x_6$	$x_7$
+	+	+	+	-	-	+
+	-	+	-	-	+	+
+	-	+	+	-	+	-
+	+	+	-	+	+	-
+	+	-	-	-	-	+
+	-	+	+	-	-	+
+	-	-	-	+	+	+
+	-	-	+	-	-	+
-	+	+	-	+	-	-
+	-	-	+	-	+	-
+	-	+	-	+	-	-
-	+	+	+	-	-	+
-	+	+	+	+	-	-
+	-	-	+	+	+	-
-	-	-	-	-	-	-
+	-	-	-	+	-	-
-	+	+	+	+	-	+
-	-	+	+	-	+	-
+	-	-	-	-	+	-
-	-	-	-	+	+	+
-	-	+	-	-	+	+
+	-	+	-	+	+	-
-	+	+	-	+	+	-
-	+	-	-	-	+	+
-	-	-	+	+	-	+
+	+	-	-	+	+	+
+	+	+	+	+	-	+
-	-	-	-	-	-	+
-	-	+	-	+	-	+
+	+	-	-	+	-	+
-	-	-	-	-	+	+
+	+	-	-	-	-	-

Table 2

Design  $F_3$  of Example 9. The signs  $+$  and  $-$  correspond to  $+1$  and  $-1$ .

thesis, Department of Mathematics, University of Warwick, 2007.

- [18] M. D. McKay, R. J. Beckman, and W. J. Conover. A comparison of three methods for selecting values of input variables in the analysis of output from a computer code. *Technometrics*, 21(2):239–245, 1979.
- [19] M. B. Monagan, K. O. Geddes, K. M. Heal, G. Labahn, S. M. Vorkoetter, J. McCarron, and P. DeMarco. *Maple 10 Programming Guide*. Maplesoft, Waterloo ON, Canada, 2005.
- [20] T. Mora and L. Robbiano. The Gröbner fan of an ideal. *J. Symb. Comp.*, 6(2-3):183–208, 1988. Computational aspects of commutative algebra.
- [21] I. Müller. Corner cuts and their polytopes. *Beiträge Algebra Geom.*, 44(2):323–333, 2003.
- [22] S. Onn and B. Sturmfels. Cutting corners. *Adv. Appl. Math.*, 23(1):29–48, 1999.
- [23] J.L. Peixoto. Hierarchical variable selection in polynomial regression models. *Am. Stat.*, 41(4):311–313, 1987.
- [24] G. Pistone, E. Riccomagno, and M.P. Rogantin. Algebraic statistics methods in DOE (with a contribution by Maruri-Aguilar, H.). In A. Zhigljavsky and L. Pronzato, editors, *Algebra and geometry in statistics and*

- design*. (Forthcoming).
- [25] G. Pistone, E. Riccomagno, and H. P. Wynn. *Algebraic Statistics*, volume 89 of *Monographs on Statistics and Applied Probability*. Chapman & Hall/CRC, Boca Raton, 2001.
  - [26] G. Pistone and H.P. Wynn. Generalised confounding with Gröbner bases. *Biometrika*, 83(3):653–666, 1996.
  - [27] B. Sturmfels. *Gröbner bases and convex polytopes*, volume 8 of *University Lecture Series*. American Mathematical Society, Providence, RI, 1996.
  - [28] U. Wagner. On the number of corner cuts. *Adv. Appl. Math.*, 29(2):152–161, 2002.
  - [29] H. Wu and C. F. J. Wu. Clear two-factor interactions and minimum aberration. *Ann. Statist.*, 30(5):1496–1511, 2002.