Understanding aliasing using Gröbner bases

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ABSTRACT: The now well-established Gröbner basis method in experimental design (see the authors' monograph "Algebraic Statistics") had the understanding of aliasing as a key motivation. The basic method asks: given an experimental design, what is estimable, or more generally what is the alias structure? The paper addresses the following related question: given a set of conditions which the design is known to satisfy, what can we say about the alias structure? Some classical and non-classical construction methods are included.

KEYWORDS: Aliasing; Gröbner basis; polynomial conditions

1 The Gröbner basis method

We summarise the method briefly in a number of steps.

Step 1 Define a design $D \subset \mathbf{R}^d$ as a set of n distinct points: $D = \left[a^{(i)}\right]_{i=1}^{n}$.

Step 2 Set up a series of polynomial equations whose solutions give precisely D. This, mathematically, amounts to representing the design as a zero dimensional algebraic variety. The design ideal, $\mathrm{Ideal}(D)$, is the set of all polynomials whose zeros include the design points.

Step 3 Select a so-called monomial ordering τ. This is a total well-ordering on the monomials such that $x^\alpha \prec_\tau x^\beta$ implies $x^\alpha x^\gamma \prec_\tau x^\beta x^\gamma$ for all $\gamma \neq 0$.

Step 4 Generate a Gröbner basis for $\mathrm{Ideal}(D)$, given τ, namely a special representation of D as the solutions of polynomial equations

$$\{g_j(x) = 0 : j = 1, \ldots, k\}$$

The full details are omitted.

Step 5 List the leading terms $l_j(x) = \mathrm{LT}\,(g_j(x))$, $j = 1, \ldots, k$ with respect to the monomial ordering τ.

Step 6 List all monomials not divisible by any leading term $l_j(x)$ ($j = 1, \ldots, k$). Call this list $\mathrm{Est}_\tau(D)$ and note that

(i) $\#\mathrm{Est}_\tau(D) = n$, that is the sample size of the design.

(ii) If $\mathrm{Est}_\tau(D) = \{x^\alpha : \alpha \in L\}$ then the monomial terms are the basis of a saturated and estimable regression model

$$\sum_{\alpha \in L} \theta_\alpha x^\alpha$$

with non singular X-matrix

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

(iii) $\mathrm{Est}_\tau(D)$ is an order ideal, that is if $x^\alpha \in \mathrm{Est}_\tau(D)$ then $x^\beta \in \mathrm{Est}_\tau(D)$ for any β component wise smaller than α.

A lot can be said about this process with regard to appropriate computer algebra. For example methods are available for directly computing the Gröbner basis and $\mathrm{Est}_\tau(D)$ from D. See Pistone, Riccomagno and Wynn (2000) for details. For the present paper we note simply that the equations $\{g_j(x) = 0 : j = 1, \ldots, k\}$ defining the design essentially also give some alias structure. For example each leading term can be written

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

so that $g_j(x) = l_j(x) - \sum_{\alpha \in L} \theta_\alpha^{(j)} x^\alpha$. That is to say "higher order" terms with respect to τ can be written in terms of polynomials constructed from monomials in $\mathrm{Est}_\tau(D)$. Apart from the fact that the equations are dependent on τ all the alias structure can be captured from such equations. A generic member of the ideal $\mathrm{Ideal}(D)$ is written $\sum_{j=1}^k s_j(x) g_j(x)$ where the $s_j(x)$'s are generic polynomials. Setting this to zero for arbitrary $s_j(x)$ gives all possible alias relations.

2 A theorem on aliasing

Historically there have been many combinatorial constructions of experimental design of which the standard Abelian group construction of symmetric and asymmetric factorial design is perhaps the most celebrated. In such constructions one exhibits a set of conditions which the designs must satisfy. For example to construct a 2^{3-1} the equations are

$$x_1^2 = 1, \qquad x_2^2 = 1, \qquad x_3^2 = 1, \qquad x_1 x_2 x_3 = 1$$

In the previous section this could be considered as Step 2.
In this section we discuss some simple properties that can be predicted for $\mathrm{Est}_\tau(D)$ given the construction equations but in advance of computing $\mathrm{Est}_\tau(D)$ itself.
The equation $x_1x_2x_3 = 1$ for the 2^{3-1} above implies that the interaction $x_1x_2x_3$ and the constant term are aliased, in particular the vector obtained by evaluating $x_1x_2x_3$ at the design points is the unit vector, $(1,\ldots,1)$. Theorem 1 generalises this observation.

Theorem 1 *Let the design D be known to satisfy the polynomial equation*

$$h(x) = 0$$

in $\mathbf{R}^d$ and let τ be a monomial ordering. Let $M(\neq \emptyset)$ be the set of monomials with non zero coefficients in h. Then

$$M \not\subseteq Est_\tau(D)$$

Proof. This is by contradiction. Suppose $M \subseteq \mathrm{Est}_\tau(D)$. Then

$$h(x) = \sum_{\alpha \in M \subseteq L} \phi_\alpha x^\alpha$$

where $\mathrm{Est}_\tau(D) = \{x^\alpha : \alpha \in L\}$ and all $\phi_\alpha \neq 0$ for α such that $x^\alpha \in M$. But this is false since all x^α are linearly independent over D and $h(x) = 0$ for all $x \in D$.
A proof relying on more classical arguments from matrix theory is as follows. Let $h(x) = \sum_{\alpha\in M} \phi_\alpha x^\alpha$ and consider the matrix $X = \{x^\alpha\}_{x\in D,\alpha\in M}$ with columns $X(\alpha) = \{x^\alpha\}_{x\in D}$. The matrix X is singular because the condition $h(x) = 0$ implies that the linear combination of the columns of X, $\left\{\sum_{\alpha\in M} \phi_\alpha X(\alpha)\right\}$ is the zero vector. Thus the monomials x^α, $\alpha \in M$ are linearly dependent over D and cannot all be included in a model identifiable by D. $\square$

To repeat the result of the theorem: any M must have at least one "non zero" term not in $\mathrm{Est}_\tau(D)$. Note also that if $x^\beta \notin \mathrm{Est}_\tau(D)$ it also follows from Gröbner basis theory that $x^\gamma \notin \mathrm{Est}_\tau(D)$ for all $\gamma > \beta$ component wise.

Corollary 1 *If $h(x) = x^\alpha - c$ for some index α and constant c then if $D \neq \emptyset$ then x^α cannot be in $Est_\tau(D)$.*

Proof. Since D is not empty the constant must be in $\mathrm{Est}_\tau(D)$. This follows from Step 6 (iii). Thus by Theorem 1, $x^\alpha \notin \mathrm{Est}_\tau(D)$. $\square$

Typically in construction we may know that $h_j(x) = 0$ on D for $j = 1, \ldots, r$. Then Theorem 1 applies to each corresponding M_j.
Sometimes we may construct designs as exactly all solutions of $h_j(x) = 0$, $j = 1, \ldots, r$

$$D = \{x : h_j(x) = 0, \qquad j = 1, \ldots, r\}$$

However it is advisable to replace this by the Gröbner basis representation to obtain a more tractable description of aliasing.
Example 1 Factorial design. The corollary makes a strong connection to the fractional factorial construction mentioned above since those consist typically of solving sets of equations of the form

$$\{x^{\alpha(j)} - c_j : j = 1, \ldots, r\}$$

3 Further examples

Example 2 Mixture. Here a basic equation is $\sum x_i - 1 = 0$. Theorem 1 simply says that not all of 1 and x_i, $i = 1, \ldots, d$ can be in $\mathrm{Est}_\tau(D)$ confirming the standard redundancy in this case. See Giglio, Riccomagno and Wynn (2000).
Example 3 Other groups. Any design D invariant under a group G on $\mathbf{R}^d$ will preserve the maximal invariants, $\pi_j(x)$, under G. Thus candidates for $h_j(x)$ are

$$h_j(x) = \pi_j(x) - c_j$$

As a very simple example consider designs on a circle in $\mathbf{R}^2$ satisfying

$$x_1^2 + x_2^2 = 1$$

Then we can conclude that both of x_1^2 and x_2^2 cannot be in $\mathrm{Est}_\tau(D)$. Since maximal invariants are constant on orbits any design constructed as an orbit will be invariant

$$D = \{x = G(x_0) : \text{ for a point } x_0 \in D\}$$

In the above example one can easily construct arbitrary large designs in this way and still not have x_1^2 and x_2^2 in $\mathrm{Est}_\tau(D)$. This can easily be extended to rotations in $\mathbf{R}^d$.
An important class of groups in design theory are reflection groups. Indeed the conditions above $x_1^2 = x_2^2 = x_3^2 = 1$ and $x_1x_2x_3 = 1$ are precisely a set of invariants for the subgroup generated by the reflections

$$(x_1, x_2, x_3) \longrightarrow \left\{ \begin{array}{l} (-x_1, -x_2, x_3) \\ (-x_1, x_2, -x_3) \end{array} \right.$$

and the design $D = \{(1,1,1), (1,-1,-1), (-1,1,-1), (-1,-1,1)\}$ is an orbit.

Example 4 Lattices. One generator lattice designs are equally spaced designs on the integer grid defined as

$$D = \{gk \pmod{n} : k = 0, \ldots, n-1\}$$

where g is a vector of integers. If the components of g and n have greatest common divisor equal to one, then D has exactly n distinct points. For $g = (1, 2)$ and $n = 5$, $D = \{(0,0), (1,2), (2,4), (3,1), (4,3)\}$. The Gröbner basis computed modulo 5 and with respect to any term-ordering for which x_2 is smaller than x_1, includes the polynomial $x_1 + 2x_2$. Thus every point in D has to satisfy the equation $x_1 + 2x_2 = 0 \pmod{5}$. The full Gröbner basis is

$$\begin{array}{l} x_1 + 2x_2, \\ x_2^5 - x_2 \end{array}$$

and $\mathrm{Est}_\tau(D)$ is $\left\{1, x_2, x_2^2, x_2^3, x_2^4\right\}$. This shows algebraically that modulo 5 the design D is a one dimensional object.
Over the real numbers and with respect to a lexicographic term ordering (see Cox, Little and O'Shea, 1996) with again x_2 smaller than x_1 the Gröbner basis is

$$\begin{array}{rcl} g_1(x) & = & x_2^5 - 10x_2^4 + 35x_2^3 - 50x_2^2 + 24x_2, \\ g_2(x) & = & x_1 + 5/6x_2^4 - 20/3x_2^3 + 50/3x_2^2 - 83/6x_2 \end{array}$$

with the same $\mathrm{Est}_\tau(D)$. The condition $\pi(x) = x_1 + 2x_2$ is rewritten over $\mathrm{Est}_\tau(D)$ as

$$-5/6x_2^4 + 20/3x_2^3 - 50/3x_2^2 + 95/6x_2 = \pi(x) - g_2(x)$$

With respect to an ordering that does not favour either x_1 or x_2 so strongly, namely `tdeg` (see Char, Geddes, Gonnet, Leong, and Monogan, 1991) the set $\mathrm{Est}_\tau(D)$ is $\left\{1, x_1, x_2, x_1x_2, x_2^2\right\}$. This example shows that term orderings can be chosen to determine the structure of $\mathrm{Est}_\tau(D)$ as far as the design allows.

4 Conclusion

The theory and examples in this paper are relatively simple but, we hope, show the power of the method. The challenge is to revisit many of the classical and some of the more recent constructions in design, such as lattices, to relate the special algebra used in each case to the wider Gröbner basis theory. The list should include notions such as blocking, dummying, trend resistance, cross-over which are of considerable practical importance, but where aliasing is not yet fully understood.

References

Char, B., Geddes, K., Gonnet, G., Leong, B. and Monogan, M. (1991). *MAPLE V Library Reference Manual.* Springer-Verlag, New York.

Cox, D., Little, J. and O'Shea, D. (1996). *Ideals, Varieties, and Algorithms.* Springer, New York (second edition).

Giglio, B., Riccomagno E. and Wynn, H.P. (2000). Gröbner basis methods in mixture experiments and generalisations. In: Atkinson, A., Bogacka, B. and Zhigljavsky, A. (eds). *Optimum Design 2000. Improceedings of "Optimum experimental designs: Prospects for the new millennium?.*

Pistone, G., Riccomagno E. and Wynn, H.P. (2000). *Algebraic Statistics.* Chapman and Hall, New York.