ENBIS-16

The Algebraic method in experimental design

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Polynomial regression

We are familiar with the use of polynomials throughout statistics.

$$x_1, x_2^2, x_1x_2, \ldots$$

EG a second order polynomial response surface in tw0 factors is

$$f(x_1, x_2) = \theta_{00} + \theta_{10}x_1 + \theta_{01}x_2 + \theta_{20}x_1^2 + \theta_{11}x_1x_2 + \theta_{02}x_2^2$$

Polynomial are made up of monomials. Consider a set of k factors:

$$x = (x_1, \ldots, x_k)$$

and non-negative integers $\alpha = (\alpha_1, \ldots, \alpha_k)$ a monomial is

$$x^\alpha = x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_k^{\alpha_k}.$$

A monomial x^α can be represented by its exponent vector α and we can list the monomial is a model either directly or by listing a set of exponents. We shall often use the notation

$$\{x^\alpha, x \in M\}.$$

Ideals

Definition

A monomial ideal I is an ideal for which a collection of monomials $f_1, \ldots, f_m$ such that any $g \in I$ can be expressed as a sum

$$g = \sum_{i=1}^{m} g_i(x) f_i(x).$$

The idea is that given a monomial ordering and an ideal expressed in terms of the G-basis, $I = \langle g_1, \ldots, g_m \rangle$, any polynomial f has a unique remainder with respect the quotient operation $K[x_1, \ldots, x_k]/I$. That is

$$f = \sum_{i=1}^{m} s_i(x) g_i(x) + r(x)$$

We call the remainder $r(x)$ the *normal form* of f with respect to I and write $NF(f)$. Or, to stress the fact that it may depend on $\prec$, we write $NF(f, \prec)$.

The algebraic method in design

We should think of design as lists of points,

$$D = \{x^{(1)}, \ldots x^{(n)}\},$$

in R^k. As algebraic varieties they have associated ideal

$$I(D) = \{f : f(x) = 0,\ x \in D\}$$

The use of polynomials to define design is clearly not new. For example a 2^k full factorial designs give by $\{\pm 1, \ldots, \pm 1\}$ is expressed the by the solution of the simultaneous equations:

$$\{x_i^2 - 1 = 0,\ i = 1, \ldots, k\}.$$

To obtain fractions we impose additional equations: e.g. $x_1 \ldots x_k = 1$.

Step by step approach

- Choose a design D
- Select a monomial term ordering, $\prec$
- Compute Gröbner basis for $I(D)$ for given monomial ordering, $\prec$.
- The quotient ring

$$K[x_1, \ldots, x_k]/I(D)$$

  of the ring of polynomials $K[x_1, \ldots, x_k]$ in $x_1, \ldots, x_k$ forms is a vector space spanned by a special set of monomials: $x^\alpha, \alpha \in L$. These are all the monomials not divisible by the leading terms of the G-basis and $|L| = |D|$.
- The set of multi-indices L has the "order ideal" property: $\alpha \in L$ implies $\beta \in L$ for any $0 \leq \beta \leq \alpha$. For example, if $x_1^2 x_2$ in the model so is $1, x_1, x_2, x_1 x_2$. (Hierarchical model).

- Any function $y(x)$ on D has a unique polynomial interpolator given by

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

such that $y(x) = f(x), \ x \in D$.
- The cardinality of the design and the quotient basis (model) is the same: $|L| = |D|$.
- The X-matrix is $n \times n$, has full rank n and has rows indexed by the design points and columns indexed by the basis:

$$X = \{x^\alpha\}_{x \in D, \alpha \in L}$$

Response surface design

Response surface design, non-standard: a 16-point design which is a 5^2 factorial with all internal points (a 3^2 design) removed:

$$\begin{array}{cccc} (2,0) & (2,1) & (2,2) & (1,2) \\ (0,2) & (-1,2) & (-2,2) & (-2,1) \\ (-2,0) & (-2,-1) & (-2,-2) & (-1,-2) \\ (0,-2) & (1,-2) & (2,-2) & (2,-1) \end{array}$$

The design ideal is generated by the following polynomials $x_2^5 - 5x_2^3 + 4x_2, x_1^5 - 5x_1^3 + 4x_1, x_1^2x_2^2 - 4x_1^2 - 4x_2^2 + 16$. It can be shown that for any term ordering, the above polynomials form a so-called reduced Gröbner basis and thus the design identifies a single model with terms $1, x_2, x_2^2, x_2^3, x_2^4, x_1, x_1x_2,\ x_1x_2^2, x_1x_2^3, x_1x_2^4, x_1^2, x_1^2x_2, x_1^3,\ x_1^3x_2, x_1^4, x_1^4x_2$.

Graeco Latin square

$$\begin{matrix} A\alpha & B\beta & C\gamma & D\delta \\ B\gamma & A\delta & D\alpha & C\beta \\ C\delta & D\gamma & A\beta & B\alpha \\ D\beta & C\alpha & B\delta & A\gamma \end{matrix}$$

Code up the design point using indicator functions.
Estimable terms

1, u[4], u[3], u[2], t[4], t[3], t[2], c[4], c[3], c[2], r[4], r[3], r[2], t[4]u[4], t[4]u[3], t[4]u[2]

$$Checkdegreesorfreedom:$$

16 - $(1+4\ \times 3) = 3$ df for interactions

Fans: a Latin Hypercube example

Design $d = 3, n = 6$

$$(0,0,0),(1/5,1,4/5),(2/5,3/5,2/5),$$

$$(3/5,4/5,1/5),(4/5,1/5,1)(1,2/5,3/5)$$

The collection of all models identifiable is called the *algebraic fan*
This design identifies 27 different models which can be classified in only six types of models, up to permutations of variables:

$1, x_1, x_1^2, x_1^3, x_1^4, x_1^5$ (3 models); $1, x_1, x_1^2, x_1^3, x_1^4, x_2$ (6 models); $1, x_1, x_1^2, x_1^3, x_2, x_1x_2$ (6 models); $1, x_1, x_2, x_1^2, x_1x_2, x_2^2$ (3 models); $1, x_1, x_2, x_3, x_1^2, x_1^3$ (3 models) and $1, x_1, x_2, x_3, x_1^2, x_1x_2$ (6 models).

The fan of fractions of 2^d

- Very rich families of models, designs with enormous fans

Name	d	n	Fan size
2^{4-1}_{III}	4	8	4
2^{4-1}_{IV}	4	8	12
PB8	7	8	218
2^{7-2}_{IV}	7	32	132
2^{7-2}_{IV} (mga)	7	32	1708
2^{7-2} (rnd)	7	32	$\sim 270,000$
PB12	11	12	$\sim 300,000$

- Exact computations only feasible for small cases.
- Aliasing strructure for PB designs very complicated

Aliasing

Let $I(D)$ be the design ideal and for two polynomials f, g define

$$f(x) \sim_D g(x)$$

to mean $f(x) = g(x),\ x \in D$. This is equivalent to

$$f(x) - g(x) \in I(D).$$

Again equivalently we have, with respect to a particular monomial ordering

$$NF(f) = NF(g)$$

The G-basis for the design ideal gives the aliasing structure:

$$LT(g) = \sum_{\alpha \in L} c_\alpha x^\alpha, \quad g \in G$$

. We can think of any large term as mapped first to a $LT(g)$.

A duality result

Given a design D embedded in a full factorial F, that is to say a fraction of a full factorial, we can consider the complementary design (fraction) $\bar{D} := F \setminus D$. Our main result says that the basis of the complementary design is the Alexander dual (relative to F) of the basis of the original design. Put as succinctly as possible:

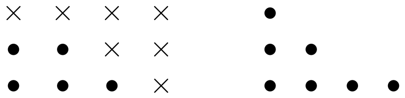
$$L^*(D) = L(\bar{D}) \tag{1}$$

Let $\prec$ be a fixed monomial ordering; let F be a full factorial design F with a fraction $D \subset F$. Then the bases of the quotient rings of D and the complementary design $\bar{D} = F \setminus D$ are Alexander dual, relative to F.

An example

A subset of a 4×3 design.

The crosses represent term exponents in $L(F) \setminus L(D)$. The Alexander dual $L^*(D)$ is obtained by flipping the crosses to give the right panel in the same figure. In this example, the Alexander dual of $L(D) = \{1, x_1, x_2, x_1^2, x_1x_2, x_1^2\}$ relative to the 4×3 full factorial is $L^*(D) = \{1, x_1, x_2, x_1^2, x_1x_2, x_2^2, x_1^3\}$.



Transepts 1. Interpolation on transepts

Consider the equation $x_1 x_2 = 0$. The G-basis of $< x_1, x_2 >$ is itself. This says that we take all terms

$$1, x_1, x_1^2, \ldots x_2 x_2^2, \ldots$$

which means all polynomial additive models

$$\theta_{00} + \theta_{10} x_1^2 + \theta_{20} x_1^2 + \cdots + \theta_{01} x_2^2 + \theta_{01} x_2^2 + \cdots$$

Now combine it with a design $< x_1^2 - 1, x_2^2 - 1 >$ We want to interpolate on the lines $x_1 x_2 = 0$ AND the points $(\pm 1, \pm 1)$. We need to represent OR that is union of varieties:

$$< x_1 x_2 (x^2 - 1), x_1 x_2 (x_2^2 - 1) >$$

The leading terms are

$$x_1^3 x_2, \quad x_1 x_2^3$$

Models

$\uparrow$						
o	x	x	x	x	x	
o	X	x	x	x	x	
o	o	o	x	x	x	
o	o	o	X	x	x	
o	o	o	o	o	o	$\rightarrow$

Using the Normal Form

Truncate the Taylor expansion of some function. Eg

$$(1+\exp(x_1))(1+exp(x_2))$$

Truncated form up to degree 3.

$$1+x_1+\frac{x_1^2}{2}+\frac{x_1^3}{6}+\cdots+\frac{x_2^2}{2}+\frac{x_2^3}{6}+\ldots$$

$$x_1x_2+\frac{x_1^2x_2}{2}+\frac{x_1x_2^2}{2}+\frac{x_1^2x_2^2}{4}+\cdots$$

$$\frac{x_1^3x_2}{6}+\frac{x_1x_2^3}{6}+\frac{x_1^3x_2}{6}+\frac{x_1x_2^3}{6}+\frac{x_1^3x_2}{12}+\frac{x_1^2x_2^3}{12}+\frac{x_1^3x_3}{36}$$

Normal forms wrt $< x_1x_2(x^2-1), x_1x_2(x_2^2-1) >$

$$1+x_1+\frac{x_1^2}{2}+\frac{x_1^3}{6}+\cdots+x_1+\frac{x_2^2}{2}+\frac{x_2^3}{6}+\ldots$$

$$\frac{49}{12}x_1x_2+\frac{7}{12}x_1^2x_2+\frac{7}{12}x_1x_2^2+\frac{1}{4}x_1^2x_2^2$$

A general class of designs

Observe on hyperplanes, lines, points. We wish to develop an aliasing theory for such *hyperplane arrangements*.
Simple example: 3 line in R^2.

$$(x_1 + x_2 - 1)(x_1 - x_2 - 1)(2x_1 + x_2 - 1)$$

Multiply out: $2x_1^3 + \dots$ Clear that with the right $\prec$ we have $LT = x_1^3$

$$\begin{array}{cccccc}
\uparrow & \uparrow & \uparrow & & & o \\
o & o & x & x & x & \\
o & o & o & x & x & x \\
o & o & o & x & x & x \\
o & o & o & X & x & x
\end{array}$$

We need to distiguish the following two points
1. Observing on trancepts (see above). This is quotienting wrt the transept ideal: $< x_1 x_2 >$ and we have

$$
\begin{array}{ccccccc}
\uparrow & & & & & & \\
o & x & x & x & x & x & \\
o & x & x & x & x & x & \\
o & x & x & x & x & x & \\
o & X & x & X & x & x & \\
o & o & o & o & o & o & \rightarrow
\end{array}
$$

2. Tie down: the values are fixed on the ideals eg zero on $x_1 = x_2 = 0$.
But then add a design eg

$$(\pm 1, \pm 1)$$

A differencing trick

Take the quotient ring defined by

$$< x_1x_2(x^2 - 1), x_1x_2(x_2^2 - 1) >$$

and remove the terms defined by $< x_1x_2 >$. Solution:

$$\{x_1x_2,\ x_1^2x_2,\ x_1x_2^2,\ x_1^2x_2^2\}$$

$$\begin{array}{ccccccc}
\uparrow & & & & & & \\
x & x & x & x & x & x & \\
x & X & x & x & x & x & \\
x & o & o & x & x & x & \\
x & o & o & X & x & x & \\
x & x & x & x & x & x & \rightarrow
\end{array}$$

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