Complexity of experimental designs and polynomial models via Betti numbers

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Order of the talk

1. Generalised confounding
2. Weighted orders and zonotopes
3. The fan of a design
4. Hilbert zonotope
5. State polytope etc
6. $2^k$ regular fractions
7. Simplicial complexes, Betti number: results
8. Further work
9. References
Rings, polynomial division (Cox et al., 1996)

- \( \mathbb{R}[x] = \mathbb{R}[x_1, \ldots, x_d] \) 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 \( \tau \) is a total ordering in monomials in 
  \( T^d = \{ x^\alpha : \alpha \in \mathbb{Z}^d_{\geq 0} \} \), compatible with monomial simplification: i) \( x^\alpha \succ 1, \alpha \neq 0 \), 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 \( G_\tau \) is a finite subset of \( I(\mathcal{D}) \) such that 
  \[ \langle \text{LT}(g) : g \in G_\tau \rangle = \langle \text{LT}(f) : f \in I(\mathcal{D}) \rangle. \]
- For any \( f \in \mathbb{R}[x] \), unique remainder \( r \) in division of \( f \) by \( I(\mathcal{D}) \)
  \[ f = \sum_{g \in G_\tau} gh + r \]
Quotient rings (Cox et al., 1996)

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

Generalised confounding (Pistone and Wynn, 1996)

- 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 $\mathcal{D}$

\begin{equation*}
G_\tau = \{x_1^2 + 2x_1x_2 + x_2^2 - x_1 - x_2, x_2^3 - x_2, x_1x_2^2 - x_1x_2 - x_2^2 + x_2\}
\end{equation*}

- 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 $\pm 1$. For any term ordering, its
design ideal $I(D)$ 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 $F$
has six runs and for the standard term order in CoCoA, the
model identified is $\{1, x_1, x_2, x_3, x_1x_3, x_2x_3\}$.

- Confounding by normal form: $NF(x_1x_2x_3) = x_1 - x_2 + x_3$.

- Technique applicable to essentially, any design whose points
have continuous factors: LH, RSM, optimal,...

...linear independence with a term order, but much more!
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 $w \in \mathbb{Z}^d_{\geq 0}$, $w \neq 0$. 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. [8]** 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 $\succeq_w$ in $B$. 
Equivalence classes of vectors [8]

**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: \( B = \{ x_1, x_1x_2, x_2^3 \} \)

Representative

\[
\begin{align*}
C_1 &: \quad x_2^3 \succ w \quad x_1x_2 \succ w \quad x_1 \\
C_2 &: \quad x_1x_2 \succ w \quad x_2^3 \succ w \quad x_1 \\
C_3 &: \quad x_1x_2 \succ w \quad x_1 \succ w \quad x_2^3
\end{align*}
\]

\((0, 1)\) \quad (5, 2) \quad (4, 1)
Equivalence classes and Minkowski sums [8]

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

$$Z(V) = \sum_{v \in V} [0, v],$$

(2)

where $[0, v]$ is the line segment between $0$ and $v$.

**Minkowski sum** of $A, B \subset \mathbb{R}^d$ is

$$A + B = \{a + b : a \in A, b \in B\}$$

**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 \( \Pi_{d-1} \).
A column selection algorithm (Babson et al., 2003)

- 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.

\[
\begin{array}{ccccccc}
1 & x_1 & x_2 & x_1^2 & x_1x_2 & x_2^2 & x_1^3 & \cdots \\
1 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 1 & 0 & 0 & 1 \\
1 & 0 & 1 & 0 & 0 & 1 & 0 \\
1 & 1 & -1 & 1 & -1 & 1 & 1 \\
1 & -1 & 1 & 1 & -1 & 1 & -1 \\
\end{array}
\]

By row elimination, the methodology retrieves $G_w$ for $I(D)$.

It is a variation of the FGLM algorithm for change of basis Faugere et al. (1993).
The fan of a design

• As we scan over all possible term orders, we obtain the algebraic fan of \( \mathcal{D} \), see (Caboara et al., 1997 and Maruri, 2007).

• Not all identifiable hierarchical models belong to the algebraic fan, i.e. \( \emptyset \subset A \subset S \subset \mathcal{C}_{d,n} \).

\[ A = \{ \cdots , \cdots \} , \ S \setminus A = \{ \cdots \} \]

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

\[ S(I) = \text{conv}(\bar{\alpha}_L : L \in A) + \mathbb{R}_{\geq 0}^d \]
Constructing the fan

One to one correspondence between:
Models retrieved by algebra↔ vertexes of state polyhedron

1. Reverse search and change of basis. Particular construction for every ideal $I(\mathcal{D})$. Software available (Gfan).
2. Hilbert zonotope (Onn and Sturmfels, 1999 and Babson et al., 2003)

$$\mathcal{H}_n^d = \sum_{v \in D(V_n^d)} [0, v].$$

Universal construction for any $I(\mathcal{D})$, depends only on $d, n$. 
Idea behind $H_n^d$: to generate the universal set of $w$-ordering vectors it is sufficient to order the set $V_n^d = \{\text{union of all staircases with } n \text{ elements in } d \text{ undeterminates}\}$.

⇒ 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\textsuperscript{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 \( \text{Hilb}_{n}^{d} \).
Hilbert zonotope, $d = 2$

**Theo. [??]** The cones in of $\mathcal{N}(\mathcal{H}_n^2) \cap \mathbb{R}_\geq^2$ are generated by the directions of $[0, n - 1]^2$. 
Hilbert zonotope, higher dimensions

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

Any hints?
Factorial designs with two levels: $2^d$

- Widely used in industrial experimentation
- Orthogonality properties
- “Regular” fractions available $2^{d-r}$
- Criteria: resolution, generator wordlength
- Highly fractioned, non-regular, for screening: Plackett Burman
- Close link to Hadamard matrices
- Study the alias structure
- Polynomial dynamical systems (Dimitrova et al. (2007)):
Regular fractions: the Abelian group method

We start with a $d$-letter alphabet $A, B, \ldots$ etc which form an Abelian group $G_d$ under the condition $A^2 = B^2 = \ldots = I$, $I$ is the identity, and $AB = BA$. Then we consider a subgroup $G_r$ of order $r$ generated by $r$ algebraically independent words $(G_1, G_2, \ldots, G_r)$. We label the actual factors by lower case words $a, b, c, \ldots$ which take levels $\pm 1$. The subgroup $G_r$ splits the full factorial design

$$\{\pm 1, \pm 1, \ldots, \pm 1\}$$

into $2^{d-r}$ blocks in the following way. Let $g = (g_1, \ldots, g_r)$ be the lower case version of $G_1, G_2, \ldots, G_r$. Then the blocks are given by the solutions of

$$\{a^2 = b^2 = \cdots = 1, g = e\}$$

where $e$ ranges over all $2^r$ $r$-vectors $(\pm 1, \pm 1, \ldots, \pm 1)$. 
Example 1: $2^{4-1}, \{ABCD\}$

Let $d = 4$ and take the defining contrast subgroup

\[\{I, ABCD\}\]

We take as our design the block given by

\[\{a^2 = 1, b^2 = 1, c^2 = 1, d^2 = 1, abcd = 1\}\]

Consists of the $2^{4-1} = 8$ points:

\[(1, 1, 1, 1), (-1, -1, 1, 1), (-1, 1, -1, 1), (-1, 1, 1, -1)\]
\[(1, -1, -1, 1), (1, -1, 1, -1), (1, 1, -1, -1), (-1, -1, -1, -1)\]

It is common to write out the aliased terms as rows in a table.
Alias table

\[\begin{align*}
I &= ABCD \\
A &= BCD \\
B &= ACD \\
C &= ABD \\
D &= ABC \\
AC &= BD \\
AB &= CD \\
AD &= BC
\end{align*}\]
Simple results for regular fractions

• Basic theory: each row is an alias class. Eg in the second row, $A = BCD$ means $a \sim bcd$ in that $a = bcd$ on the design, or $a - bcd \in I(D)$.

• For any monomial ordering, the models selects the lowest term in the alias table wrt the ordering (proof: column selection algorithm)

• The Normal Form of any monomial is a monomial.
• The G-basis elements only have two terms.
• Two leading terms with common letters cannot be in same alias class.
Simplicial complexes, Betti numbers etc

• The main idea: we consider that the complexity of the model and the alias structure is held in the structure of the multi-graded (graded) Hilbert series, and hence in the multi-graded (graded) Betti numbers.
• These are surprisingly complex
• We start with the model simplicial complex $\triangle$. These fall into equivalence classes as we vary the monomial ordering. Using the zonotope theory we can (theoretically) find candidate $w$-vectors.
• Betti numbers for the Stanley-Reisner ideal and its Artinian closure (adjoint the quadratics $a^2, b^2, \ldots$):

$$\triangle, \beta(I_\triangle), \beta(\overline{I_\triangle})$$
Example 1, contd.

Algebraic fan of 12 simplicial models, belonging to just three equivalence classes (up to permutations of variables).

<table>
<thead>
<tr>
<th>Class</th>
<th>(a \rightarrow b)</th>
<th>(a \rightarrow b)</th>
<th>(c \rightarrow b)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(HS(s))</td>
<td>(1 + 4s + 3s^2)</td>
<td>(1 + 3s + 3s^2 + s^3)</td>
<td></td>
</tr>
</tbody>
</table>
| \(\beta(I_{\Delta})\) | \[
\begin{array}{c}
0 \\
2: 3 \\
Total 3
\end{array}
\] | \[
\begin{array}{c}
0 \\
2: 3 \\
3: 1 \\
Total 4
\end{array}
\] | \[
\begin{array}{c}
0 \\
1: 1 \\
Total 1
\end{array}
\] |
| \(\beta(\overline{I}_{\Delta})\) | \[
\begin{array}{c}
0 \\
2: 7 \\
3: 6 \\
Total 7
\end{array}
\] | \[
\begin{array}{c}
0 \\
2: 7 \\
3: 1 \\
Total 8
\end{array}
\] | \[
\begin{array}{c}
0 \\
1: 1 \\
2: 1 \\
3: 1 \\
4: 1 \\
Total 4
\end{array}
\] |

Betti numbers for Stanley-Reisner ideal and its Artinian closure.
Vertexes of the state polytope are in one to one correspondence with models in the algebraic fan.

Schlegel diagram of the state polytope of the ideal of design $2^{4-1}$. 
Example 2: Factorial design $2^6 - 2$; \{ABCD, CDEF\}

Algebraic fan with 132 simplicial models, split into 6 equivalence classes.

(a) \hspace{2cm} (b) \hspace{2cm} (c)

(d) \hspace{2cm} (e) \hspace{2cm} (f)
<table>
<thead>
<tr>
<th>Class</th>
<th>$HS(s)$</th>
<th>$\beta(I_\Delta)$</th>
<th>$\beta(\overline{I}_\Delta)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a)</td>
<td>$1 + 4s + 6s^2 + 4s^3 + s^4$</td>
<td>0 1</td>
<td>0 1 2 3 4 5</td>
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<td>1: 2 1</td>
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<td>2: 4 8 4</td>
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<td>3: 6 12 6</td>
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<td>4: 4 8 4</td>
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<td>5: 1 2 1</td>
<td>5: 1 2 1</td>
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<td>Total 2 1</td>
<td>Total 6 15 20 15 6 1</td>
</tr>
<tr>
<td>(b)</td>
<td>$1 + 5s + 7s^2 + 3s^3$</td>
<td>0 1 2 3</td>
<td>0 1 2 3 4 5</td>
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<td>1: 1</td>
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<td>2: 3 6 4 1</td>
<td>2: 8 17 13 5 1</td>
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<td>3: 1 2 1</td>
<td>3: 1 15 32 25 8 1</td>
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<td>Total 5 8 5 1</td>
<td>4: 1 8 16 12 3</td>
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<td>Total 9 33 53 46 21 4</td>
<td>Total 10 33 53 46 21 4</td>
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<td>(c)</td>
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<td>0 1 2</td>
<td>0 1 2 3 4 5</td>
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<td>Total 4 5 2</td>
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<td>(d)</td>
<td>$1 + 6s + 7s^2 + 2s^3$</td>
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<td>2: 14 32 33 20 7 1</td>
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<td>3: 2 21 46 40 15 2</td>
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<td>Total 16 53 82 68 29 5</td>
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<td>0 1 2 3 4</td>
<td>0 1 2 3 4 5</td>
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<td>2: 8 15 12 5 1</td>
<td>2: 14 31 31 18 6 1</td>
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<td>Total 15 50 78 65 28 5</td>
<td>Total 15 50 78 65 28 5</td>
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<td>0 1 2 3 4 5</td>
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<td>Total 8 14 9 2</td>
<td>3: 16 38 35 14 2</td>
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<td>Total 14 46 69 55 23 4</td>
<td>4: 3 8 7 2</td>
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<td>Total 14 46 69 55 23 4</td>
<td>Total 14 46 69 55 23 4</td>
</tr>
</tbody>
</table>
Schlegel diagram of the state polytope of the ideal of design $2^6 - 2$. 
\begin{align*}
I &= ABCD = CDEF = ABEF \\
A &= BCD = ACDEF = BEF \\
B &= ACD = BCDEF = AEF \\
C &= ABD = DEF = ABCEF \\
D &= ABD = CEF = ABDEF \\
E &= ABCDE = CDF = ABF \\
F &= ABCDF = CDE = ABF \\
BF &= ABCDF = BCDE = AE \\
DE &= ABCE = CF = ABDF \\
CE &= ABCD = DF = ABCF \\
BE &= ABCDE = CBDF = AF \\
BD &= AC = BCEF = ADEF \\
CD &= AB = EF = ABCDEF \\
BC &= AD = BDEF = ACEF \\
BDE &= ACE = BCF = ADF \\
BCE &= AED = BDF = ACF
\end{align*}
Example: Plackett Burman design

Highly fractioned factorial 12 runs in 11 factors.

Algebraic fan of enormous size (order $10^6$), but models classified in just 19 classes.

Work in progress...
References