Algebraic techniques in design of experiments

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Abstract

Techniques from algebraic geometry were introduced in design of experiments by Pistone and Wynn (1996). The techniques they introduced identify models of a low degree and provide a natural extension to basic concepts such as confounding and fractions of designs.

I intend to describe the basic ideas of the algebraic method, specially work relating term orderings with geometrical results. I will also present some of our recent work on aberration which leads to Nyquist-type lower bounds for models identified with algebra.

Order of the talk

1. Algebraic analysis of experiments
   a Generalised confounding
   b Examples
2. Weighted orders and zonotopes
3. The fan of a design
   a A column selection algorithm
   b Hilbert zonotope
4. Linear aberration
   a Examples
   b Bounds for minimal aberration
   c Comparison of designs
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1. Algebraic analysis of experiments

Rings, polynomial division (Cox et al., 1996 [5])

- $\mathbb{R}[x] = \mathbb{R}[x_1, \ldots, x_d]$ the polynomial ring.
- The ideal generated by a finite set of points $\mathcal{D} \subset \mathbb{R}^d$ is $I(\mathcal{D}) = \{f \in \mathbb{R}[x] : f(x) = 0, x \in \mathcal{D}\} \subset \mathbb{R}[x]$.
- A term order τ is a total ordering in monomials in $T^d = \{x^\alpha : \alpha \in \mathbb{Z}^d_{\geq 0}\}$, compatible with monomial simplification: i) $x^\alpha \succ 1, \alpha \neq \mathbf{0}$, ii) $x^\alpha \succ x^\beta \Rightarrow x^{\alpha+\gamma} \succ x^{\beta+\gamma}$ for $x^\alpha, x^\beta, x^\gamma \in T^d$.
- A Gröbner basis G_τ is a finite subset of $I(\mathcal{D})$ such that $\langle \mathsf{LT}(g) : g \in G_\tau \rangle = \langle \mathsf{LT}(f) : f \in I(\mathcal{D}) \rangle$.
- For any $f \in \mathbb{R}[x]$, unique remainder r in division of f by $I(\mathcal{D})$

$$f = \sum_{g \in G_\tau} gh + r \tag{1}$$

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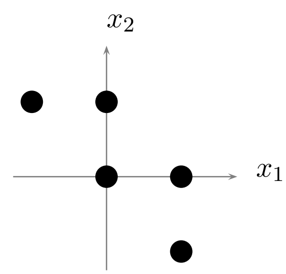
Quotient rings (Cox et al., 1996 [5])

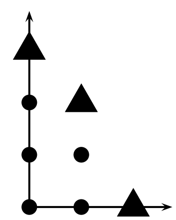
- $\mathbb{R}[\mathcal{D}]$ is the collection of polynomial functions $\phi : \mathcal{D} \mapsto \mathbb{R}$.
- The elements of $\mathbb{R}[\mathcal{D}]$ are in one to one correspondence with equivalence classes of polynomials modulo $I(\mathcal{D})$ and we have an isomorphism $\mathbb{R}[\mathcal{D}] \sim \mathbb{R}[x]/I(\mathcal{D})$.
- A basis for $\mathbb{R}[x]/I(\mathcal{D})$ is given by those monomials that cannot be divided by any of $\mathsf{LT}(g)$ for $g \in G_{\mathcal{T}}$.
- The reminder in Eq. (1) is known as the normal form of f (modulo $I(\mathcal{D})$), i.e. $\mathsf{NF}(f) = r$.

Generalised confounding (Pistone and Wynn 1996 [13])

- Design $\mathcal{D}$, n points, d factors.
- Study the $\mathcal{D}$ through the design ideal $I(\mathcal{D}) \subset \mathbb{R}[x]$.
- The support for a model is given by those monomials not divisible by the leading terms of the RGröbner basis $G_\tau \subset I(\mathcal{D})$.

Design $\mathcal{D}$





term order $\tau : x_1 \succ x_2$

Model $= \{1, x_1, x_2, x_1x_2, x_2^2\}$

$$G_\tau = \{\underline{x_1^2} + 2x_1x_2 + x_2^2 - x_1 - x_2, \underline{x_2^3} - x_2, \underline{x_1x_2^2} - x_1x_2 - x_2^2 + x_2\}$$

- Exact polynomial interpolator $=$ saturated regression model.
- Hierarchical polynomial model: staircases.
- Link with aliasing/confounding $f(x) = g(x), x \in \mathcal{D}$.

Examples

- Factorial design 2^d with levels ± 1. For any term ordering, its design ideal $I(\mathcal{D})$ has Gröbner basis $G_\tau = \{x_i^2 - 1, i = 1, \ldots, d\}$ and identifies the model $\{1, x_1\} \times \cdots \times \{1, x_d\}$
- Indicator function blends naturally to create the ideal of a design fraction, e.g. the indicator $(x_1 - x_2)(x_2 - x_3)$ removes the treatments $\pm(1, -1, 1)$ from the 2^3 design. The fraction $\mathcal{F}$ has six runs and for the standard term order in CoCoA, the model identified is $\{1, x_1, x_2, x_3, x_1 x_3, x_2 x_3\}$.
- Confounding by normal form: NF$(x_1 x_2 x_3) = x_1 - x_2 + x_3$.
- Technique applicable to essentially, any design whose points have continuous factors: LH, RSM, optimal,...

...linear independence with a term order, but much more!

2. Weighted orders and zonotopes

Term orders, weighted orders

- The requirement of a term order (total order in all of T^d) can be relaxed without losing generality. Use instead weighted order.

Def. w-**order** Let $B \subseteq T^d, B \neq \emptyset$, let $w \in \mathbb{Z}^d_{\geq 0}, w \neq \mathbf{0}$. For $x^\alpha, x^\beta \in B$ we say $x^\alpha \succeq_w x^\beta$ if $w \cdot \alpha \geq w \cdot \beta$.

- If $B = T^d$ then for any w, $\succeq_w$ is a partial order, i.e. there are ties among monomials.
- Even for finite B, it is easy to find w such that $\succeq_w$ is only partial ordering. e.g. $B = \{x_1, x_2\}$ take $w = (1, 1)$.
- But careful selection of w wrt B allows to use w-orders.

Theo. [10] Let $B \subset T^d$ be finite; let w be such that w is not orthogonal to any of $\{\alpha - \beta : x^\alpha, x^\beta \in B\}$. Then w-order is total ordering $\succ_w$ in B.

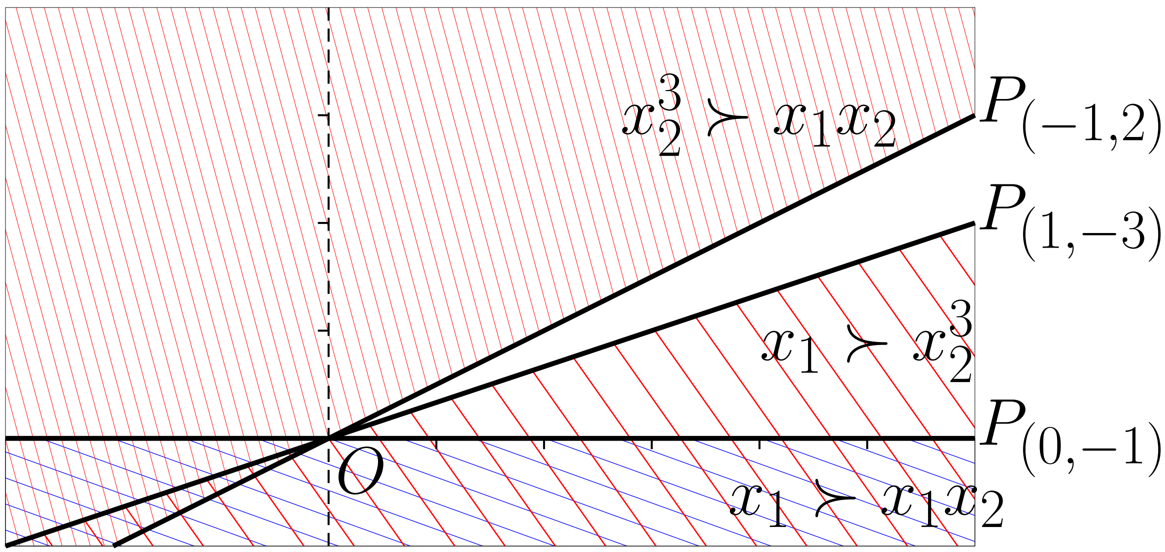
Equivalence classes of vectors [10]

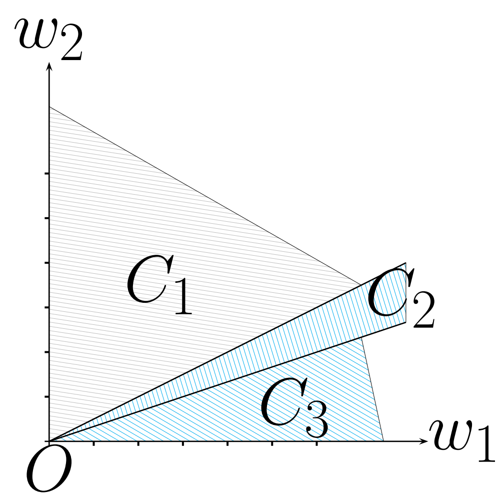
Def. Let $B \subset T^d$ be finite; let $\succ_{w_1}, \succ_{w_2}$ be total orderings in B. We say $w_1 \sim w_2$ when $x^\alpha \succ_{w_1} x^\beta$ iff $x^\alpha \succ_{w_2} x^\beta$ for all $x^\alpha, x^\beta \in B$.

For fixed B, the set of all weighing vectors that create $\succ_w$ is the equivalence class of w. It is a polyhedral cone (intersection of halfspaces) intersected with the positive integer lattice.

Theo. The central hyperplane arrangement constructed with all pairwise differences between exponents of monomials in B partitions the positive integer lattice into cones, the interior of which corresponds to equivalence classes $\sim$.

Example: $B = \{x_1, x_1x_2, x_2^3\}$





Equivalence classes and Minkowski sums [10]

Def. Let V be a finite set of vectors in $\mathbb{R}^d$. The **zonotope** of V is the Minkowski sum

$$Z(V) = \sum_{v \in V} [-v, v], \tag{2}$$

where $[-v, v]$ is the line segment between $-v$ and v.

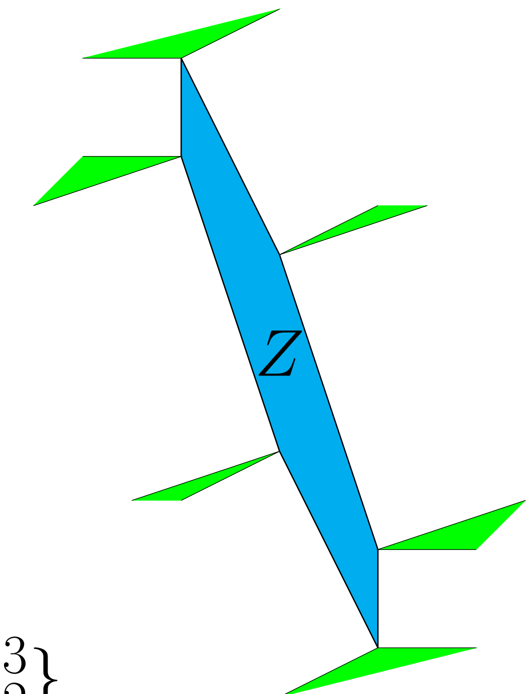
Theo. Let $B \subset T^d$ be finite, let $D = D(B) = \{\alpha - \beta : x^\alpha, x^\beta \in B\}$ and let $Z(D)$ be the zonotope of D. Then the restricted *normal fan* of $Z(D)$ partitions the positive integer lattice into the cones $\sim$.

Universal set of weighing vectors $W_+(B)$

For $B \subset T^d$ finite, there is a one to one correspondence between

Equivalence classes of ordering vectors $\leftrightarrow$ Cones in the first orthant of the normal fan of the zonotope of $D(B)$.

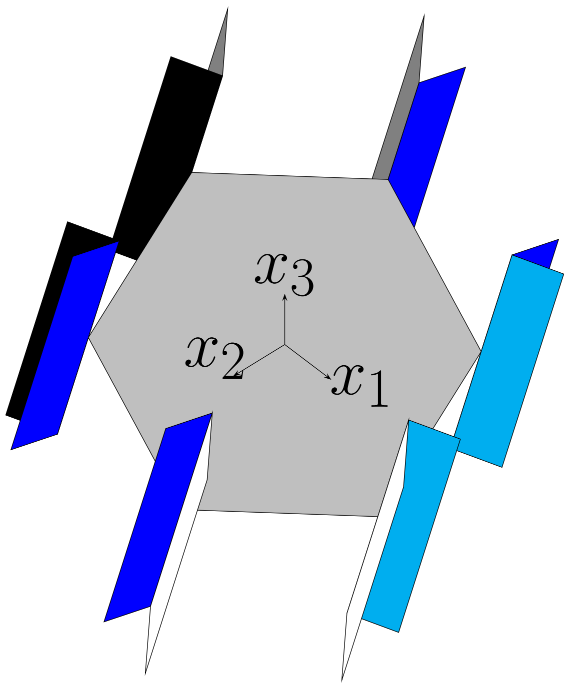
Set of representatives: $W_+(B)$



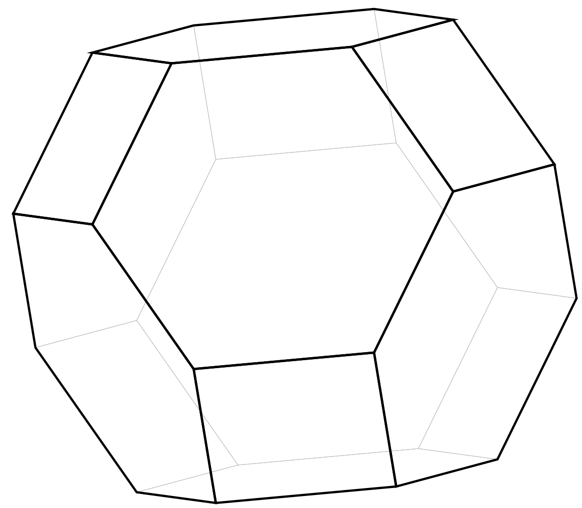
$$B = \{x_1, x_1x_2, x_2^3\}$$

Permutahedron

When $B = \{x_1, \ldots, x_d\}$ then the associated zonotope is the permutahedron Π_{d-1}.



Π_2



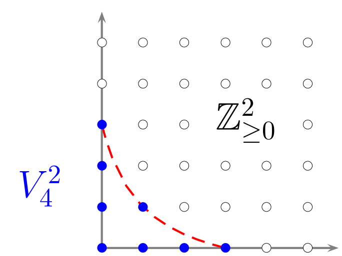
Π_3

3. The fan of a design

A column selection algorithm (Babson et al. 2003 [1])

- Compute the design model matrix for the set of terms V_n^d.
- Using a term ordering $\succ_w$, order the columns of the matrix.
- Pick the first n columns which form a linearly independent set.

1	x_1	x_2	x_1^2	x_1x_2	x_2^2	x_1^3	$\cdots$
1	0	0	0	0	0	0	
1	1	0	1	0	0	1	
1	0	1	0	0	1	0	
1	1	−1	1	−1	1	1	
1	−1	1	1	−1	1	−1	



$$V_n^d := \{x \in \mathbb{Z}^d_{\geq 0} : \prod_{i=1}^d (x_i + 1) \leq n\}$$

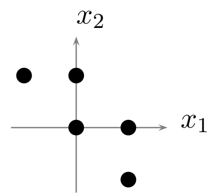
By row elimination, the methodology retrieves G_w for $I(\mathcal{D})$.

It is a variation of the FGLM algorithm for change of basis [6].

The fan of a design

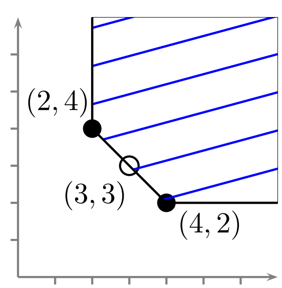
- As we scan over all possible term orders, we obtain the algebraic fan of $\mathcal{D}$, see [3][10].
- Not all identifiable hierarchical models belong to the algebraic fan, i.e. $\emptyset \subset A \subseteq S \subseteq \mathcal{C}_{d,n}$.

$\mathcal{D}$



$$A = \{ \ \vdots\!: \ , \ ::. \ \}, S \setminus A = \{ \ \vdots.. \ \}$$

- The models in A correspond to the vertexes of the state polytope $\mathcal{S}(I)$, e.g. we add up the exponent vectors for $L = \{1, x_1, x_2, x_1x_2, x_2^2\}$, $\bar{\alpha}_L = \sum_L \alpha = (2, 4)$.



$$\mathcal{S}(I) = \mathrm{conv}(\bar{\alpha}_L : L \in A) + \mathbb{R}^d_{\geq 0}$$

Constructing the fan

One to one correspondence between:

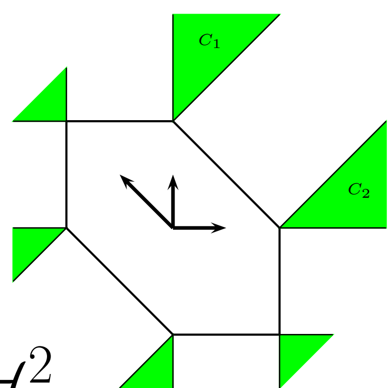
Models retrieved by algebra $\leftrightarrow$ vertexes of state polytope

1. Reverse search and change of basis. Particular construction for every ideal $I(\mathcal{D})$. Software available (Gfan).
2. Hilbert zonotope [12,1] $\mathcal{H}_n^d$. Universal construction for any $I(\mathcal{D})$, depends only on d, n.
   Idea behind $\mathcal{H}_n^d$: to generate the universal set of w-ordering vectors it is sufficient to order the set $V_n^d = \{$union of all staircases with n elements in d undeterminates$\}$.
   $\Rightarrow$ run the column selection algorithm with a universal set of w-orders.

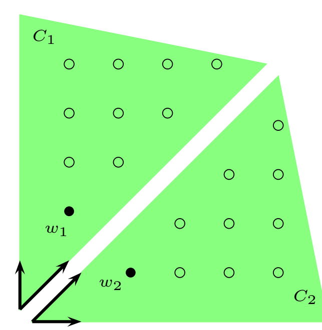
Hilbert zonotope

Hilbert schemes are algebraic varieties that parameterize families of ideals in polynomial rings i.e.Hilb$_2^2$ consists of all $I \subset R[x]$ for which $R[x]/I$ has dimension 2 as $\mathbb{R}$-vector space.

Theo. [1]: $\mathcal{H}_n^d$ is a refinement of the state polytope of every member of Hilb$_n^d$.

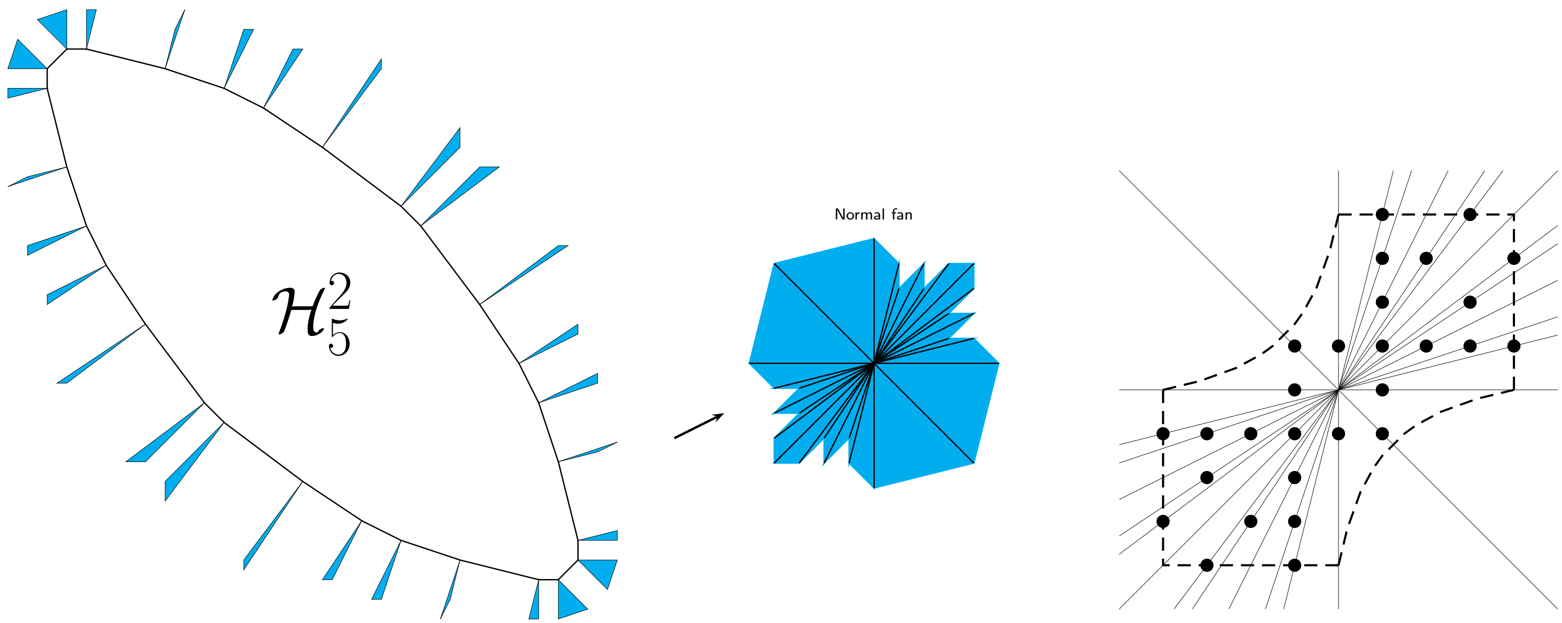


$\mathcal{H}_2^2$



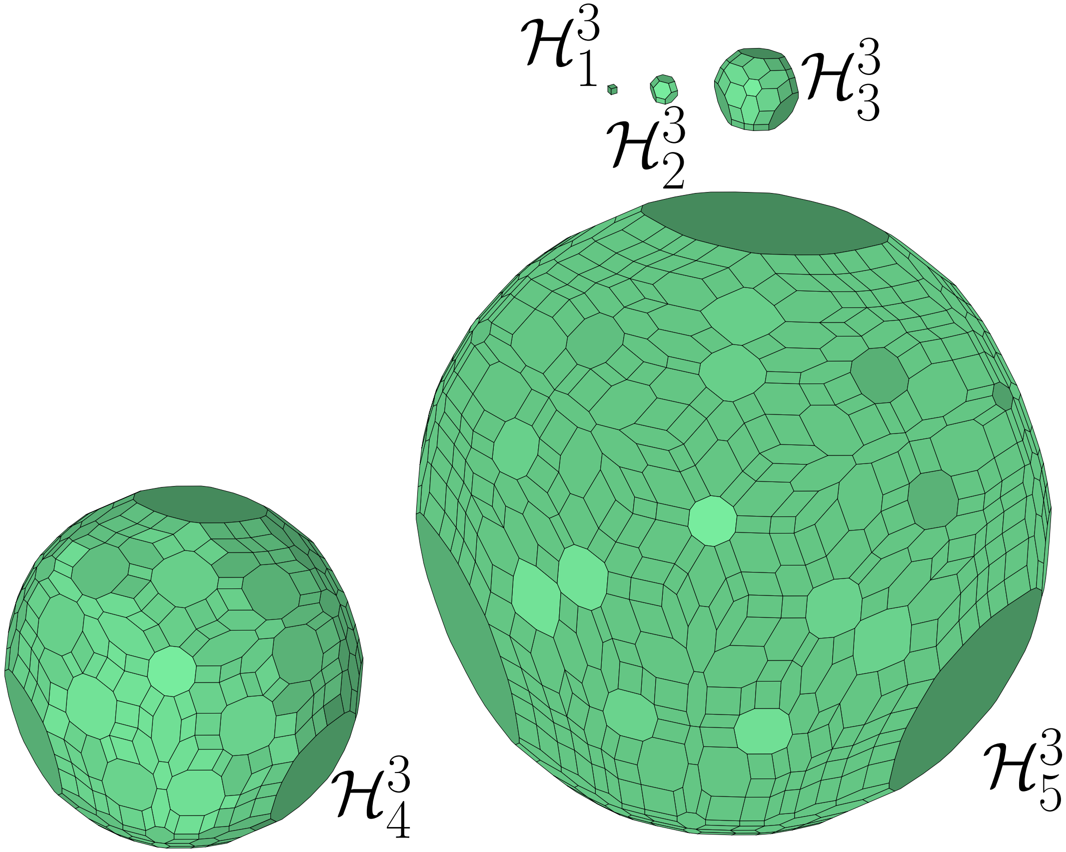
Hilbert zonotope, $d = 2$

Theo. [9] The cones in of $\mathcal{N}(\mathcal{H}_n^2) \bigcap \mathbb{R}^2_{\geq 0}$ are generated by the directions of $[0, n-1]^2$.



Hilbert zonotope, higher dimensions

For $d > 2$, the complexity of $\mathcal{N}(\mathcal{H}_n^k) \bigcap \mathbb{R}^d_{\geq 0}$ is not captured with the directions of $[0, n-1]^d$.



Any hints?

4. Linear aberration

Linear aberration

- Taking the motivation from the concept of aberration, we want to fill out lower degrees before higher:

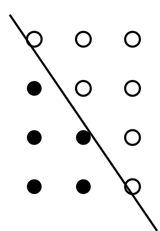
$$A(w, L) = \frac{1}{n} \sum w_i \bar{\alpha}_{L_i}$$

$w_i \geq 0$, $\sum w_i = 1$.

Theorem: Any algebraic model minimises some $A(w, L)$.

Proof. Use LP arguments for the lower boundary of $\mathcal{S}(I)$.

- **Generic** designs minimise $A(w, L)$ over $\mathcal{C}_{d,n}$ and all vectors w.
- For generic designs, algebraic models are corner cut models [12]

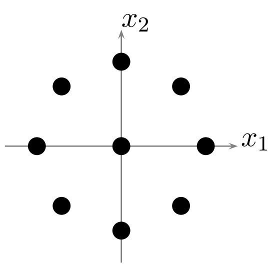
Corner cut model  $\{1, x_1, x_2, x_1 x_2\}$ is not corner cut

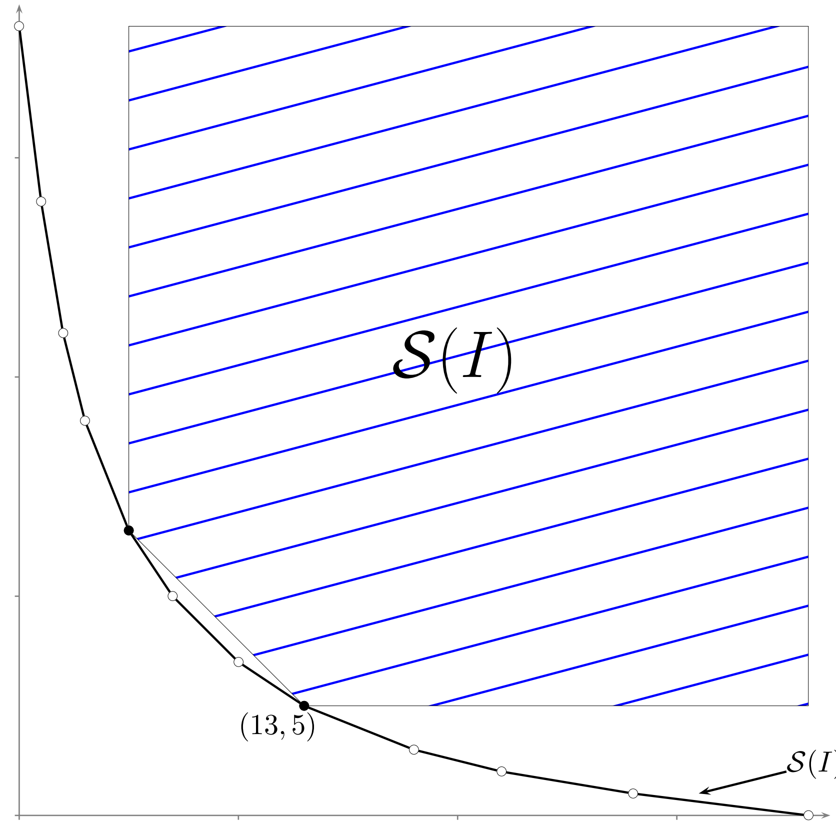
Linear aberration and algebraic models

- The state polytope summarises information about linear aberration, i.e. its vertexes correspond to models that minimise $A(w, L)$ over the set of identifiable hierarchical models S.
- The vertexes of $\mathcal{S}(I)$ correspond to algebraic models A.
- The (minimum) aberration of designs can be compared through their state polytopes.
- However, there may be non-algebraic models on the lower boundary (and thus minimising $A(w, L)$ for some w) or in the interior of $\mathcal{S}(I)$.

Example aberration 1

Central composite design (CCD, Box, 1957) with $d = 2$, $n = 9$ and axial distance $= \sqrt{2}$

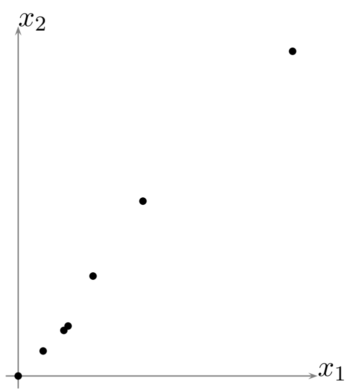




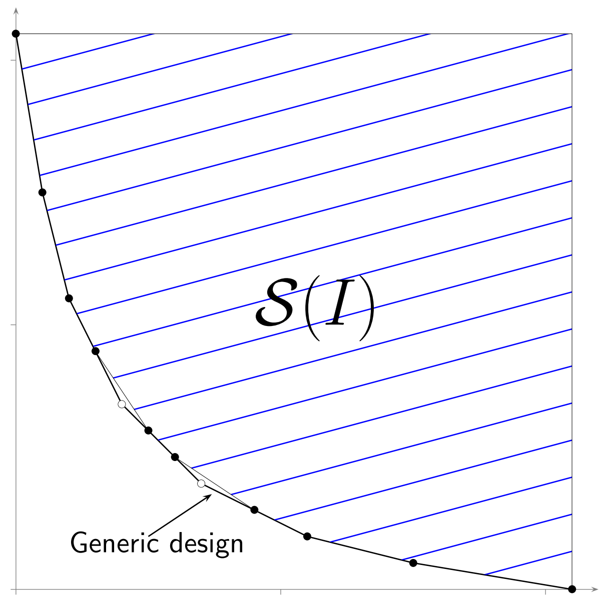
Algebraic $=\{1, x_1, x_1^2, x_1^3, x_1^4, x_2, x_1x_2, x_1^2x_2, x_2^2\}$ and its conjugate

Example aberration 2

Consider $\mathcal{D} = \{(0,0),(1,1),(2,2)(3,4),(5,7),(11,13),(\alpha,\beta)\}$, with $(\alpha,\beta) \approx (1.82997, 1.82448)$ (Onn, 1999)



$\mathcal{D}$



$\Rightarrow$ The set of algebraic models can be larger in size than the set of corner cut models. However, corner cut models are always of lowest possible degree over all vectors $c \neq 0$.

Minimal aberration (Bernstein et al. (2007) [2,8])

L a model support, $w > 0$ vector of weights, $\sum w_i = 1$

Compute the aberration: $A(w, L) = \frac{1}{n} \sum w_i \bar{\alpha}_{L_i}$

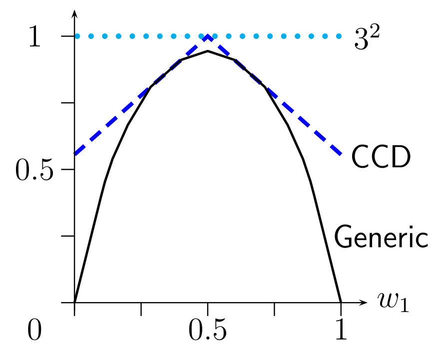


Figure 1: Minimal aberration for three designs in two factors and nine runs.

Minimal aberration. For fixed w, $A^* = \min_{L \in \mathcal{L}} A(w, L)$

Bounds for A^*: $A^+ - 1 \leq A^* \leq A^+ + 1$; $A^+ = k \cdot g(w)$

Approximate minimal aberration: $\tilde{A} = db^{1/d} g(w) - a$; $\tilde{A} \to A^*$

Comparison of designs using A^*: generic LHS, fractional 2^d

Comparison through aberration

F_1, F_2 fractional factorial designs 2^{7-2} of resolution IV with F_2 of minimum *generator aberration* (Fries & Hunter, 1980). F_3 is a randomly selected non-orthogonal fraction.

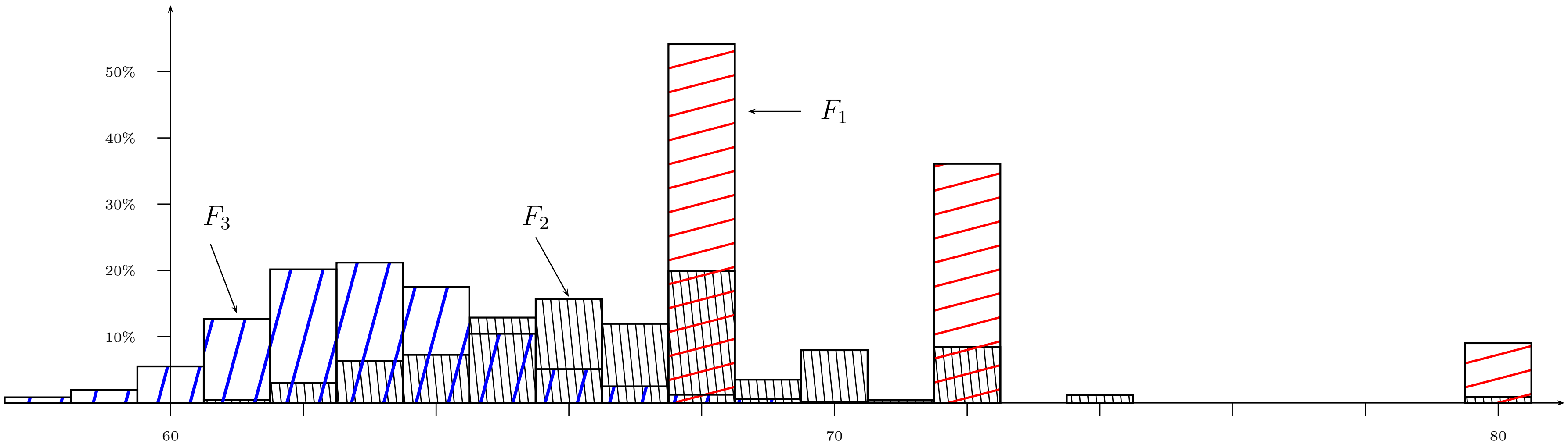


Figure 2: Histograms of relative frequencies of model degrees for fractions F_1, F_2 and F_3.

Work on progress and future work

- Universal w-orders. Extending/finding (zonotope) result to higher dimensions.
- Approximate computations? Computing algebraic fan is expensive even for, say $n = 50, d = 8$, need to retort to other methods, possibly approximate. Select w vectors at random to generate the algebraic fan.
- Aberration: Link linear aberration with traditional generator aberration and estimation capacity [4].

5. References

1. Babson, Onn, Thomas (2003). *Adv. Appl. Math.* **30**(3), 529-544.
2. Bernstein *et al.* (2007). *Minimal aberration* `arXiv:0808.3055`.
3. Caboara *et al.* (1997). Res. Rep. 33, Univ. of Warwick.
4. Cheng, Mukerjee (1998). *Ann. Statist.* **26**(6), 2289-2300.
5. Cox, Little, O'Shea (1996). *Ideals, varieties and algorithms*.
6. Faugere *et al.* (1993). *J. Symb. Comput.* **16**, 329-344.
7. Gritzmann, Sturmfels (1993). *SIAM JDM* **6**(2), 246-269.
8. Lee *et al.* (2008) *SIAM JDM* **22**(3), 901-919.
9. Maruri (2006). *RIMUT* **37**(1-2), 95-119.
10. Maruri (2007). Ph.D. Thesis, Univ. of Warwick.
11. Maruri, Notari, Riccomagno (2007). *Stat. Sin.* **17**, 1417-1440.

12. Onn, Sturmfels (1999). *Adv. Appl. Math.* **23**, 29-48.
13. Pistone and Wynn (1996). *Biometrika* **83**(3), 653-666.
14. Pistone *et al.* (2000). *Algebraic Statistics*. CRC.