The Algebraic method in experimental design: Betti numbers and interactions

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EMS2010, Bernoulli Society,
University of Piraeus, Greece, 19th August 2010
Pistone and Wynn (1996) proposed the use of algebra to identify models in experimental design. Their technique creates a (linearly independent) basis using a term ordering.

Algebraic models consists of a description of the border between the model its complement. This description is applied to fractions of factorial $2^d$ designs, where the algebraic models can be seen as simplicial complexes. A measure of the connectivity of such complexes is given by Betti numbers asociated to the monomial ideal of the model and that of its complement. Intuitively, large Betti numbers are related to models which are relatively disconnected.

The talk points to the computations we have performed to such purpose, using a Plackett-Burman designs as examples.
Order of the talk

1. Algebraic analysis of experiments
2. Hilbert series
3. Fractions of factorial designs with two levels
   a. The fan
   b. Simplicial models and Stanley Reisner ring
4. Constructing the Betti numbers
5. Example: Plackett Burman designs
   a. PB8
   b. PB12
6. Hilbert functions and the BHP theorem
7. Final comments
8. References
1. Algebraic analysis of experiments
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
  $T^d = \{ x^\alpha : \alpha \in \mathbb{Z}_{\geq 0}^d \}$, compatible with monomial
  simplification:
    1. $x^\alpha \succ 1$, $\alpha \neq 0$,
    2. $x^\alpha \succ x^\beta \Rightarrow x^{\alpha+\gamma} \succ x^{\beta+\gamma}$ 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
  $\langle \text{LT}(g) : g \in G_\tau \rangle = \langle \text{LT}(f) : f \in I(\mathcal{D}) \rangle$. 
Quotient rings (Cox et al., 1996)

• The elements of $\mathbb{R}[D]$ are in one to one correspondence with equivalence classes of polynomials modulo $I(D)$. The important isomorphisms hold

\[ \mathbb{R}[D] \sim \mathbb{R}[x]/I(D) \sim \mathbb{R}[x]/\langle LT(I(D)) \rangle \]  

(1)

• A basis (model) for $\mathbb{R}[x]/I(D)$ is given by those monomials that cannot be divided by any of $LT(g)$ for $g \in G_\tau$ (Gröbner basis).

• A model can be described through the (complement) monomial ideal associated with it.

• The computations depend on the term order selected $\tau$. By varying $\tau$ over all term orders, the collection of models is called design fan (Maruri, 2007).
2. Hilbert series
Hilbert series

A degree-by-degree description of the monomials that generate $\mathbb{R}[x]/I$ is given by the Hilbert series of $\mathbb{R}[x]/I$:

$$HS(s) = \sum_{t=0}^{\infty} H(t) s^t,$$

where $H(t) = \dim \mathbb{R}[x]_t/I_t$ is the Hilbert function. When $I = I(D)$ then $HS(s)$ encodes degree-by-degree information of the model $(L)$.

The Hilbert Series can be written alternatively as

$$HS(s) = \sum_{\alpha \in L} s^{\mid \alpha \mid},$$

with $\mid \alpha \mid$ the sum of elements in $\alpha$. The Hilbert function can be retrieved from the Hilbert Series $H(t) = \lim_{s \to 0} \frac{1}{t!} \frac{\partial^t HS(s)}{\partial s^t}$.
A finer description of the monomials generating $\mathbb{R}[x]/I$ is given by the multigraded Hilbert series. Let $W$ be a matrix of $d$ rows with integer entries ($W$ need not be square, nor full rank). The multigraded Hilbert Series of the quotient ring $\mathbb{R}[x]/I$ is defined as

$$HS_W(x) = \sum_{\alpha \in L} x^{WT\alpha},$$

where $L$ is the set of monomials which do not lie in $\langle LT(I) \rangle$. The Hilbert series is easily retrieved by using $W^T = (1, \ldots, 1)$.

Setting $W$ as identity ($d$) then $HS_W(x) = \sum_{\alpha \in L} x^{\alpha}$, and the partition $\mathbb{Z}^d = L \cup (\mathbb{Z}^d \setminus L)$ is reflected in the following relation:

$$\frac{1}{\prod_{i=1}^{d}(1-x_i)} = \sum_{\alpha \in L} x^{\alpha} + \left(\frac{1}{\prod_{i=1}^{d}(1-x_i)} - \sum_{\alpha \in L} x^{\alpha}\right)$$

$$HS(\mathbb{R}[x]/\langle 0 \rangle) = HS(\mathbb{R}[x]/I) + HS(I)$$
3. Factorial designs with two levels $2^d$
Factorial designs with two levels $2^d$

- Widely used in industrial experimentation
- Orthogonality properties
- Fractions available $2^{d-p}$
  - Criteria: resolution, generator wordlength
  - Highly fractioned for screening: Plackett Burman
  - Confounding: algebra and classic design analysis together
- Modelling of polynomial dynamical systems (Dimitrova et al. (2007)):
  - 9 point fraction of $2^5$ design
  - Reverse engineering with interpolators of PDS
  - Computation over design fan with 13 cones
The fan of fractions of $2^d$

- Very rich families of models, designs with enormous fans

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<tr>
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<td>$2^7-2$ (rnd)</td>
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<td>$\sim$ 300,000</td>
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- Exact computations only feasible for small cases.
- Complexity mirrors that of $0 - 1$ polytopes: a few relatively uninteresting cases (fractions with sizes 1, 2 or $2^d - 1, 2^d$) and for intermediate sizes the computations become very complex.
Simplicial models

The algebraic techniques above have particular characteristics when the designs are fractions of factorial designs with two levels.

- The models are squarefree, i.e. a model is a (hierarchical) subset of \( \bigotimes_{i=1}^{d} \{1, x_i\} \).
- By their squarefree and hierarchical structure, models can be seen and studied as simplicial complexes.
- We thus write \( \Delta \) for the model (i.e. basis of \( \mathbb{R}[x]/\langle LT(I(D))\rangle \)) to emphasize its simplicial structure.

**Example:** \( 2^3 \) design together with indicator \((x_1 - x_2)(x_2 - x_3)\) (6 run fraction). Model identified under \( \tau = \text{DegRevLex} \): \( \Delta_\tau = \{1, x_1, x_2, x_3, x_1 x_3, x_2 x_3\} \)
Stanley-Reisner ring

A simplicial complex has a one to one relation with a special type of monomial ideal, called the Stanley-Reisner ideal [7]. For a simplicial complex $\Delta$, let $I_{\Delta}$ be the squarefree monomial ideal created by the non-faces of $\Delta$: $I_{\Delta} = \langle x^a : a \notin \Delta \rangle$.

The complexity of the model $\Delta$ can be studied by the Stanley-Reisner ring $R[x]/I_{\Delta}$.

In the description of $R[x]/I_{\Delta}$, Betti numbers play a central role. Graded Betti number is the minimal number of generators $e_{a,j}$ in degree $i + j$. 
The ideal of leading terms $\langle \text{LT}(I(D)) \rangle$ is related to the Stanley-Reisner ideal:

$$\langle \text{LT}(I(D)) \rangle = \overline{I}_\Delta,$$

where $\overline{I}_\Delta$ is the artinian closure of $I_\Delta$. 
4. Computing the Betti numbers

Consider the following simplicial complex (model) [7]: \( \Delta = \{1, a, b, c, d, e, ab, ac, ad, ae, bc, bd, be, cd, ce, abc, abd, adc, bcd, bce\} \) and the Stanley-Reisner ideal generated by it:

\[
I_\Delta = \langle de, abe, ace, abcd \rangle \subset \mathbb{R}[a, b, c, d, e]
\]
Use \( T := \mathbb{Q}[a, b, c, d, e] \);
\( J := \text{Ideal}(de, a\, b\, e, a\, c\, e, a\, b\, c\, d) \);
Hilbert(T/J);
HilbertSeries(T/J);

\[
H(t) = \frac{5}{2}t^2 + \frac{3}{2}t + 1 \quad \text{for } t \geq 0
\]
\[
\frac{1 + 2a + 2a^2}{(1-a)^3}
\]
BettiDiagram(T/J);

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Hilbert Series (after simplification)

\[
HS = \frac{\left( 1 - de - a be - ace - abcd + abde + acde + abce \right)}{(1 - a)(1 - b)(1 - c)(1 - d)(1 - e)}
\]
BettiDiagram(J);

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Tot: 4 4 1
Alternatively we could use the Artinian closure of $\bar{I}_\Delta$ which is

$$I_\Delta = \langle de, abe, ace, abcd \rangle + \langle a^2, b^2, c^2, d^2, e^2 \rangle$$

K:=J+Ideal(a^2,b^2,c^2,d^2,e^2);
Hilbert(T/K);
HilbertSeries(T/K);

----------------------------------------------

H(0) = 1
H(1) = 5
H(2) = 9
H(3) = 5
H(t) = 0 for t >= 4
----------------------------------------------

(1 + 5a + 9a^2 + 5a^3)

----------------------------------------------
K;
BettiDiagram(T/K);

Ideal(de, abe, ace, abcd, a^2, b^2, c^2, d^2, e^2)

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A degree-by-degree description of the model border is obtained.
5. Example: Plackett-Burman designs
Plackett-Burman designs

• Small fractions of $2^d$ with $d$ factors and $n = d + 1$ runs.
• Designs constructed by circular shifts of a generator, available for $d = 7, 11, 15, 19, 23, \ldots$
• PB designs possess a complicated aliasing table, but they have an orthogonal design-model matrix for the linear model with all factors

$$E(y) = \theta_0 + \sum_{i=1}^{d} \theta_i x_i$$

• PB designs are a popular choice for screening in a first stage of experimentation.

We study their algebraic fan and describe the structure of models with the aid of Betti numbers.
Consider a Plackett-Burman (PB8) design with eight runs, seven factors $a, b, c, d, e, f, g$ and generator $+---+++ +$. 

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<th>a</th>
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Set a block term ordering $\prec_1$ for which monomials in $c, d, e$ are smaller than monomials in $a, b, f, g$. The model identified by PB8 is

$$\Delta_{\prec_1} = \{1, e, d, de, c, ce, cd, a\},$$

i.e. a simplicial complex consisting of two components. The description of $\Delta$ (degree by degree) is found by computing the Hilbert series of the quotient ring $R[a, b, c, d, e, f, g]/\langle LT(I(D))\rangle$ which is

$$HS(s) = 1 + 4s + 3s^2.$$  

The model border contains one leading monomial of degree one ($a$) and three leading monomials of degree two ($de, ce, cd$). We now examine the monomial ideal generated by the leading terms of
the design ideal
\[
\langle LT(I(\mathcal{D})) \rangle = \langle f, b, g, a^2, ac, ad, ae, c^2, e^2, d^2, cde \rangle = \overline{I}_\Delta
\]
which has three generators of degree one, seven of degree two and one of degree three. This precise description degree by degree is read from the Betti diagram of the ideal of leading terms, i.e. \( \beta_{0,1} = 3, \beta_{0,2} = 7, \beta_{0,3} = 1 \), and the border description of \( \Delta \) is also read from the Betti diagram: \( \beta_{6,8} = 1, \beta_{6,9} = 3 \).

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<td>86</td>
<td>99</td>
<td>67</td>
<td>25</td>
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**Table 1**: Betti diagram for PB8 and \( \prec_1 \).
PB8 (cont.)

In contrast, consider a term ordering $\prec_2$ which is DegRevLex. Now the Betti diagram contains much higher numbers $\beta_{0,2} = 28$ (number of leading terms of $\langle I(D) \rangle$) and $\beta_{6,8} = 7$ (number of leading monomials of $\Delta$). In other words, PB8 identifies a simplicial complex model with seven disconnected components

$$\Delta_{\prec_2} = \{1, a, b, c, d, e, f, g\}$$

and a very complex ideal of leading terms. This is the model for Equation (3).

Now repeat the analysis with a Lex term ordering $\prec_3$. The Betti diagram now shows much smaller figures $\beta_{0,1} = 4$, $\beta_{0,2} = 3$ and $\beta_{6,10} = 1$. Betti numbers reflect that the model $\Delta_{\prec_3}$ is simpler, being one simplicial complex completely connected (and
contractable)

\[ \Delta \prec_3 = \{1, e, f, g, ef, eg, fg, efg\} \]

The results for the 218 models in the algebraic fan of PB8 are summarized in Table 2, where representatives of six equivalence classes (up to permutation of factors) are shown.

<table>
<thead>
<tr>
<th>(\prec_1) (Block)</th>
<th>(\prec_2) (DegRevLex)</th>
<th>(\prec_3) (Lex)</th>
</tr>
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<tr>
<td>1 + 6s + s^2 (21)</td>
<td>1 + 7s (1)</td>
<td>1 + 3s + 3s^2 + s^3 (28)</td>
</tr>
<tr>
<td>1 + 5s + 2s^2 (84)</td>
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Table 2: Equivalence classes of models \(\Delta\) and corresponding Hilbert Series for PB8.
PB8: Comparing models

<table>
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<td>2: - - 6 26 45 39 17 3</td>
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<tr>
<td>Tot: 1 10 38 75 85 56 20 3</td>
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Disconnected model $\prec_2$ DegRevLex:

| 0 1 2 3 4 5 6 |
| 0: 1 - - - - - - |
| 1: - 21 70 105 84 35 6 |
| Tot: 1 21 70 105 84 35 6 |
PB12

This design has 12 runs in 11 factors and generator
\[+ + - + + + - - - + -].

The algebraic fan of PB12 is very complex, showing a rich variety
of simplicial models.

Despite its enormous size (around \[3 \times 10^5\]), models have been
classified in nineteen classes (up to permutations of variables),
which in turn share only ten distinct Hilbert Series.
6. Results on integer sequences that are Hilbert functions

Macaulay’s Theorem for Hilbert function growth: Let \( \mathcal{H} : \mathbb{N} \to \mathbb{N} \) a function with \( \mathcal{H}(0) = 1 \). Then \( \mathcal{H} \) is the Hilbert function of some cyclic \( R \)-module if and only if

\[
\mathcal{H}(d + 1) \leq \mathcal{H}(d)^{(d)}
\]

for all \( d \geq 1 \).

The notation \( \mathcal{H}(d)^{(d)} \) is related to the Macaulay expansion of \( \mathcal{H}(d) \) with respect to \( d \). The Macaulay expansion of an integer \( a \) with respect to \( d \) is defined as follows:

**Macaulay expansion:** Let \( a, d \in \mathbb{N} \) with \( d > 0 \). Then there are unique integers \( a_d > a_{d-1} > \cdots > a_1 \geq 0 \) such that

\[
a = \binom{a_d}{d} + \binom{a_{d-1}}{d-1} + \cdots + \binom{a_1}{1}.
\]
The sum \( a = \binom{a_d}{d} + \binom{a_{d-1}}{d-1} + \cdots + \binom{a_1}{1} \) is the Macaulay expansion of \( a \) with respect to \( d \).

Let \( a \in \mathbb{N} \). Then for \( d \in \mathbb{N}_+ \), define \( a^{\langle d \rangle} \) to be the integer

\[
a^{\langle d \rangle} = \binom{a_d + 1}{d + 1} + \binom{a_{d-1} + 1}{d - 1 + 1} + \cdots + \binom{a_1 + 1}{1 + 1},
\]

where \( a = \binom{a_d}{d} + \binom{a_{d-1}}{d-1} + \cdots + \binom{a_1}{1} \) is the Macaulay expansion of \( a \) with respect to \( d \).

**Macaulay’s theorem on Hilbert functions:** A function \( \mathcal{H} : \mathbb{N} \rightarrow \mathbb{N} \) with \( \mathcal{H}(0) = 1 \) is the Hilbert function of a cyclic module if and only if there is a lex ideal \( L \) such that \( H(R/L) = \mathcal{H} \).

**Lex ideals:** A monomial ideal \( I \subset R \) is called lex if for each \( j > 0 \), \( I \cap R_j \) is generated as a \( k \)-vector space by the first \( \dim_k(I \cap R_j) \) monomials of degree \( j \) in descending lex order.
Extremal behaviour of lex ideals with respect to Betti numbers

**Bigatti-Hulett-Pardue Theorem:** Let $I \subset R$ an ideal and let $L$ be the lex ideal such that $\mathcal{H}(R/I) = \mathcal{H}(R/L)$. Then $\beta_{i,j}^L \geq \beta_{i,j}^I$ for all $i = 1, \ldots, n$ and $j \in \mathbb{N}$.

**Example** Let $R = k[x, y, z]$ and let us consider zero dimensional ideals in $R$ of multiplicity 6.

The possible Hilbert functions are:

$[1, 2, 3], [1, 3, 2], [1, 2, 2, 1], [1, 3, 1, 1], [1, 2, 1, 1, 1], [1, 1, 1, 1, 1, 1]$

and each one has its own ideal attaining maximal Betti numbers:

$\langle x, z^3, yz^2, y^2z, y^3 \rangle, \langle y^2, xz, xy, x^2, z^3, yz^2 \rangle, \langle x, y^2, yz^2, z^4 \rangle, \langle yz, y^2, xz, xy, x^2, z^4 \rangle, \langle x, yz, y^2, z^5 \rangle, \langle y, x, z^6 \rangle$. 
7. Final remarks

• Continuing work to linking designs and Betti numbers through BHP Theorem. For observed PB designs, maximal Betti numbers for models (i.e. ideals of leading terms) are achieved.

• Link between multigraded Hilbert Series of $\mathbb{R}[x]/I(D)$ and aberration

$$A(w, L) = \frac{1}{n} w^T \nabla HS(x)|_{x=1}$$

• Link with Betti results and traditional generator aberration and estimation capacity (Cheng & Mukerjee, 1998 [2]).
8. References


Thank you!