Generalised design: interpolation and statistical modelling over varieties

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Abstract

Designs are commonly defined as sets of points. We extend the definition to sets of algebraic varieties and explore the implications on the models that are identifiable for such designs. The case when all the algebraic varieties are hyperplanes is studied and a bound on the total degree of models identifiable in such case is given. We also present initial results on interpolation of convergent series over algebraic varieties.

Key words: Algebraic variety, design ideal, hyperplane arrangement, interpolation.

1 Introduction

The basic setting for interpolation is to construct a function $f(x)$ that coincides with observed data at n given x-values. That is, for a finite set of distinct interpolating design points $x_1, \ldots, x_n \in \mathbb{R}^k$ and a set of values $y_1, \ldots, y_n \in \mathbb{R}$, to build a function such that $f(x_i) = y_i$, $i = 1, \ldots, n$. Here k is the number of factors. Approaches to this problem range from statistical oriented techniques such as kriging, see Stein (1999), to more algebraic techniques involving polynomials, splines or operator theory, see Phillips (2003) and Sakhnovich (1997). We do not attempt to present here a complete survey of interpolation theory, for which we refer to the appropriate sources. It is convenient to consider statistical regression analysis as fitting and analysing submodels of a basic interpolator. This interpolator can be though of as the saturated case, in which there are the same number of free parameters as design points.

An important instance of interpolation arises when the function is a polynomial function, see the survey by Gasca & Sauer (2000) and also Sauer (1998). For instance, interpolation in one dimension can be solved with the classic

Lagrange interpolation formula

$$f(x) = \sum_{j=1}^{n} y_j \prod_{m=1}^{n} \frac{x - x_m}{x_j - x_m}.$$

Pistone and Wynn (1996) used algebraic geometry techniques for a multdimensional interpolation problem. They showed how the interpolating polynomial can be constructed as a linear combination of monomials using Gröbner bases theory. This technique has been applied to design of experiments and analysis of discrete probabilities and statistical modelling. There is now a small but expanding literature in this area, see the monograph by Pistone, Riccomagno & Wynn (2001) and the recent survey by Pistone, Riccomagno & Rogantin (2006).

The aim of the present paper is to discuss the extension of algebraic interpolation when instead of interpolating being over a finite set of points, it is carried out over a general algebraic variety.

In Sections 1.1 and 1.2 we present the basic definitions of the algebraic theory and revisit briefly interpolation over point sets in Section 1.3. The extension of designs to varieties is discussed in Section 1.4. In Section 2 we discuss a particular case of the extension, that is, when the variety under consideration is a unions of intersections of hyperplanes. We first study the case when the interpolating sets are defined solely by unions of $k-1$ dimensional hyperplanes (Section 2.1) and then approach the general case with unions of intersections of varieties (Section 2.2). In Section 3 we study the "fill-up" of varieties with design points.

In Section 4 we discuss the normal form of analytic functions with respect to varieties. A particular instance occurs when a reduced interpolator is sought for a set of given prescribed polynomial functions over interpolating varieties. A useful algorithm due to Becker & Weispfenning (1991) is surveyed in Section 5. In Section 6 we discuss further extensions to the work.

1.1 Rings of polynomials and ideals

For basic definitions and a comprehensive treatment of the subject we refer the reader to the book by Cox et al. (1997) and the volume by Kreuzer & Robbiano (2000).

Let $x_1, \ldots, x_k$ be indeterminates. A monomial is the power product $x^\alpha := x_1^{\alpha_1} \cdots x_k^{\alpha_k}$, where the elements of the vector of exponents $\alpha = (\alpha_1, \ldots, \alpha_k)$ are non-negative integers. The total degree of a monomial x^α is $\alpha_1 + \cdots + \alpha_k$. The set of all monomials with integer exponents is $T^k = \{x^\alpha : \alpha \in \mathbb{Z}^k_{\geq 0}\}$, where

$\mathbb{Z}^k_{\geq 0}$ is the set of all k-tuples with non-negative integer entries.

Let $\mathbb{F}$ be a field, that is, a set that satisfies the field axioms for the operations of sum and product. Examples of fields are the set of rational, real and complex numbers (represented by $\mathbb{Q}, \mathbb{R}, \mathbb{C}$). Most of the results we present are valid for other fields. However, we are specially concerned with the three cases above mentioned as they appear most frequently in applications.

A polynomial is a finite combination of monomials in T^k with coefficients in $\mathbb{F}$. The set of all such polynomials has the structure of a ring under the usual operations of sum and product of polynomials. It is called the polynomial ring and it is represented by $\mathbb{F}[x_1, \ldots, x_k]$. When there is no ambiguity we write $\mathbb{F}[x]$.

A term ordering $\prec$ on $\mathbb{F}[x]$ is a total ordering on T^k that satisfies 1) $1 \prec x^\alpha$ for all $x^\alpha \in T^k, \alpha \neq 0$ and 2) if $x^\alpha \prec x^\beta$ then $x^\alpha x^\gamma \prec x^\beta x^\gamma$ for all $x^\alpha, x^\beta, x^\gamma \in T^k$. The leading term of $f \in \mathbb{F}[x]$ is the greatest term of f under $\prec$, with non-zero coefficient, and we write $\mathrm{LT}_\prec(f)$.

A polynomial ideal is a non-empty subset I of $\mathbb{F}[x]$ that satisfies i) I contains the zero polynomial, ii) I is closed under polynomial sum and iii) if $f \in I$ and $h \in \mathbb{F}[x]$ then $hf \in I$.

Given a set of polynomials $f_1, \ldots, f_m \in \mathbb{F}[x]$, the set $I = \{\sum_{i=1}^m f_i h_i : h_1, \ldots, h_m \in \mathbb{F}[x]\}$ is a polynomial ideal. We say that $f_1, \ldots, f_m$ is a generating set for I and we write $I = \langle f_1, \ldots, f_m \rangle$. The Hilbert basis theorem states that any polynomial ideal has a finite set of generators, see (Cox et al. 1997, Section 2§5) for details.

An important generating set for an ideal is the Gröbner basis. Given a term ordering $\prec$ and a polynomial ideal I, a Gröbner basis for I is a finite subset $G \subset I$ such that $\langle \mathrm{LT}_\prec(g) : g \in G \rangle = \langle \mathrm{LT}_\prec(f) : f \in I \rangle$. A finite set of polynomials $G \subset I$ that is a Gröbner basis for I for every term ordering $\prec$ is called a universal Gröbner basis for I. Gröbner basis were first proposed in Buchberger (1966), and their computation is implemented in software packages such as CoCoAand Singular, see CoCoATeam (2007), Greuel, Pfister & Schönemann (2005).

1.2 Varieties and quotient rings

An affine variety V is the subset of $\mathbb{F}^k$ constructed by the solutions of a finite set of polynomial equations. The ideal of a variety V is the polynomial ideal generated by such equations and we refer to it as $I(V)$. There is a correspondence between operations between varieties and operations between ideals, for example the ideal of a finite union of varieties is the intersection of the individual variety ideals, see the algebra-geometry dictionary in (Cox et al. 1997, Chapter 4).

Two polynomials $f, g \in \mathbb{F}[x]$ are congruent modulo I if $f - g \in I$. The quotient ring $\mathbb{F}[x]/I$ is the set of equivalence classes for congruence modulo I. We are interested in studying the congruence created by the ideal of a variety. The quotient ring $\mathbb{F}[x]/I(V)$ is isomorphic, as $\mathbb{F}$-vector space, to the set of polynomial functions defined on V, $\mathbb{F}[V]$, see (Cox et al. 1997, Section 5§2). For a fixed term ordering $\prec$, let G be a Gröbner basis for $I(V)$ and let $L(I(V), \prec)$ be the set of all monomials in T^k that cannot be divided by the leading terms of the Gröbner basis G, that is

$$L_{\prec}(I(V)) := \{x^\alpha \in T^k : x^\alpha \text{ is not divisible by } \mathrm{LT}_{\prec}(g), g \in G\} \tag{1}$$

This set of monomials is known as the set of standard monomials, and when there is no ambiguity, we refer to it simply as $L(V)$. The following proposition is taken from (Cox et al. 1997, Section 5§3, Proposition 4).

Proposition 1 *Let $I(V) \subset \mathbb{F}[x]$ be an ideal. Then $\mathbb{F}[x]/I(V)$ is isomorphic as a $\mathbb{F}$-vector space to $S = Span(L(V))$, where $Span(L(V))$ is the set of all polynomials with monomials in $L(V)$ and coefficients in $\mathbb{F}$.*

In other words, the monomials in $L(V)$ are linearly independent modulo $I(V)$ and thus form a basis for the quotient ring $\mathbb{F}[x]/I(V)$. By the isomorphism above mentioned, $L(V)$ forms also a basis for polynomials on V, $\mathbb{F}[V]$, see (Cox et al. 1997, Sections 5§2 and 5§3). The division of a polynomial f by the elements of a Gröbner basis for $I(V)$ leads to a remainder r with monomials in $L(V)$, which is called the normal form of f.

Theorem 1 *(Cox, Little & O'Shea 1997, Section 2§3, Theorem 3) Let $I(\mathcal{V})$ be the ideal of a variety V; let $\prec$ be a fixed term order on $\mathbb{F}[x]$ and let $G = \{g_1, \ldots, g_m\}$ be a Gröbner basis for $I(V)$ with respect to $\prec$. Then every polynomial $f \in \mathbb{F}[x]$ can be expressed as $f = \sum_{i=1}^m g_i h_i + r$, where $h_1, \ldots h_m \in \mathbb{F}[x]$ and r is comprised only of monomials in $L(V)$.*

We have that $f - r \in I(V)$ and we say that the normal form r interpolates f. That is, f and r coincide as polynomial functions over V. When there is no ambiguity, we write only $r = \mathrm{NF}(f, V)$ to denote the normal form of f with respect to the ideal $I(V)$ and a given term ordering.

1.3 Designs of points

Pistone & Wynn (1996) realised that identifiability problems in experimental design can be solved by using the isomorphism between $\mathbb{F}[x]/I(V)$ and $\mathbb{F}[V]$. They set $\mathbb{F} = \mathbb{R}$ and define an experimental design $\mathcal{D}$ as a finite set of distinct points in $\mathbb{R}^k$. In other words, set $V = \mathcal{D}$. The design ideal $I(\mathcal{D})$ is the set of all polynomials in $\mathbb{R}[x]$ that vanish on the design points. For a fixed term ordering $\prec$, a model identifiable by $\mathcal{D}$ is given by the terms in $L(\mathcal{D})$.

An ideal I is radical if whenever a power f^m of a polynomial f is in I, then $f \in I$. The ideal of a variety $I(V)$ is always a radical ideal, see (Cox et al. 1997, Section 1§4, Exercise 8). In other words, taking points with no duplicities for $\mathcal{D}$ makes $I(\mathcal{D})$ a radical ideal. See Cohen et al. (2001) for considerations when there are duplicities in $\mathcal{D}$. In this paper we consider radical ideals defined by varieties.

The most elementary experimental design is that with a single point $d_1 = (d_{11}, \ldots, d_{1k}) \in \mathbb{R}^k$. As a variety, d_1 is the simultaneous solution of the set of equations $\{x_1 - d_{11} = 0, \ldots, x_k - d_{1k} = 0\}$, that is, d_1 is the intersection of d varieties and generates the ideal $I(d_1) = \langle x_1 - d_{11}, \ldots, x_k - d_{1k} \rangle$. A design $\mathcal{D}$ is the union of points

$$\mathcal{D} = \bigcup_{i=1}^{n} d_i = \{d_1, \ldots, d_n\} \tag{2}$$

and its design ideal is the intersection of ideals for single points:

$$I(\mathcal{D}) = \bigcap_{i=1}^{n} I(d_i). \tag{3}$$

Consider the design $\mathcal{D} = \{(0,0), (1,0), (1,1), (2,1)\} \subset \mathbb{R}^2$. Its design ideal $I(\mathcal{D})$ is constructed as the intersection of the ideals for single points. For any term ordering $\prec$, the set $G = \{x_1^3 - 3x_1^2 + 2x_1, x_1^2 - 2x_1x_2 - x_1 + 2x_2, x_2^2 - x_2\}$ is a Gröbner basis for $I(\mathcal{D})$. If we set a term order for which $x_2 \prec x_1$ then the leading terms of G are x_1^3, x_2^2 and x_1^2 and thus $L(\mathcal{D}) = \{1, x_1, x_2, x_1x_2\}$. Any real-valued polynomial function defined over $\mathcal{D}$ can be expressed as a linear combination of monomials in $L(\mathcal{D})$. That is, for any function $f : \mathcal{D} \to \mathbb{R}$, there is a unique representative $c_0 + c_1x_1 + c_2x_2 + c_{12}x_1x_2 \in \text{Span}(L(\mathcal{D}))$ where the constants c_0, c_1, c_2, c_{12} are real.

If instead of defining a function we observe real values y_i for every point $d_i \in \mathcal{D}$, then the representative $\hat{y} \in \text{Span}(L(\mathcal{D}))$ is an interpolator for the data y_i. Being an interpolator, $\hat{y}$ satisfies $\hat{y}(d_i) = y_i$ for all $d_i \in \mathcal{D}$. In statistical terms, $\hat{y}$ is a saturated model. For example, if we observe the data $2, 1, 3, -1$ at the points in $\mathcal{D}$ then $\hat{y} = 2 - x_1 + 5x_2 - 3x_1x_2$ is the saturated model for the data.

The algebraic fan of a finite set of points (design) $\mathcal{D}$ is the set of all $L(\mathcal{D})$ obtained as $\prec$ varies over all term orderings, see Caboara et al. (1997). For our example, if we consider a term order in which $x_1 \prec x_2$, then we identify $L(\mathcal{D}) = \{1, x_1, x_2, x_1^2\}$. An interpolator can be constructed with this set of monomials.

Recent developments on the algebraic approach is that on mixture designs by Maruri-Aguilar et al. (2006) and on indicator functions by Pistone et al. (2006).

1.4 Designs of varieties

The main purpose of this paper is to generalise the concept of experimental design from point sets to algebraic varities. We shall at some stage need to discuss the issue of observation on varieties, but we first cover the generalisation of the last section to varieties.

A design is defined as a union of varieties, each separate variety V_i in this union can be considered as a generalised "point". Thus generalising Equation (2) we define

$$\mathcal{D} = \bigcup_{i=1}^{n} V_i \tag{4}$$

so that Equation (5) is generalised to

$$I(\mathcal{D}) = \bigcap_{i=1}^{n} I(V_i). \tag{5}$$

We turn our attention to the quotient ring $\mathbb{F}[x]/I(V)$, which given a term order $\prec$ and a Gröbner basis G, has a basis $L(V)$, as defined in Equation (1). When any of the varieties V_i are not points, $L(V)$ is infinite and we can intepret members of the quotient ring as the infinite dimensional vector spaces $\text{Span}(x^\alpha : x^\alpha \in L(V))$. The question of whether any elements of this vector space represents a convergent infinite power series in $\mathbb{R}^k$ will be discussed briefly in Sections 4 and 5.

At the heart of this approach is an issue relating to whether we are considering interpolation over $\mathbb{R}^k$ or over $\mathbb{C}^k$. Proposition 1 and indeed much of the theory depends on $\mathbb{F}$ being an algebraically closed field.

Suppose our variety is $V = \{x \in \mathbb{F} : x^3 = 1\}$. As a real variety (setting $\mathbb{F} = \mathbb{R}$), there is only one solution: $d_1 = 1$. As a complex variety (considering $\mathbb{C} = \mathbb{R}$) it has three solutions: one real, d_1, and two complex $d_2 = (-1+i\sqrt{3})/2$ and $d_3 = (-1 - i\sqrt{3})/2$, with $i = \sqrt{-1}$. For any term ordering, the Gröbner basis is $\{x^3-1\}$ with leading term x^3 and thus $L(V)=\{1,x,x^2\}$. We can proceed to complex quadratic interpolation over $\mathcal{D}=\{d_1\cup d_2\cup d_3\}$. With real observations y_i at d_i, $i=1,2,3$ we obtain the interpolator

$$\begin{aligned}\hat{y}(x) = & \frac{1}{3}(y_1+y_2+y_3)+\frac{x}{6}(2y_1-y_2-y_3)+\frac{x^2}{6}(2y_1-y_2-y_3)\\ & +\frac{i\sqrt{3}}{6}(y_3-y_2)\left(x-x^2\right) \end{aligned} \tag{6}$$

which is complex. However if we only allow real interpolation we only have d_1 as the design and we can only fit a constant.

The variety corresponding to the 2−dimensional circle C is also revealing. The variety C is the set of solutions to $x_1^2+x_2^2=1$. Its ideal $I(C)$ is generated by $x_1^2+x_2^2-1$, which forms a Gröbner basis for any term ordering. Formally for any term order such that $x_1 \prec x_2$, the leading term of the Gröbner basis is x_2^2 and $L(C)=\{x_1^{\alpha_1}x_2^{\alpha_2}:\alpha_1=0,1,2,\ldots,\alpha_2=0,1\}$. But the circle equation has complex solutions as well, for instance consider $u\in\mathbb{R}, u>1$ and thus any point $z=u+i\sqrt{u^2-1}\in\mathbb{C}^2$ is also a solution of the circle and therefore belongs to C. An early discussion on some properties of real algebraic varieties is due to Whitney (1957).

Despite the issue regarding the complex parts of varieties we may use the theory to generate real interpolators. We can explain this with the above example: $I(V)=\langle x^3-1\rangle$. Any real polynomial $p(x)$ has a quadratic normal form with respect to $\langle x^3-1\rangle$. This is because $p(x)$ induces values over the complex part of the variety. The normal form can be considered as a complex interpolator but may be *used* as a real interpolator. The "penalty" we pay is that the interpolator remains quadratic. Thus the polynomial $p(x)=1+x+x^2+x^3$ has normal form $r(x)=x^2+x+2$ with respect to $\langle x^3-1\rangle$. Now $p(x)$ itself has value 4 at d_1 and 1 at d_2 and d_3. Putting these values into $\hat{y}(x)$ at (1.6) yields $r(x)$.

Informally, we can consider the real interpolator $r(x)$ "forgets" about the complex part. The explanation for this important phenomenon is that normal forms over $\mathbb{Q}$ or $\mathbb{R}$ will have coefficients in $\mathbb{Q}$ or $\mathbb{R}$, so that we never "see" complex terms. However, as seen in this example, the variety itself may have a complex components and the size of the quotient ring will be larger than if we just take the real subvariety; in the example $x=1$.

Another important point, which we shall discuss in Section 3 is whether we can embed point set designs within a variety and identify an model based on a finite set of quotient ring basis basis elements. We shall refer to this as "fill-up". We are able to establish a conjecture on this issue in an important special case namely when all the varieties are linear.

2 Interpolation on hyperplanes

2.1 Unions of hyperplanes (hyperplane arrangements)

We study ideals created by arrangements of hyperplanes. They give rise to principal ideals, which are relatively simple algebraic structures.

The ($k-1$ dimensional) affine hyperplane directed by a non-zero vector $a \in \mathbb{R}^k$ and with real intercept c is termed as $H(a, c)$, i.e.

$$H(a,c) = \left\{x = (x_1, \ldots, x_k) \in \mathbb{R}^k : l_a(x) - c = 0\right\}$$

with $l_a(x) := \sum_{i=1}^{n} a_i x_i$. Now for a set of vectors $a_1, \ldots, a_n \in \mathbb{R}^k$ and real scalars $c_1, \ldots, c_n$, the hyperplane arrangement $\mathcal{A}$ is the union of the affine hyperplanes $H(a_i, c_i)$, that is

$$\mathcal{A} = \bigcup_{i=1}^{n} H(a_i, c_i). \tag{7}$$

The combinatorial properties of hyperplane arrangements have long been studied in mathematical literature, see (Grünbaum 2003, Chapter 18). We are concerned with polynomial ideals related to hyperplane arrangements. The set of all polynomials that vanish on the hyperplane $H(a, c)$ is a polynomial ideal, which we refer to as $I(H(a, c))$. The ideal $I(H(a, c))$ is generated by the single polynomial $l_a(x) - c$, that is $I(H(a, c)) = \langle l_a(x) - c\rangle$. The following lemma summarizes the properties of $I(H(a, c))$.

Lemma 2 *(1) For any $\prec$, $\{l_a(x)-c\}$ is a Gröbner basis for $I(H(a, c))$, and (2) $I(H(a, c))$ is a radical ideal.*

The polynomial

$$Q_{\mathcal{A}}(x) := \prod_{i=1}^{n} (l_{a_i}(x) - c) \tag{8}$$

is called the defining polynomial of $\mathcal{A}$. Let $I(\mathcal{A})$ be the set of polynomials that vanish on $\mathcal{A}$. The ideal $I(\mathcal{A})$ is generated by $Q_{\mathcal{A}}(x)$, that is $I(\mathcal{A}) = \langle Q_{\mathcal{A}}(x)\rangle$. The following lemma generalises Lemma 2.

Example 1 If $\mathcal{A}$ is composed of the k coordinate hyperplanes, that is, a_i is the i-th unit vector and $c_i = 0$ for $i = 1, \ldots, k$, then its defining polynomial is $Q_{\mathcal{A}}(x) = x_1 \cdots x_k$. Another instance is the *braid arrangement*, which plays an important role in combinatorial studies of arrangements. It has defining polynomial $Q_{\mathcal{A}}(x) = \prod(x_i - x_j - 1)$, where the product is carried on $i, j : 1 \leq i < j \leq k$, see Stanley (1996).

Lemma 3 *Let $\mathcal{A}$ be a hyperplane arrangement with defining polynomial $Q_{\mathcal{A}}(x)$; let $I(\mathcal{A})$ be the polynomial ideal generated by $\mathcal{A}$. Then*

(1) $\{Q_{\mathcal{A}}(x)\}$ is Gröbner basis for $I(\mathcal{A})$, for any $\prec$ and
(2) if no two hyperplanes of $\mathcal{A}$ are coincidental, then the ideal generated by $Q_{\mathcal{A}}(x)$ is radical.

We summarize the properties obtained so far. The ideal $I(\mathcal{A})$, generated by an arrangement of hyperplanes $\mathcal{A}$, is a principal ideal, that is, it is generated by a single polynomial. The defining polynomial $Q_{\mathcal{A}}(x)$ is a Gröbner basis for $I(\mathcal{A})$, for any $\prec$. For the rest of the section we only work with arrangements that have no coincidental hyperplanes, and therefore $I(\mathcal{A})$ is a radical ideal.

The set of standard monomials $L(\mathcal{A})$ is composed by those monomials that cannot be divided by the leading term of $Q_{\mathcal{A}}(x)$ with respect to a given term order $\prec$. In the example of k coordinate hyperplanes, for any term order, the set of standard monomials is composed of those monomials that cannot be divided by $\mathrm{LT}_{\prec}(Q_{\mathcal{A}}(x)) = x_1 \cdots x_k$.

For other hyperplane arrangements, the leading term of $Q_{\mathcal{A}}(x)$ depends on the actual term order used. The following result for computing the leading term of a product of polynomials will be used together with the definition of $Q_{\mathcal{A}}(x)$ in Equation (8).

Lemma 4 *Let $\prec$ be a fixed term order in $\mathbb{R}[x]$ and let $p, q \in \mathbb{R}[x]$. Then $LT_{\prec}(pq) = LT_{\prec}(p)LT_{\prec}(q)$.*

In the next corollaries, Lemma 4 is extended to a finite product of polynomials and simplified for the leading term of $Q_{\mathcal{A}}(x)$ in (1.8).

Corollary 5 *Let $\prec$ be a fixed term ordering on $\mathbb{R}[x]$ and let $f_1, \ldots, f_m$ be polynomials in $\mathbb{R}[x]$. Then $LT_{\prec}(\prod_{i=1}^{m} f_i) = \prod_{i=1}^{m} LT_{\prec}(f_i)$.*

In a similar form as for designs of points, we can define the algebraic fan of a variety $\mathcal{D}$ as the set of all $L(\mathcal{D})$ obtained as $\prec$ varies over all term orderings. The correctness of this extension follows from the results of Mora & Robbiano (1988).

Corollary 6 *Consider a hyperplane arrangement $\mathcal{A}$ with defining polynomial as in Equation (8). Then*

(1) A necessary and sufficient condition for uniquely determining the leading term of $Q_{\mathcal{A}}(x)$ is to define an initial ordering on $x_1, \ldots, x_k$.

(2) The cardinality of the algebraic fan of $\mathcal{A}$ has the upper bound $k!$.

A special instance of $\mathcal{A}$ occurs when the vectors $a_1, \ldots, a_n$ all have its elements different than zero. In such case the algebraic fan of $\mathcal{A}$ has exactly $k!$ bases. The following corollary characterises the total degree of monomials identified

Corollary 7 *Let $\mathcal{A}$ be an arrangement of n hyperplanes ($k-1$ dimensional hyperplanes). Then for any term ordering, the total degree of $LT_{\prec}(Q_{\mathcal{A}}(x))$ is n.*

2.2 Generalised linear designs (GLDs)

The union in Equation (7) can be generalised to include not the just $k-1$ dimensional hyperplanes, but unions of intersections of hyperplanes. That is, using the definition of a design of Equation (4), the design is $\mathcal{D} = \cup V_i$ and every variety V_i is built as the intersection of n_i hyperplanes, $V_i = \bigcap_{j=1}^{n_i} H_{i,j}$, and the design is the union of intersections of hyperplanes

$$\mathcal{D} = \bigcup_{i=1}^{n} \bigcap_{j=1}^{n_i} H_{i,j}$$

Consequently, the design ideal is the intersection of unions of ideals

$$I(\mathcal{D}) = \bigcap_{i=1}^{n} \bigcup_{j=1}^{n_i} I(H_{i,j}).$$

The standard approach for designs of points of Section 1.3 is built using this idea, and is already a field of growing interest under the heading of "ideals of points". It would be interesting to extend algorithms for ideals of point to GLDs.

Example 2 Consider the design $\mathcal{D}$ in $\mathbb{R}^3$ constructed by the union of the following eleven affine sets: $V_1, \ldots, V_8$ are the eight hyperplanes $\pm x_1 \pm x_2 \pm x_3 - 1 = 0$, and V_9, V_{10}, V_{11} are the three lines in direction of the every coordinate axis. The ideal for each of the eight hyperplanes is constructed by Lemma 2, i.e. by its linear generator. The variety V_9 is the axis x_1 and thus it is the intersection of the hyperplanes $x_2 = 0$ and $x_3 = 0$, we have $I(V_9) = \langle x_2, x_3 \rangle$. Similarly $I(V_{10}) = \langle x_1, x_3 \rangle$ and $I(V_{11}) = \langle x_1, x_2 \rangle$. The design ideal is $I(\mathcal{D}) = \cap_{i=1}^{11} I(V_i)$. For a lexicographic term ordering in which $x_3 \prec x_2 \prec x_1$, the Gröbner basis of $I(\mathcal{D})$ has three polynomials whose leading terms have total degree ten and are $x_1^9 x_2, x_1^9 x_3, x_1^8 x_2 x_3$. Samples taken from this design have the potential to estimate a full model of total degree nine in three variables (see the next section for similar constructions).

3 "Fill-up"

Even though we can create a theory of interpolation by specifying, or "observing" polynomial function on varieties we may wish to carry out statistical or numerical methods according to the standard theory. That is we may wish to observe at a point set design $\mathcal{D}_n$ which is a subset of the variety design $\mathcal{D}$: $\mathcal{D}_n \subset D$. (We us the $\mathcal{D}_n$ notation only in this section.) Note that for the quotient rings: $L_n = L(\mathcal{D}_n) \subset L = L(\mathcal{D})$. The question remains: given any finite subset $L' \subset L$ can we find a $\mathcal{D}_n \subset \mathcal{D}$ so that $L' \subseteq L_n$

An interesting case is the circle. Can we "achieve" L' from some finite design on the circle? The authors are able, in fact, to prove this with a sufficiently large equally spaced design around the circle, and a little help from discrete Fourier analyis. Noting that we can show that the result is true for the circle which is irreducible over $\mathbb{C}$ and false for $x^3 - 1$, which is reducible. We state the general case as a conjecture.

Conjecture 8 *If V is a single irreducible variety in $\mathbb{C}$ and the quotient ring has basis $L(V)$, then for any model with finite support on $L' \subset L(V)$, then there is a finite experimental design with points on the real part of V such that the model is identifiable.*

The extension of the conjecture to unions of varieties is to take $\mathcal{D} = V_i$ where each V_i is irreducible and take $\mathcal{D}_n = \cup \mathcal{D}_{n,i}$ where $\mathcal{D}_{n,i}$ lies in the real part of $V_i, \ \ i = 1, \ldots, n$.

We can prove this extension for the class of generalised linear designs of the last subsection. We believe that the construction may be of some use in the important inverse problem: finding a design which allows identification of a given model.

Proof. Let $\mathcal{D} = \bigcup V_i$ be a GLD. Take a finite set of monomial $L' \subset L(\mathcal{D})$ and construct a polynomial in this basis:

$$p(x) = \sum_{\alpha} \theta_\alpha x^\alpha, \ \alpha \in L'$$

Note that for a GLD each V_i is an intersection of affine linear subspaces and is therefore irreducible (so long as there are no redundant copies, which we shall assume). Select such a V_i and consider the values of $p(x)$ on this variety. Suppose $\dim(V_i) = d_i$, then by a linear coordinatisation of the variety we can reduce the design problem on the variety to the identification of a model of a particular order on $\mathbb{R}^{d_i}$. But with a sufficiently large design $\mathcal{D}_{n_i}$ on V_i we can carry out this identification and therefore can completely determine the value of $p(x)$ on the variety. Carrying out such a construction for each variety gives

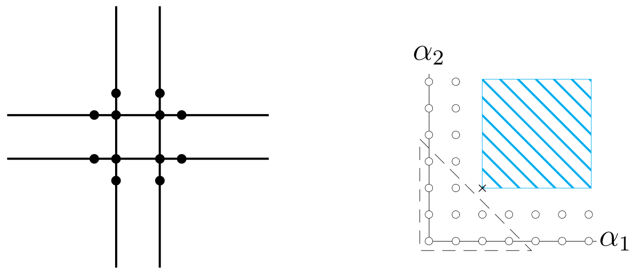

Fig. 1. Hyperplane arrangement $\mathcal{A}$ of Example 3 with selected points $\mathcal{D}' \subset \mathcal{A}$ (left) and exponents $\alpha = (\alpha_1, \alpha_2)$ for monomials in $L(\mathcal{A})$ (right). The symbol $\times$ in the right diagram corresponds to the leading term $x_1^2 x_2^2$, while the shaded area contains monomials not in $L(\mathcal{A})$. The dashed triangle highlights monomials for a model of total degree three or less.

the design

$$\mathcal{D}_n = \bigcup_i \mathcal{D}_{n_i}.$$

(Common points are allowed.) Then the values on $p(x)$ are completely known on each variety and the normal form over $\mathcal{D}$ recaptures $p(x)$, which completes them proof. A shorthand version is: fix a polynomial model on each V_i and the normal form (remainder) is fixed. ■

This raises a number of issues which we have not room to explore. It points to a sequential algorithms in which we "fix" the values on V_1, reduce the dimension of the model as a result, fix the reduced model on V_2 and so on.

Example 3 Take $k = 2$ and the design $\mathcal{D}$ as the union of the four lines $x_1 = \pm 1, x_2 = \pm 1$, i.e. $I(\mathcal{D}) = \langle (x_1^2 - 1)(x_2^2 - 1) \rangle$. For any $\prec$, by Lemma 4, we can take the single leading term $x_1^2 x_2^2$ and $L(\mathcal{D})$ is given by

$$\{x_1^{\alpha_1} x_2^{\alpha_2} : \{\alpha_1 = 0, 1\} \cup \{\alpha_2 = 0, 1\}\}.$$

Take the model with all terms of degree three or or less, which has ten terms. On $x = 1$ the model is cubic in x_2 so that four distinct points are enough to fix it. Thus a design with four distinct pints on each line is enough. The design $\mathcal{D}'$ in Figure 1, namely $\{(\pm 1, \pm 1), (\pm 1, \pm 2), (\pm 2, \pm 1)\}$ twelve points and satisfies our needs.

4 Reduction of power series by ideals

Let us revisit the basic theory. A polynomial $f \in \mathbb{F}[x]$ can be reduced by the ideal $I(\mathcal{D}) \subset \mathbb{F}[x]$ to an equivalent polynomial f' such that they take the same values over the ideal variety. By Theorem 1, this reduced expression is $f' = \mathrm{NF}(f, \mathcal{D})$ and clearly $f - f' \in I(\mathcal{D})$, that is f and f' coincide as polynomial functions over $\mathcal{D}$.

Example 4 Consider the hyperplane arrangement $\mathcal{A}$ constructed with the lines $x_1 = x_2$ and $x_1 = -x_2$. We have $I(\mathcal{A}) = \langle x_1^2 - x_2^2 \rangle$. Now for $l = 1, 2, \ldots$, consider the polynomial $f_l = (x_1 + x_2)^l$. For a term ordering in which $x_2 \prec x_1$, we have that $\mathrm{NF}(f_l, \mathcal{A}) = 2^{l-1}(x_1 + x_2)x_2^{l-1}$, for instance $\mathrm{NF}((x_1 + x_2)^5, \mathcal{A}) = 16(x_1 + x_2)x_2^4 = 16x_1x_2^4 + 16x_2^5$.

The above procedure is simply polynomial division by an ideal: the normal form of a polynomial. It is also possible to compute the normal form of a convergent series. Given a convergent series of the form

$$f(x) = \sum_{i=0}^{\infty} \alpha_i x^{\alpha_i},$$

its expansion on the variety $\mathcal{D}$ is determined by computing the remainder for every monomial in the series, that is, to compute the normal form $\mathrm{NF}(x^{\alpha_i}, \mathcal{D})$. We thus produce the series remainder

$$\mathrm{NF}(f, \mathcal{D}) = \sum_{i=0}^{\infty} \alpha_i \mathrm{NF}(x^{\alpha_i}, \mathcal{D}). \tag{9}$$

Full definition or normal forms (remainders) of power series is omitted. See in Apel et al. (1996) for a discussion of the convergence in (9). Under suitable conditions $\mathrm{NF}(f, \mathcal{D})$ coincides with $f(x)$ over $\mathcal{D}$.

We may also take the normal form of convergent power series. For example by substituting $x^3 = 1$ in the expansion for e^x we obtain

$$\begin{aligned}
\mathrm{NF}(e^x, \langle x^3 - 1 \rangle) = & 1 + \frac{1}{3!} + \frac{1}{6!} + \frac{1}{9!} + \ldots + x\left(1 + \frac{1}{4!} + \frac{1}{7!} + \frac{1}{10!} + \ldots\right) \\
& + x^2\left(\frac{1}{2!} + \frac{1}{5!} + \frac{1}{8!} + \ldots\right) \\
= & \frac{1}{3}e + \frac{2}{3}e^{-\frac{1}{2}} \cos\left(\frac{\sqrt{3}}{2}\right) \\
& + x\left(\frac{1}{3}e - \frac{1}{3}e^{-\frac{1}{2}} \cos\left(\frac{\sqrt{3}}{2}\right) + \frac{1}{3}e^{\frac{1}{2}} \sin\left(\frac{\sqrt{3}}{2}\right)\right) \\
& + x^2\left(\frac{1}{3}e - \frac{1}{3}e^{-\frac{1}{2}} \cos\left(\frac{\sqrt{3}}{2}\right) - \frac{1}{3}e^{\frac{1}{2}} \sin\left(\frac{\sqrt{3}}{2}\right)\right)
\end{aligned}$$

We confirm that $\mathrm{NF}(e^x, \langle x^3 - 1 \rangle) = e^x$ at d_1, d_2, d_3. As a comparison, the truncated Taylor expansion at $x = 1$, namely $\frac{1}{2}e(1 + x^2)$ is equal to e^x at d_1, but not at d_2, d_3. Here is a more complex example for $k = 2$.

Example 5 Consider the ideal $I = \langle x_1^3 + x_2^3 - 3x_1x_2 \rangle$. The variety $\mathcal{D}$ that corresponds to I is the well-known Descartes' *folium*. For a term ordering in which $x_2 \prec x_1$, the leading term of the ideal is x_1^3. Now we consider the function $f(x) = \sin(x_1 + x_2)$, whose Taylor series expression

$$\begin{aligned} f(x) &= \sum_{i=1}^{\infty} \frac{(-1)^i}{(2i+1)!} (x_1 + x_2)^{2i+1} \\ &= (x_1 + x_2) - \frac{1}{3!}(x_1 + x_2)^3 + \frac{1}{5!}(x_1 + x_2)^5 + \dots \end{aligned} \tag{10}$$

converges absolutely on $\mathbb{R}^2$.

We now obtain a ideal-reduced expression for $f(x)$. The coefficients for every term of Equation (10) which is divisible by x_1^3 is absorbed into the coefficient of some of the monomials in $L(\mathcal{D})$. For the second term in the summation we have the following remainder

$$\mathrm{NF}\left(-\frac{(x_1 + x_2)^3}{3!}, I\right) = -\frac{1}{2}\left(x_1^2 x_2 + x_1 x_2^2 + x_1 x_2\right)$$

We note that some that there is some overlapping when computing normal forms, for instance the normal form for the third term in the summation is

$$\mathrm{NF}\left(\frac{(x_1 + x_2)^5}{5!}, I\right) = \frac{3}{40} x_1^2 x_2^3 - \frac{3}{40} x_2^5 + \frac{1}{8} x_1^2 x_2^2 + \frac{1}{4} x_1 x_2^3 - \frac{1}{40} x_2^4 + \frac{3}{40} x_1 x_2^2$$

We observe that the monomial $x_1 x_2^2$ absorbed some of the terms of the second and third terms. In general, this phenomena is to be expected when computing reduction of a power series.

The sum of the normal forms for first ten terms of Equation (10) is

$$\begin{aligned} \tilde{f}(x) = {} & x_2 + x_1 - \frac{1}{2} x_1 x_2 - \frac{17}{40} x_1 x_2^2 - \frac{1}{2} x_1^2 x_2 - \frac{1}{40} x_2^4 + \frac{137}{560} x_1 x_2^3 \\ & + \frac{1}{8} x_1^2 x_2^2 - \frac{41}{560} x_2^5 - \frac{167}{4480} x_1 x_2^4 + \frac{1}{16} x_1^2 x_2^3 + \frac{167}{13440} x_2^6 \\ & - \frac{4843}{492800} x_1 x_2^5 - \frac{17}{896} x_1^2 x_2^4 + \frac{2201}{492800} x_2^7 + \frac{197343}{25625600} x_1 x_2^6 \\ & + \frac{89}{44800} x_1^2 x_2^5 - \frac{65783}{76876800} x_2^8 - \frac{4628269}{5381376000} x_1 x_2^7 + \frac{1999}{5913600} x_1^2 x_2^6 \\ & + \frac{118301}{1793792000} x_2^9 - \frac{305525333}{1463734272000} x_1 x_2^8 - \frac{308387}{1076275200} x_1^2 x_2^7 + \dots \end{aligned}$$

The equality $\tilde{f}(x) = \sin(x_1 + x_2)$ is achieved over $\mathcal{D}$ by summing the normal forms for all terms in Equation (10).

5 Becker-Weispfenning interpolation

Becker & Weispfenning (1991) produced an algorithm for interpolation on varieties. Their algorithm obtains a polynomial interpolator for a set of pre-specified functions defined on a set of varieties in $\mathbb{R}[x]$.

Its basic ingredients are a design $\mathcal{D} = \bigcup_{i=1}^{n} V_i$, whose corresponding ideals are generated in parametric form and a set of pre-specified polynomial functions, one for every variety. Let $V_1, \ldots, V_n \subset \mathbb{R}^k$ be the set of varieties; for $i = 1, \ldots, n$ let $g_{i1}, \ldots, g_{ik} \in \mathbb{R}[z]$ be the set of parametric generators for the ideal of the variety $I(V_i)$, i.e. $I(V_i) = \langle x_1 - g_{i1}, \ldots, x_k - g_{ik} \rangle \subset \mathbb{R}[x, z]$. For every variety V_i, a polynomial function $f_i(z) \in \mathbb{R}[z]$ is pre-specified. Now for indeterminates $w_1, \ldots, w_n$, let I^* be the ideal generated by the set of polynomials

$$\bigcup_{i=1}^{n} \{w_i (x_1 - g_{i1}), \ldots, w_i (x_n - g_{in})\} \bigcup \left\{ \sum_{i=1}^{n} w_i - 1 \right\} \qquad (11)$$

We have $I^* \subset \mathbb{R}[x, y, z]$. The technique of introducing dummy w_i variables is familiar from the specification of point ideals: when any $w_i \neq 0$ we must have $x_j - g_{ij} = 0$ for $j = 1, \ldots, k$, that is, we select the i-th variety ideal. The statement $\sum w_i - 1 = 0$ prevents all the w_i being zero at the same time. If several w_i are non-zero the corresponding V_i are active. Consistency of the parametrization in this case is a necessary, but not sufficient, condition for the method to work.

Let $\prec$ be a term order for which $x^\alpha \prec w^\beta z^\gamma$; set $f^* = \sum_{i=1}^{m} w_i f_i(z)$ and let $f' = \mathrm{NF}(f^*, I^*)$. The interpolation problem has solution if the normal form of f^* depends only on x, that is if $f' \in \mathbb{R}[x]$. Although the solution does not always exist, an advantage of the approach is the freedom to parametrise each variety separately from a functional point of view, but using a common parameter z.

Example 6 (Becker & Weispfenning 1991, Example 3.1) We consider interpolation over $\mathcal{D} = V_1 \cup V_2 \cup V_3 \subset \mathbb{R}^2$ The first variety is the parabola $x_2 = x_1^2 + 1$, therefore defined through the parameter z by $g_{11} = z, g_{12} = z^2 + 1$.

The second and third varieties are the axes x_1 and x_2 and therefore $g_{21} = z, g_{22} = 0$ and $g_{31} = 0, g_{32} = z$. The prescribed functions over the varieties are $f_1 = z^2, f_2 = 1$ and $f_3 = z + 1$. The ideal I^* is constructed using the set in Equation (11) and we set $f^* = w_1 f_1 + w_2 f_2 + w_3 f_3$. Now for a lexicographic term order $\prec$ in which $x^\alpha \prec w^\beta z^\gamma$, we compute the normal form of f^* with respect to I^* and obtain $f' = x_2 + 1$.

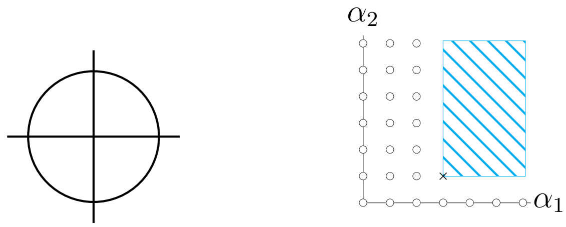

Fig. 2. Variety for the ideal $\langle x_1x_2(x_1^2+x_2^2-2)\rangle$ (left) and exponents $\alpha=(\alpha_1,\alpha_2)$ for monomials in $L(\mathcal{D})$ (right). The symbol $\times$ in the right diagram corresponds to the leading term $x_1^3x_2$, while the shaded area contains monomials not in $L(\mathcal{D})$.

6 Discussion

The material covered has been mostly about interpolation, but one of the main applications is to statistical modelling. In the "standard" theory explained in Section 1.3, we may start with a saturated interpolator over the design, but consider fitting statistical submodels using standard regression methods.

In, when a design is a union of varieties, questions remain: what is the interpretation of observation on a variety? What constitutes an observation? What method of statistical analysis should be used?

We do not resolve all these issues here. Rather we present the ideas as a guide to experimentation on varieties in the following sense. If we take design points on $\mathcal{D}=\bigcup_{i=1}^n V_i$ then the quotient ring provides an indication of the models we may fit. For any finite set of points $\mathcal{D}'\subset\mathcal{D}$ we know, in advance, that $L(\mathcal{D}')\subset L(\mathcal{D})$. Varieties give a taxonomy which informs experimentation.

As an example consider the structure consisting of a circle with a cross, see Figure 2. For any term ordering, the polynomial $g=x_1x_2(x_1^2+x_2^2-2)=x_1^3x_2+x_1x_2^3-2x_1x_2$ is a Gröbner basis for $I(\mathcal{D})$. Now, for a term order in which $x_2\prec x_1$, we have $\mathrm{LT}_\prec(g)=x_1^3x_2$ and $L(\mathcal{D})=\{x_1^{\alpha_1}x_2^{\alpha_2}$ for $\alpha_1=0,1,2,\alpha_2=1,2,\ldots$ and $\alpha_1=0,1,\ldots,\alpha_2=0\}$, see Figure 2. So under mild conditions we expect to estimate any submodel $L'\subset L(\mathcal{D})$. For instance, if we are interested in $L'=\{1,x_1,x_2,x_1^2,x_1x_2,x_2^2\}$ then a good subset of $\mathcal{D}$ which not only estimates L' but is also orthogonal is

$$\mathcal{D}'=\{(\pm1,\pm1)\}\cup\{(0,\pm\sqrt{2}),(\pm\sqrt{2},0)\}\cup\{(0,0)\}.$$

This is the well-known central composite design of response surface methodology.

It may be that there is a structural reason for only being able to observe on a variety. In several areas of science one may only observe on a transect, but may wish to reconstruct or predict the phenomenon off the transect. The present approach gives a guide to what is achievable off the transect, given perfect estimation on the transect. Elsewhere in this volume there is emphasis on probability models defined in discrete sets. Typically the set may be product sets which allow independence. A simple approach but with deep consequences is to consider not interpolation of data (y-values) in a variety, but $\log p$ where p is a probability (difficulties arise when $p = 0$, much of which are solved by power product models and the theory of toric ideals). It is a challenge, therefore, to consider $\log p$ models in varieties, that is, distributions in varieties. One may count rather than observe real continuous y-values. With counts we may be able to reconstruct a distribution on the transect. The issue would be to reconstruct the full distribution off the transect. We finish with an example which may point to a theory of reconstructing distributions.

Example 7 Reconstruction of bivariate normal from transects. Suppose we have a general bivariate Normal distribution $(X_1, X_2)^T \sim N((\mu_1, \mu_2)^T, \Sigma)$ where

$$\Sigma = \begin{pmatrix} \sigma_1^2 & \sigma_1\sigma_2\rho \\ \sigma_1\sigma_2\rho & \sigma_2^2 \end{pmatrix}.$$

Now $\log p(x_1, x_2)$ is a quadratic form, there are five unknown parameters. Imagine that we have perfect transect sampling on a number of line transects. This means that we know the value of the distribution on the transects. The question is: what is the minimum number of such transects needed to reconstruct the distribution and are there any conditions on their location. It is clear that this is achievable with three transects but not, in general, from two. Using the "fill up" ideas, three transects each with three points "fits" the quadratic for $k = 2$. This generalises to the fact that three $(k-1)-$dimensional transects are enough to reconstruct a degree 2 polynomial in $\mathbb{R}^k$.

Finally, we remark that is $\log p$ is polynomial on a variety then p itself sets up an exponential statistical model on the variety. We trust that the development of such a theory would be in the spirit of this volume and the very valuable work of its dedicee.

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Appendix: Proofs of Lemma 4 and Corollary 6

Proof. Let $p(x)$ be $\sum_{i=0}^{s} b_i x^{a_i}$ and $q(x) = \sum_{j=0}^{t} d_j x^{c_j}$, where for $i = 0, \ldots, s$ and $j = 0, \ldots, t$, the coefficients of p and q are $b_i, d_j \neq 0$. Without loss of generality, assume that the monomials of p and q are ordered by the term ordering $\prec$ as $x^{a_0} \prec \cdots \prec x^{a_s}$ and $x^{c_0} \prec \cdots \prec x^{c_t}$. We thus have $\mathrm{LT}_{\prec}(p) = x^{a_s}$ and $\mathrm{LT}_{\prec}(q) = x^{c_t}$.

The divisibility condition of term orders imposes the following pre-order on the monomials of pq

$$
\begin{array}{ccccccc}
x^{a_0}x^{c_t} & \prec \cdots \prec & x^{a_{s-1}}x^{c_t} & \prec & x^{a_s}x^{c_t} \\
\curlyvee & & \curlyvee & & \curlyvee \\
x^{a_0}x^{c_{t-1}} & \prec \cdots \prec & x^{a_{s-1}}x^{c_{t-1}} & \prec & x^{a_s}x^{c_{t-1}} \\
\curlyvee & & \curlyvee & & \curlyvee \\
\vdots & \ddots & \vdots & & \vdots \\
\curlyvee & & \curlyvee & & \curlyvee \\
x^{a_0}x^{c_0} & \prec \cdots \prec & x^{a_{s-1}}x^{c_0} & \prec & x^{a_s}x^{c_0}
\end{array}
$$

The largest term of this pre-order is $x^{a_s}x^{c_t}$, with coefficient $b_s d_t$. The claim follows as $b_s d_t \neq 0$ by hypothesis. ■

Proof of Corollary 6
Proof.

(1) An initial ordering is a total ordering on the undeterminates $x_1, \ldots, x_k$. We extend any initial ordering to the term 1 by imposing the condition $1 \prec x_i$, $i = 1, \ldots, k$. Then for $i = 1, \ldots, k$, the initial ordering is sufficient and necessary to uniquely determine the leading term of the polynomial $(l_{a_i}(x) - c)$. By Lemma 4 and Corollary 5, this result is extended to determine the leading term of $Q_{\mathcal{A}}(x)$.
(2) We verify the bound by observing that the number of initial orderings on $x_1, \ldots, x_k$ is the number of permutations of k elements.

■

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