The algebraic method in experimental designs

Hugo Maruri-A.

School of Mathematical Sciences
Queen Mary, University of London

Slow morning on algebraic statistics
Collegio Carlo Alberto, Moncalieri 11th January 2014
Abstract

The algebraic approach to identify models in experimental designs represents a set of points (design) by a polynomial ideal and produces sets of monomials which satisfy desirable statistical properties such as hierarchy and identifiability.

In this talk I will describe recent developments on the relation between designs and identified models. Three topics form the core of the talk: a) a description of the design based on the graded degree of models, also known as aberration; b) a description of the complexity of identifiable monomial models in terms of Betti numbers and c) a description of models identified by complementary fractions in terms of Alexander duality. Further, I will describe some current medium and long term research aims.

This talk presents results from joint work with S. Onn, Y. Bernstein, E. Riccomagno, H. Wynn and E. Sáenz-de-Cabezón.
The algebraic approach

The design $\mathcal{D}$ is a collection of points in $\mathbb{R}^d$. We are interested in identifying models for the response over the design. This is known as a direct problem in design of experiments.

The design ideal $I(\mathcal{D}) \subset R$, $R := \mathbb{R}[x_1, \ldots, x_d]$ is the set of polynomials that vanish on $\mathcal{D}$. The isomorphisms between $\mathbb{R}[\mathcal{D}]$ (as vector spaces), $R/I(\mathcal{D})$ and $R/\langle LT(I(\mathcal{D})) \rangle$ allow the search for a basis to be that of the search for standard monomials of the design ideal $I(\mathcal{D})$.

This is achieved by Gröbner bases computations: fix term ordering $\tau$, compute the reduced Gröbner basis $G_\tau$ for $I(\mathcal{D})$ and retrieve the basis as those monomials that cannot be divided by the leading terms of $G_\tau$.

For a given design $\mathcal{D}$, the collection of models obtain by varying over all term orders $\tau$ is called the algebraic fan of $\mathcal{D}$. 
Examples

The $2^k$ design with points $(\pm 1, \ldots, \pm 1)$ has Universal Gröbner basis
\[
\{x_i^2 - 1, i = 1, \ldots, d\}
\] and its fan has the sole model
\[
\bigotimes_{i=1}^{d} \{1, x_i\}.
\]

Design \(\{(0, 0), (1, 0), (0, 1), (1, -1), (-1, 1)\}\) identifies the models
\[
L_1 = \{1, x_1 x_2, x_1 x_2, x_1^2\} \quad \text{and} \quad L_2 = \{1, x_1, x_2, x_1 x_2, x_2^2\}
\]

\[
\mathcal{D} \quad \dot{\bullet} \quad x_1 \quad A = \{\ldots, \ldots, \ldots\}, \quad S \setminus A = \{\ldots\}
\]

The design \((n = 16)\) with design ideal
\[
I(\mathcal{D}) = \langle x_i^2 - 1, i = 1, \ldots, 6\rangle
\]
\[
+ \langle x_1 x_2 x_3 x_4 - 1, x_3 x_4 x_5 x_6 - 1\rangle
\]
and \text{deglex} identifies \(\{1, x_1, x_2, x_3, x_4, x_5, x_6, x_1 x_4, x_1 x_6, x_2 x_6, x_2 x_4, x_3 x_6, x_4 x_6, x_5 x_6, x_2 x_4 x_6, x_1 x_4 x_6\}\); and with \text{lex} \(\{1, x_2, x_4, x_5, x_6, x_2 x_4, x_2 x_5, x_2 x_6, x_4 x_5, x_4 x_6, x_5 x_6, x_2 x_4 x_5 x_6, x_2 x_4 x_6, x_2 x_5 x_6, x_4 x_5 x_6, x_2 x_4 x_5 x_6\}\)
Staircases

Consider the log representation of a polynomial model, i.e. a model with the terms $1, x_1, x_1x_2$ will be represented by $(0 \choose 0), (1 \choose 0), (1 \choose 1)$.

The log representation of a hierarchical polynomial model is called a staircase; and let $\binom{\mathbb{N}^d}{n}_{stair}$ be the family of $n$-term staircases in $d$ variables.

Example: $d = 2, n = 4$, $\binom{\mathbb{N}^2}{4}_{stair} = \{\lambda_i\}_{i=1}^5$.

\[
\begin{array}{cccccc}
\quad & \bullet & \bullet & \bullet & \bullet & \bullet \\
\lambda_1 & \lambda_2 & \lambda_3 & \lambda_4 & \lambda_5 \\
\text{i.e.} & x^{\lambda_3} = \{1, x_1, x_2, x_1x_2\}
\end{array}
\]
Counting stairs

\[ \sum_{n=0}^{\infty} \# \binom{\mathbb{N}^2}{n}_{\text{stair}} \cdot z^n = \prod_{k=1}^{\infty} \frac{1}{1-z^k} = 1 + z + 2z^2 + 3z^3 + 5z^4 + 7z^5 + 11z^6 \ldots \]

\[ \sum_{n=0}^{\infty} \# \binom{\mathbb{N}^3}{n}_{\text{stair}} \cdot z^n = \prod_{k=1}^{\infty} \frac{1}{(1-z^k)^k} = 1 + z + 3z^2 + 6z^3 + 13z^4 + 24z^5 + 48z^6 \ldots \]

The class \( \binom{\mathbb{N}^d}{n}_{\text{stair}} \) has been previously referred in literature\(^1\) as “well-formed”, “hierarchical” or “hierarchically well-formulated” models.

Generating stairs

Algorithm by Onn\(^2\), enhanced by the local step method of Bates \textit{et al}\(^3\).

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\(^1\)MN83, P90, BGW03
\(^2\)OS99, BOT03
\(^3\)BGW03
Cutting corners

A corner cut is a staircase that can be separated by its complement by a single hyperplane. For fixed dimension and number of terms, the set of corner cuts is referred to as \( \binom{N^2}{n} \text{cut} \).

Staircase \( \lambda_3 \) is not a corner cut.
Fan of a design

Let $\mathcal{D} \subset \mathbb{R}^d$, $\# \mathcal{D} = n$ be a design with no replications. The fan of $\mathcal{D}$ is the set of all staircase models $\lambda_i \in \left( \mathbb{N}^d \right)_{stair}$ such that $|\mathcal{D}^{\lambda_i}| \neq 0$.

Computing the fan of a design: algebraic (gfan, universal term orderings) “algebraic fan” vs simply numeric approach (rank, determinant) “statistical fan”.

Example: Consider $\mathcal{D}_1 = \{ (2,0), (-1,2), (-2,4)(-4,1) \}$. Its fan has all staircases, except the one for $\{1, x_1, x_2, x_1 x_2 \}$. However, $x_1 x_2 \equiv \frac{2}{5} x_1 - \frac{8}{5} x_2 - \frac{4}{5}$ over $\mathcal{D}_1$.

Example: Consider the factorial $2^2$ design ($\mathcal{D}_2$). Its fan has only one model, namely $\{1, x_1, x_2, x_1 x_2 \}$. We have $x_1^2 \equiv 1$, $x_1 x_2^2 \equiv x_1$ etc.
Maximal, minimal fan designs

Minimal fan designs identify a single staircase model.

Maximal fan designs identify all staircases in \( \binom{N^2}{n}_{stair} \)

Generic designs identify all corner cut staircases in \( \binom{N^2}{n}_{cut} \)

**Theorem** (Onn, Sturmfels) If the design is generic, its algebraic fan is the set of corner cuts.

In other words, the algebraic approach may identify a smaller set of models than the numerical (rank, determinant) approach.
Size of the set of corner cuts vs set of staircases

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{chart.png}
\caption{Graph showing the size of the set of corner cuts vs set of staircases for different values of $k$.
\label{chart}
\end{figure}
Minimal aberration (Bernstein et al. (2010))

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

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

For fixed $w$, define

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

This value is achieved for algebraic models in a generic design.

**Theorem** [1] In a generic design, minimal aberration $A^*$ obeys the following bounds:

$$A^+ - 1 \leq A^* \leq A^+ + 1$$

with $A^+ = (nd!)^{\frac{1}{d}} \frac{d}{d+1} g(w)$ and $g(w) = \sqrt[\frac{1}{d}]{w_1 \cdots w_d}$
Example: minimal aberration \( d = 2 \)

The graphs include \( A^*, A^+ \) and \( A^+ \pm 1 \) of Theorem; also approximate \( \tilde{A} \) is shown.

The border of the model (Betti)

For a polynomial ideal $I$, the *ideal of leading terms* $LT(I)$ is the monomial ideal generated by the leading terms of polynomials in $I$. In this part of the talk, $I$ denotes a monomial ideal.

The Hilbert function $H_{R/I}$ counts the number of monomials not in $I$, for each degree. E.g. for $I = \langle x^3, y^2 \rangle$ we have $H_{R/I} = 1, 2, 2, 1$.

The generating function for those terms is the *multigraded Hilbert series* $HS_{R/I}$. In the current example $HS_{R/I} = 1 + x + y + x^2 + xy + x^2y$.

We can however compute the Hilbert function and the Hilbert series for terms in $I$, and we have the following equality for $HS$:

$$
\sum_{\alpha \geq 0} x^\alpha = \sum_{\alpha \in I} x^\alpha + \sum_{\alpha \notin I} x^\alpha
$$

$$
\frac{1}{\prod_{i=1}^{d}(1 - x_i)} = HS_I + HS_{R/I}
$$
The table of Betti numbers describes the composition of (numerators of) sums, i.e. entry \((i, j)\) contains number of terms of degree \(i + j\).

\[
\frac{1}{(1-x)(1-y)} = \frac{y^2 + x^3 - x^3y^2}{(1-x)(1-y)} \quad \text{ } \quad \bigcup \quad \quad + \quad (1 + x + y + x^2 + xy + x^2y)
\]

\[
\begin{array}{ccc}
0: & 1 & - \\
1: & - & 1 \\
2: & 1 & - \\
3: & - & 1 \\
4: & - & 1 \\
\end{array}
\]

\[
\begin{array}{cccc}
0 & 1 & 2 & 1 \\
0: & 1 & - & - \\
1: & - & 1 & - \\
2: & - & 1 & - \\
3: & - & - & 1 \\
\end{array}
\]

\[
\frac{1}{(1-s)^2} = \frac{s^2 + s^3 - s^5}{(1-s)^2} + (1 + 2s + 2s^2 + s^3)
\]
We can only compare tables of Betti numbers for ideals that have the same Hilbert function. In such case, the following theorem guarantees existence of an ideal (called \textit{lex segment ideal}) that attains maximal Betti numbers.

\textbf{Theorem}[Bigatti-Hulett] Let $I \subseteq R$ and $L$ be the lex ideal such that $H_{R/I} = H_{R/L}$. Then $\beta_{i,j}(R/L) \geq \beta_{i,j}(R/I)$ for all $i, j$.

For generic designs, the models in the algebraic fan are corner cuts. In two dimensions, the relation between ideals generated by corner cuts staircases and lex-segment ideals is one-to-one. In other words, the models in the algebraic fan are precisely those that maximise Betti numbers.

For more than two dimensions, the relationship between lex-segment ideals and ideals which are the complement of corner cut staircases and is not necessarily one-to-one. For some cases, the ideal of a corner cut model may attain maximal Betti number despite not being a lex-segment ideal, while in other cases it may not attain maximal Betti numbers.
Example. Generic design $n = 7$, $d = 3$. Fan with 36 models, of which 3 are not lex segment, yet they still attain maximal Betti numbers [3].
We give conditions on weighing vector $w$ for identification of corner cut models whose ideals are lex segment ideals. The weights used are $w = (C - \gamma^{d-1}, C - \gamma^{d-2}, \ldots, C - 1)$.

Alexander duality

Echelon (staircase) designs

Echelon designs exhibit hierarchy in the set of indexes. These designs identify a single model.

Example: full factorial design

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

Other example
The Alexander dual of a simplicial complex $\Delta$ in a ground set $V$ is the simplicial complex $\Delta^*$ constructed by those subsets of $V$ whose complement is not in $\Delta$, see [5] and [2].

Example. Model with directing monomials $x_1x_2x_3$ and $x_3x_4$

$L = \{1, x_1, x_2, x_3, x_4, x_1x_2, x_1x_3, x_2x_3, x_3x_4, x_1x_2x_3\}$ and

$L^* = \{1, x_1, x_2, x_3, x_1x_3, x_2x_3\}$.

Equivalently, if $L$ is considered as a simplicial complex, its Stanley-Reisner ideal [5] is $I_L = \langle x_1x_4, x_2x_4 \rangle$. Thus $L^*$ has directing monomials $x_2x_3$ and $x_1x_3$, obtained as complements of generators of $I_L$. 
Alexander dual as ‘flip operation’

The designs are fractions of two-level factorial designs. To obtain Alexander dual of $L$, consider $L(F)$ of full factorial

$L(F) = \{x^\alpha : \alpha \in \bigotimes_{i=1}^d \{0, 1\}\}$. and Alexander dual $L^*$ of $L$ is

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

The Alexander duality results are not confined to designs with two levels and hold for designs with an arbitrary number of levels. The Alexander dual of a model is computed relative to a grid in which the model is embedded.

$$L^*(D) = \{n - 1 - \alpha : \alpha \in L(F) \setminus L(D)\}.$$
Model for the complement is Alexander dual

**Theorem** Let $D$ and $\bar{D}$ be complementary non empty fractions of a full factorial design $F$; let $\prec$ be a given term order. Then the algebraic models for $D$ and $\bar{D}$ are Alexander duals, relative to the grid of the model for design $F$.

Alexander duality

The model for a fraction of a full factorial design has a natural dual: the Alexander dual, which is the model for the complement of the fraction.

Design \[ \mathcal{D} = \{(0, 0), (1, 0), (0, 1), (1, 1), (1, 2), (2, 2), (3, 1), (3, 2), (4, 3)\} \]

Model \[ L = 1, y, y^2, y^3, x, xy, xy^2, x^2, x^2y \]

Complementary design \[ \mathcal{D}^c = \text{Grid} \setminus \mathcal{D} \]

Model is Alexander dual \[ L^c = \{x_{\max} / x^{\alpha} : x^{\alpha} \in \text{Grid} \setminus L\} \]
Regular fractions of $2^d$

Alexander duality is performed over the alias’ table. For example, the 8 point fraction of $2^5$ with generators $x_1x_2x_3 = x_3x_4x_5 = 1$ yields

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Self-dual designs

For regular $1/2$ fractions of factorial designs $2^d$, the models are self-Alexander duals and thus the algebraic fan (collection of models) of $\mathcal{D}$ equals that of $\overline{\mathcal{D}}$ and state polytopes of both designs coincide.

For some $1/2$ non-regular fractions self duality and fan equality still holds.

But it is not difficult to find examples where self duality does not hold, despite equality of state polytopes.
Other constructions: reflections [4]

The model identified by reflections of an echelon design remains echelon and its model shares the same structure of that for the original design.
Reflections of an echelon design and Alexander duality

By Alexander duality, the complement of an echelon design remains so, thus its reflections lead to a model stemming from the Alexander dual.

Design (and complement)  Model (and A. dual)

Reflected designs  Model (and A. dual)
Reflections of a non-echelon design

Design (and complement)

Model (and A. dual)

Reflected design

Although Alexander duality holds for models, the design structure is not inherited to the model for the reflected design.
7. References


Thank you!
Towards inverse problems

For a given polynomial model, a problem of interest is to determine a design (set of points) such that the model is a) identifiable and b) satisfies some desirable criteria.

In statistics this is a well established problem (optimal design) which is subject of research interest: Isaac Newton Institute programs on design (2008,2011), ICODOE, mODa triennial cycle, DEMA &c.

Optimal designs are usually proposed for a particular model of interest. However, if there is no particular preference for a model, can we still aim for an optimal design?

Recall D-optimality: its objective is to minimize the volume of the confidence ellipsoid of the parameter estimates. \( \min(X^T X)^{-1} \) equivalently \( \max X^T X \) (vast literature, Kiefer-Wolfowitz, Fedorov, Wynn)
Types of optimality studied

• All stairs: **Fan D-optimality** What we obtain is a generic design (Caboara *et al* 1997) which also satisfies statistical desirable properties.

• Union of stairs: Embed the models in a **general model**. Here the design has more points than a given individual model (staircase) but it has the ability to discriminate between models (Atkinson and Cox, 1974).
Fan D-optimality (all stairs)

Construct $\mathcal{D}$ such that

$$f = \prod_{\lambda \in \binom{\mathbb{N}^d}{n}_{\text{stair}}} |X_\lambda'X_\lambda| = \prod_{\lambda \in \binom{\mathbb{N}^d}{n}_{\text{stair}}} |\mathcal{D}_\lambda|^2$$

is maximized over choice of $\mathcal{D}$ in a region $\mathcal{X} \subset \mathbb{R}^d$. We can weight every model by $\alpha_\lambda$ to reflect model preferences (Laüter, 1974).

$f : \mathbb{R}^{dn} \rightarrow \mathbb{R}$ has the following properties of symmetry (here written for $d = 2$):

- $f(x_{1i}, x_{2i}) = f(x_{2i}, x_{1i})$
- $f(x_{1i}, x_{2i}) = f(\pm x_{1i}, \pm x_{2i})$
- $f(p_i) = f(p_{\pi(i)})$ where $p_i = (x_{1i}, x_{2i})$ and $\pi(i)$ is a permutation of the indexes of $p_i$
Example: Consider $\mathcal{X} = [-1, 1]^d$, $d = 2$ and $n = 2$. A fan D-optimal design for the models $\{1, x_1\}$, $\{1, x_2\}$ is $\mathcal{D} = \{(-1, -1), (1, 1)\}$.

**Theorem** If $\mathcal{D}^* \subset \mathcal{X} \subset \mathbb{R}^2$ is a fan D-optimal design, then any design obtained by rotating $\mathcal{D}^*$ a multiple of $\frac{\pi}{2}$ radians is also fan D-optimal. Here $\mathcal{X}$ is either $[-1, 1]^2$ or the unit circle.

**Theorem** A fan D-optimal design for $n = 2$ in the region $\mathcal{X} = [-1, 1]^d$ is given by any two opposite vertexes of the hypercube.
More examples for $d = 2$ and $\mathcal{X} = [-1, 1]^2$.

$n = 3$ The fan D-optimal design is

$$\mathcal{D} = \left\{ \left( \begin{array}{c} -1 \\ 1 \end{array} \right), \left( \begin{array}{c} -\frac{4}{3} + \frac{\sqrt{13}}{3} \\ 1 \end{array} \right), \left( \begin{array}{c} 1 \\ 4 \frac{3}{3} - \frac{\sqrt{13}}{3} \end{array} \right) \right\}.$$  

$n = 4$ The fan D-optimal design is

$$\mathcal{D} = \left\{ \left( \begin{array}{c} a \\ 1 \end{array} \right), \left( \begin{array}{c} 1 \\ -a \end{array} \right), \left( \begin{array}{c} -a \\ -1 \end{array} \right), \left( \begin{array}{c} -1 \\ a \end{array} \right) \right\},$$

where $a = \frac{\sqrt{14}\sqrt{2} - 7}{7}$.

Solving the problem with Simulated Annealing\(^4\)
Using the algebra for optimization

Maximize \( f(x) = \prod_{\lambda \in \mathcal{C}} |X'_{\lambda}X_{\lambda}| \) over \( \chi = [-1, 1]^k \)

The Kuhn-Tucker (KT) conditions for the previous problem are

- \( L_i(x) = 0 \) (gradient equations)
- \( \lambda_i \geq 0, \ x_i \leq 1 \) and \( \lambda_i(x_i - 1) = 0 \)
- \( \mu_i \geq 0, \ -x_i \leq 1 \) and \( \mu_i(-x_i - 1) = 0 \)

where \( L(x) = f(x) - \sum_i \lambda_i(x_i - 1) + \sum_i \mu_i(x_i + 1) \) and \( i = 1, \ldots, kn \).
Using algebra to solve KT conditions

1. Create the KT ideal $I_{KT} \subset \mathbb{R}[x, \lambda, \mu]$ by

$$I_{KT} = \langle L_i(x), \lambda_i(x_i - 1), \mu_i(-x_i - 1) \rangle$$

2. Eliminate the Lagrange multipliers $\lambda$ and $\mu$, i.e. using the elimination ideal

$$\text{Elim}(I_{KT}, \{\lambda, \mu\}) := I_{KT} \cap \mathbb{R}[x] \subset \mathbb{R}[x]$$

3. Solve the above system.

Difficulties:

- Verifying sufficiency of KT conditions.
- The complexity of $f$ and high dimensionality of both $x$ and $\lambda, \mu$.
- $I_{KT} \cap \mathbb{R}[x]$ is generally not zero-dimensional.
Example 4: Optimal design in $[-1, 1]^2$ for estimating the models 
$\{1, x_1, x_1^2\}, \{1, x_1, x_2\}, \{1, x_2, x_2^2\}$

Coordinates for three points: $x_{11}, \ldots, x_{23}$

Lagrange multipliers: $\lambda_1, \ldots, \lambda_6, \mu_1, \ldots, \mu_6$

$I_{KT} = \langle g_1, \ldots, g_{18} \rangle$ and $I_{KT} \cap \mathbb{R}[x] = \langle g'_1, \ldots, g'_{74} \rangle$

To simplify the computation, we set the coordinates of some points to be on the border, i.e. $D = \{(-1, x_{21}), (x_{12}, -1)(1, 1)\}$. Now $I_{KT} \cap \mathbb{R}[x]$ is generated by six equations, two of which depend on $x_{12}, x_{21}$:

$$(x_{12} - 1)^2(x_{12} + 1)^2(x_{21} - x_{12})(x_{12}x_{21} - x_{12} - x_{21} - 3)(x_{21} - 1)^2(x_{21} + 1)^2,$$
$$(x_{12} - 1)^2(x_{12} + 1)^2(x_{12}x_{21} - x_{12} - x_{21} - 3)(3x_{21}^2 - 8x_{21} + 1)(x_{21} - 1)^2(x_{21} + 1)^2$$

By solving the previous equations, we obtain the feasible value $x_{12} = \frac{4-\sqrt{13}}{3}$. 
The general model approach

If we define \( V_n^d := \bigcup (N_n^d)_{stair} \), this is the log representation of the general model which contains all \( n \)-term stairs. We can then apply traditional optimality techniques for discriminating subsets of a large polynomial model.

- Easy construction of \( V_n^d \), against the problem of listing stairs
- Direct application of optimality criteria
- What’s the link between the two approaches?
References