Two polynomial representations of experimental design

Roberto Notari, Dipartimento di Matematica, Politecnico di Torino
Turin, Italy (roberto.notari@polito.it)

Eva Riccomagno, Dipartimento di Matematica, Università di Genova
Genoa, Italy (riccomagno@dima.unige.it)

Maria-Piera Rogantin, Dipartimento di Matematica, Università di Genova
Genoa, Italy (rogantin@dima.unige.it)

Abstract
In the context of algebraic statistics an experimental design is described by a set of polynomials called the design ideal. This, in turn, is generated by finite sets of polynomials. Two types of generating sets are mostly used in the literature: Gröbner bases and indicator functions. We briefly describe them both, how they are used in the analysis and planning of a design and how to switch between them. Examples include fractions of full factorial designs and designs for mixture experiments.

AMS Subject Classification: 62K15, 13P10

Key words: Algebraic Statistics, Factorial design, Gröbner basis, Indicator function, Mixture design.

1 Introduction
In the algebraic statistics literature two types of polynomial representations of an experimental design are studied: the Gröbner type (see Pistone and Wynn (1996), Pistone et al. (2001)) and the indicator function type (see Fontana et al. (2000), Ye (2003), Pistone and Rogantin (2007b)). In this paper we compare them, describe how to derive them from the design points and how to use them in the analysis of the design properties by unifying and completing results from the literature. Mainly we provide an original and efficient algorithm to switch between the two representations. The diagram below summarizes the paper.

\begin{align*}
\text{Points coordinates} & \quad \text{Generating set} \\
\downarrow & \quad \times \\
\text{Indicator function} & \quad \Rightarrow \\
& \quad \text{Gröbner representation}
\end{align*}

In Section 2 the two representations are described and their relative practical advantages are discussed. Algebraic algorithms to move along the four down-arrows of the diagram are discussed. In Section 3 a theorem and an algorithm to change representation are given which do not require the knowledge of the coordinates of the points. This is represented by the horizontal arrows in the diagram.

The horizontal arrows are particularly important in the planning stage of the experiment. This is because designs with a given confounding structure can be easily defined through generating sets and actual point coordinates are unknown until the corresponding system of equations is solved. The actual number of points in the design can be computed from the design ideal using the Hilbert function, as we do in Section 4. An implementation of the algorithms in the general-purpose mathematics software package Maple is provided in the Appendix. In Section 5 a large design for a screening experiment from the chemical literature is studied.

We use the dedicated symbolic softwares CoCoA, see CoCoATeam (2005), and the general purpose software Maple, see Char et al. (1991). The provided algorithms can be easily implemented in other softwares.
Example 1. To illustrate the main points of our discussion we use the two simple designs, $\mathcal{F}_A$ and $\mathcal{F}_P$, below

$$\mathcal{F}_A = \{(1, 0), (-1, 0), (0, 1), (0, -1)\}$$
$$\mathcal{F}_P = \{(1, 0, 0), (0, 1, 0), (0, 0, 1), (1/3, 1/3, 1/3), (1/2, 1/2, 0), (1/2, 0, 1/2), (0, 1/2, 1/2)\}$$

Note that the components of each point of $\mathcal{F}_P$ sum to one.

2 The two representations

We begin with some unavoidable algebraic notions. Relevant references to polynomial algebra can be found in the textbooks by Cox et al. (1997, 2005) and Kreuzer and Robbiano (2000, 2005).

Let $k$ be a computable numerical field, and $k^m$ be the affine $m$–dimensional space. We consider a design with $m$ factors, where the levels of each factor are coded with integer, rational, real or complex numbers. In practical situations $k$ is the set of the rational numbers $\mathbb{Q}$. For the indicator function representation, we need an extension of $\mathbb{Q}$ to include the imaginary unit and some irrational real numbers. This is a computable set. Then, a design $\mathcal{F}$ is a finite set of $n$ distinct points in $k^m$. Let $R = k[x_1, \ldots, x_m]$ be the polynomial ring in $m$ indeterminates with coefficients in $k$. The indeterminates in $R$ correspond to the design factors.

Three notions from algebraic geometry/commutative algebra are corner stones.

- **Ideal of a design.** The design ideal of $\mathcal{F}$ is

  $$I(\mathcal{F}) = \{f \in R|f(\zeta) = 0 \text{ for all } \zeta \in \mathcal{F}\}.$$  
  
  $I(\mathcal{F})$ is an ideal, i.e. $f + g \in I(\mathcal{F})$ for all $f, g \in I(\mathcal{F})$ and $fg \in I(\mathcal{F})$ for every $f \in I(\mathcal{F})$ and $g \in R$. The Hilbert Basis theorem states that every polynomial ideal is finitely generated. Thus, there exist $f_1, \ldots, f_r \in I(\mathcal{F})$ such that

  $$f \in I(\mathcal{F}) \text{ if, and only if, } f = \sum_{i=1}^{r} s_i f_i \text{ for some } s_i \in R.$$  

  The set of generators $f_1, \ldots, f_r$ is not unique. The ideal generated by $f_1, \ldots, f_r$ is indicated by $\langle f_1, \ldots, f_r \rangle$. Conversely, given an ideal $I$, the set of zeros of $I$ is, by definition, an algebraic variety and corresponds to the zero-set of any of its generator sets.

- **Interpolation.** For any $k$–valued function $F$, defined on a design $\mathcal{F}$, there exist (interpolating) polynomials $f \in R$ such that $f(\zeta) = F(\zeta)$ for all $\zeta \in \mathcal{F}$.

- **Quotient space.** A standard algebraic construction is the quotient ring $R/J$ for any ideal $J \subseteq R$. The relation $\sim$ defined as $\{f \sim g \text{ if, and only if, } f - g \in J\}$ is an equivalence relation. The elements of $R/J$ are the equivalence classes of $\sim$. $R/J$ inherits a ring structure from $R$ by defining sum and product of classes as $[f] + [g] = [f + g], [f][g] = [fg]$.

  If $f, g \in R$ interpolate the same function $F$ defined on the design $\mathcal{F}$, that is to say, $f$ and $g$ are aliased on $\mathcal{F}$, then $f - g$ is zero if evaluated on each $\zeta \in \mathcal{F}$, and so $f - g \in I(\mathcal{F})$. Hence, there exists a unique class in $R/I(\mathcal{F})$ that contains all the polynomials interpolating the same function $F$.

In algebraic geometry a design $\mathcal{F}$ is seen as a zero-dimensional variety. The focus both in algebraic statistics and in this paper switches from the design $\mathcal{F}$ to its ideal $I(\mathcal{F})$. As we shall see below, the Gröbner representation and the indicator function representation of $\mathcal{F}$ are nothing else than two sets of generators of $I(\mathcal{F})$. Replicated points can be considered but some technical issues, which are briefly illustrated in Example 2, occur which are outside the scope of this paper.
Example 2. In \( \mathbb{Q}[x_1, x_2] \) consider the two ideals \( I_1 \) and \( I_2 \) defined as \( I_1 = \langle x_1, x_2^2 \rangle \) and \( I_2 = \langle x_1 + x_2, x_2^3 \rangle \). The zero sets of \( I_1 \) and \( I_2 \) are equal and consist of the point \((0,0)\) with multiplicity two, as can be easily checked by solving the two systems of equations \( x_1 = x_2^2 = 0 \) and \( x_1 + x_2 = x_2^3 = 0 \). But the two ideals are not equal because the polynomial \( x_1 \) is in \( I_1 \) but not in \( I_2 \) and conversely \( x_1 + x_2 \) is in \( I_2 \) but not in \( I_1 \).

In general, questions like equality of ideals \((I_1 = I_2)\), membership of a polynomial to an ideal \((x_1 \in I_1 \text{ and } x_1 \notin I_2)\), intersection and sum of ideals can be handled by using computer algebra software.

\[ \square \]

2.1 Indicator function

To define the indicator function of \( \mathcal{F} \) we must consider \( \mathcal{F} \) as a subset of a larger design \( \mathcal{D} \subset \mathbb{k}^m \). Usually, but not necessarily, \( \mathcal{D} \) has the structure of a full factorial design. The indicator function \( F \) of \( \mathcal{F} \subset \mathcal{D} \) is the response function

\[
F(\zeta) = \begin{cases} 
1 & \text{if } \zeta \in \mathcal{F} \\
0 & \text{if } \zeta \in \mathcal{D} \setminus \mathcal{F}.
\end{cases}
\]

(2.1)

The polynomial indicator function for two level fractional factorial designs were introduced in Fontana et al. (1997) and Fontana et al. (2000) and independently in Tang and Deng (1999) with a slightly different presentation. An extension to two-level designs with replicates is in Ye (2003) and to multilevel factors, using orthogonal polynomials with integer coding, in Cheng and Ye (2004).

The case of factorial designs is treated in Pistone and Rogantin (2007b), where the \( n_j \) levels of each factor are coded by the \( n_j \)-th roots of the unity, \( j = 1, \ldots, m \). With this coding an orthonormal base of the response space on the design is formed by the set of all the monomial terms:

\[
\{ x^\alpha, \; \alpha \in L \} \quad \text{and} \quad L = \{ \alpha = (\alpha_1, \ldots, \alpha_m), \; \alpha_j = 0, \ldots, n_j - 1 \; \text{and} \; j = 1, \ldots, m \}.
\]

The indicator function \( F \) is a real valued polynomial with complex coefficients: \( \sum_{\alpha \in L} b_\alpha \; X^\alpha(\zeta), \; \zeta \in \mathcal{D} \). In this case, the coefficients are related to many interesting properties of the fraction in a simple way: orthogonality among the factors and interactions, projectivity, aberration and regularity. For instance, the fraction is regular if and only if all the coefficients are equal to the ratio between the number of fraction points and the number of the full design points; the level of a simple factor of an interaction occurs equally often in the fraction if and only if the coefficient of the corresponding term is zero; two simple factors or interactions are orthogonal if and only if the coefficient of the term with exponent the sum of the two exponents is zero; a fraction is an orthogonal array of strength \( s \) if and only if the coefficients of the terms of order lower than \( s \) are zero.

Example 3. The fraction of a \( 3^4 \) full factorial design \( \mathcal{F}_R = \{ (1, 1, 1, 1), (1, \omega_1, \omega_1, \omega_1), (1, \omega_2, \omega_2, \omega_2), (1, \omega_1, \omega_1, \omega_2), (1, \omega_1, \omega_2, \omega_1), (1, \omega_2, \omega_1, \omega_1), (1, \omega_2, \omega_2, \omega_1), (1, \omega_2, \omega_1, \omega_2) \} \), where \( 1, \omega_1, \omega_2 \) are the cubic roots of the unity, is a regular fraction; in fact, its indicator function is

\[
F = \frac{1}{9} \left( 1 + x_2x_3x_4 + 5x_2^2x_3^2 + 3x_1x_3x_4^2 + 5x_1x_2x_4^2 + 3x_1x_2x_3x_4 + x_1x_3x_2^2 + x_2^2x_3^2x_4 \right).
\]

The fraction points are 1/9 of the \( 3^4 \) design; in fact the constant term is 1/9. Moreover, each factor is orthogonal to the constant term as shown by the fact that the coefficients of the terms of order 1 are 0. Any two factors are mutually orthogonal; in fact the coefficients of the terms of order 2 are 0. The interaction terms appearing in the indicator function are the “defining words” of the regular fraction.

Example 4. The fraction of a \( 2^5 \) full factorial design \( \mathcal{F}_O = \{ (1, 1, 1, 1, 1), (1, 1, -1, -1, 1), (1, 1, -1, 1, -1), (1, 1, 1, -1, -1), (1, 1, 1, -1, 1), (1, 1, 1, 1, -1) \} \) is an orthogonal array of strength 2; in fact, its indicator function

\[
F = \frac{1}{2} - \frac{1}{4} x_1x_2x_3 + \frac{1}{4} x_1x_2x_5 + \frac{1}{4} x_1x_2x_3x_4 + \frac{1}{4} x_1x_2x_3x_5.
\]
contains only terms of order greater than 2, together with the constant term.

When the coordinates of the points in $F$ and $D$ are known, the indicator function $F$ can be computed using some form of interpolation formula for Equation (2.1). The CoGrA function IdealAndSeparatorsOfPoints is used in Example 6. If the complex coding is used, the coefficients of the indicator function of a fraction of a full factorial design can be easily computed from the sum of the values of each monomial response on all the fraction points: $b_\alpha = \frac{1}{n^2} \sum_{\zeta \in F} x_\alpha(\zeta)$.

Example 5. We consider the fraction $F = \{(-1, -1, 1), (-1, 1, -1)\}$ of the $2^3$ full factorial design. All the monomial responses on $F$ are

\[
\begin{array}{c|cccc|cccc}
1 & x_1 & x_2 & x_3 & x_1x_2 & x_1x_3 & x_2x_3 & x_1x_2x_3 \\
1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\
1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 \\
\end{array}
\]

and the coefficients $b_\alpha$ are:

\[
b_{(0,1,0)} = b_{(1,0,0)} = b_{(0,1,1)} = b_{(1,0,0)} = b_{(1,1,1)} = \frac{2}{4} \quad b_{(0,0,0)} = b_{(0,1,1)} = -\frac{2}{4}.
\]

Hence, the indicator function is $F = \frac{1}{2} \left(1 - x_1 - x_2x_3 + x_1x_2x_3\right)$.

Example 6 (Continuation of Example 1). The indicator function of $F_A$ as subset of a $3^2$ factorial design is

\[
F = -2x_1x_2 + x_1^2 + x_2^2.
\]

A CoGrA algorithm for the computation is provided in Item 1 of the Appendix. If the levels are coded with the 3-rd roots of the unity, the indicator function is

\[
F = \frac{4}{9} \left(1 + x_1 + x_2 - x_1^2 - x_2^2 - x_1x_2 - x_1x_2^2 - x_1^2x_2 - x_1^2x_2^2\right).
\]

We can check that there are no mutually orthogonal terms. The indicator function of $F_P$ will be computed in Example 13.

### 2.2 Gröbner bases

When working with polynomial ideals, it is useful to choose a standard form for writing the polynomials. This can be done by choosing a term ordering. That is an order relation on the monomials of $R$, compatible with the product of monomials. In more details, a monomial is written as $x^\alpha = x_1^{\alpha_1} \cdots x_m^{\alpha_m}$ with $\alpha = (\alpha_1, \ldots, \alpha_m)$ and $\alpha_i \in \mathbb{Z}_{\geq 0}$ for all $i = 1, \ldots, m$. The ordering relation $>$ is a term ordering if 1) $x_\alpha > x_\beta$ 1 for all exponents $\alpha$ and 2) if $x^\alpha > x^\beta$ then $x^{\alpha + \gamma} > x^{\beta + \gamma}$ for all $\alpha, \beta, \gamma \in \mathbb{Z}_{\geq 0}^m$. The leading term of $f \in R$ with respect to $>$ is the largest term of $f$ with respect to $>$ and we write $LT_>(f)$, or $LT(f)$ if no confusion arises.

Example 7. The lexicographic term ordering is defined as $x_1^{\alpha_1} \cdots x_m^{\alpha_m} > x_1^{\beta_1} \cdots x_m^{\beta_m}$ if $\alpha_1 = \beta_1, \ldots, \alpha_{i-1} = \beta_{i-1}, \alpha_i > \beta_i$, for some $i \in \{1, 2, \ldots, m\}$. In the tdeg ordering $x_1^{\alpha_1} \cdots x_m^{\alpha_m} > x_1^{\beta_1} \cdots x_m^{\beta_m}$ if, and only if, $\sum \alpha_i > \sum \beta_i$ or $\sum \alpha_i = \sum \beta_i$ and the right-most nonzero entry of $(\alpha_1 - \beta_1, \ldots, \alpha_m - \beta_m)$ is negative.

Given a term ordering $>$ and an ideal $I \subseteq R$, let $LT_>(I) = \langle LT_>(f) : f \in I \rangle$ be the set of leading terms of all polynomials in $I$.

**Definition 1.** Let $I$ be an ideal, $>$ a term ordering and $G = \{g_1, \ldots, g_t\} \subseteq I$.

1. $G$ is a Gröbner basis (sometimes called a standard basis) of $I$ if $LT_>(I)$ is generated by $\langle LT_>(g) : g \in G \rangle$.

2. $G$ is a reduced Gröbner basis if for all $g \in G$ the coefficient of the leading term of $g$ is 1 and no term of $g$ lies in $\langle LT_>(G \setminus \{g\}) \rangle$. 


Note that a Gröbner basis of an ideal $I$ is a particular generator set of $I$. For every ideal $I$ and term ordering $\succ$, there exist Gröbner bases of $I$ and a unique reduced Gröbner basis, see (Cox et al., 1997, Ch.2). Gröbner bases of $I$ can be computed from any generator set of $I$ with the Buchberger algorithm which is implemented in most softwares for algebraic computation. For every ideal there is a finite number of reduced Gröbner bases as the termdorden varies, see Mora and Robbiano (1988).

Example 8 (Continuation of Example 1). For any term ordering for which $x_1 \succ x_2$ the reduced Gröbner basis representation of $I(\mathcal{F}_A)$ is given by the three polynomials $g_1 = x_1^2 + x_2^2 - 1$, $g_2 = x_3^2 - x_2$ and $g_3 = x_1 x_2$. The polynomial $g_1$ indicates that the points of $\mathcal{F}_A$ are on the unit circle, $g_2$ that the factor corresponding to $x_2$ has three levels $0, \pm 1$ and $g_3$ that at least one coordinate of each point in $\mathcal{F}_A$ is zero.

The reduced Gröbner basis of $I(\mathcal{F}_P)$ for any term ordering such that $x_1 \succ x_2 \succ x_3$ has five elements

\[
\begin{align*}
h_1 &= x_1 + x_2 + x_3 - 1 \\
h_2 &= x_3(x_3 - 1/2)(x_2 + x_3/2 - 1/2) \\
h_3 &= x_3(x_2^2 + x_3^2/2 - x_2/2 - 3/4x_3 + 1/4) \\
h_4 &= (x_2 - x_3)(x_3^2 + x_2x_3 + x_3^2 - 3/2x_3 - 3/2x_3 + 3/2) \\
h_5 &= x_3(x_3 - 1/3)(x_3 - 1/2)(x_3 - 1)
\end{align*}
\]

In $h_1$ we can recognize the sum to one condition for a mixture design and in $h_5$ the levels of the $x_3$ factor.

If we fix a Gröbner basis of an ideal $I \subseteq R$, then for every equivalence class $[f] \in R/I$ there exists a unique $f' \in [f]$ written as combination of monomials not divisible by any monomial in $\text{LT}(I)$. The polynomial $f'$ is called the normal form of $f$ and we write $\text{NF}(f)$, see Cox et al. (1997). Hence, Gröbner bases give a tool to effectively perform sum and products in the quotient ring $R/I$.

Given a design $\mathcal{F}$, the quotient ring $R/I(\mathcal{F})$ is a vector space of dimension equal to the cardinality of $\mathcal{F}$. A monomial basis of $R/I(\mathcal{F})$ can be used as support for a statistical (saturated) regression model as the corresponding information matrix is invertible. A vector space basis of $R/I(\mathcal{F})$ can be determined by using Gröbner bases, and the procedure, which we call Gbasis/LT, is the following. The monomials which are not in $\text{LT}(I(\mathcal{F}))$ are linearly independent over $\mathbb{F}$. They are those monomials which are not divided by any of $\text{LT}(g)$ for all $g$ in a Gröbner basis of $I(\mathcal{F})$. This is equivalent to the fact that the columns of the matrix $X = [\zeta^\alpha]_{\zeta \in \mathcal{F}, \alpha \in L}$ are linearly independent (Pistone et al., 2001). where $L$ is the set of the exponents of the elements of $\text{Est}_\mathcal{F}$.

Example 9 (Continuation of Example 1). In the setting and notation of Example 8 the leading terms of the Gröbner basis elements of $I(\mathcal{F}_A)$ are $\text{LT}(g_1) = x_1^2$, $\text{LT}(g_2) = x_3^2$ and $\text{LT}(g_3) = x_1x_2$. The four monomials $1, x_1, x_2, x_2^2$ are not divisible by these leading terms, equivalently the first four columns of $X$ below give an invertible matrix.

\[
X = \begin{bmatrix}
1 & x_1 & x_2 & x_2^2 & x_3^2 \\
1 & 0 & 1 & 0 & 1 \\
1 & -1 & 0 & 0 & 1 \\
1 & 0 & -1 & 1 & 0 \\
\end{bmatrix}
\]

The linear response model build on any combination of the first four columns of $X$ is identified. The last column lists the design points. From $g_1 = x_1^2 + x_2^2 - 1$ we deduce that $x_1^2 = 1 - x_2^2$, that is the fifth column of $X$ is the difference between the first column and the fourth column.

For $\mathcal{F}_P$, we have $\text{Est}_{\mathcal{F}_P} = \{1, x_3, x_3^2, x_2, x_2x_3, x_3^2\}$. Note that there is no term involving $x_1$ as $g_1 = x_1 + x_2 + x_3 - 1$ confounds $x_1$ with $x_2$ and $x_3$ (see Section 2.3).

The design ideal embeds all possible aliasing relations imposed on polynomial responses by a design. A Gröbner basis is a special finite set of aliasing relations among polynomial responses defined on the fraction and are a basis of all other alias relations, see Holliday et al. (1999). Other special finite sets can be found using the indicator function. Theorem 4 and Example 10 in Pistone et al. (2007) present an algorithm based on the computation of the normal form, with respect to the full design, of all the monomial responses multiplied by the indicator function of the fraction. Knowledge of the problem to be modelled indicates whether the sets of aliasing relations from the indicator function or from the Gröbner bases are more informative.
2.3 Designs for experiments with mixtures

We need to refer here a short summary of [Maruri-Aguilar et al. (2007)]. Each point \( \zeta = (\zeta_1, \ldots, \zeta_m) \in k^m \) of a design \( \mathcal{F} \) for a mixture experiment satisfies the conditions that \( \zeta_i \geq 0 \) for all \( i = 1, \ldots, m \) and \( \sum \zeta_i = 1 \). The polynomial \( \sum x_i = 1 \in I(\mathcal{F}) \) and thus not all the linear terms can be in the support of a regression model simultaneously. In particular the Gbasis/LT procedure applied to a design for a mixture experiment returns slack models which include the identity/intercept and miss completely one factor. For a mixture design \( \mathcal{F} \subset k^m \) there exists, well defined, a unique cone passing through \( \mathcal{F} \) and the origin:

\[
\mathcal{C}_\mathcal{F} = \{ a \zeta : \zeta \in \mathcal{F} \text{ and } a \in \mathbb{R} \} \subset k^m.
\]

This can be thought of as a projective variety. The Gbasis/LT procedure is specialized to mixture designs exploiting the fact that projective varieties and homogeneous polynomials are naturally associated. Consider a term order, the cone \( \mathcal{C}_\mathcal{F} \) and all homogeneous polynomials of degree \( s \) in \( R \). Compute a Gröbner basis of \( \mathcal{C}_\mathcal{F} \), its leading terms and the set of monomials of degree \( s \) not divisible by the leading terms. Then, the information matrix for this set and \( \mathcal{F} \) is invertible (see [Maruri-Aguilar et al. (2007)])

Example 10. Consider the design \( \mathcal{F} = \{(0, 0, 1), (0, 1, 0), (1, 0, 0), (1/3, 1/3, 1/3)\} \subset \mathcal{F}_P \), and any term ordering such that \( x_1 \succ x_2 \succ x_3 \). Then \( I(\mathcal{C}_\mathcal{F}) = \{x_1 x_3 - x_2 x_3, x_1 x_2 - x_2 x_3, x_2^2 x_3 - x_2 x_3^2\} \). The leading terms are underlined. In Table 2.1 various homogeneous models identified by \( \mathcal{F} \) are given. Notice that they are Kronecker models generalizing those in [Draper and Pukelsheim (1998)].

| \( s \) | list of monomials of degree \( s \) | degree \( s \) standard monomials |
|---|---|---|
| 0 | \( x_1, x_2, x_3 \) | \( x_1, x_2, x_3 \) |
| 1 | \( x_1^2, x_1 x_2, x_2^2, x_1 x_3, x_2 x_3, x_3^2 \) | \( x_1^2, x_2^2, x_2 x_3, x_3^2 \) |
| 2 | \( x_1^3, x_1^2 x_2, x_1 x_2^2, x_1 x_3^2, x_2 x_3, x_2^2 x_3, x_1^2 x_3, x_2 x_3^2, x_3^3 \) | \( x_1^3, x_2^3, x_2 x_3, x_3^3 \) |
| \( s > 3 \) | \( x_1^s, x_1^{s-1} x_2, x_1^{s-2} x_2^2, \ldots, x_3^s \) | \( x_1^s, x_2^s, x_2 x_3^{s-1}, x_3^s \) |

Example 11 (Continuation of Example 1). The set \( \{x_2^3 x_3 - x_2 x_3^2, x_2^2 x_3 - x_1 x_3^2, x_2 x_3^2 - x_2 x_3^2\} \) is the reduced Gröbner basis of \( I(\mathcal{C}_{F_P}) \) with respect to the tdeg ordering with \( x_1 \succ x_2 \succ x_3 \). For \( s = 3 \), \( \text{Est}_{F_P} = \{x^3, xy^2, y^3, x y z, x z^2, y z^2, z^3\} \) gives the support for a homogeneous saturated regression model identified by \( \mathcal{C}_{F_P} \).

We need to observe now that ratios of homogeneous polynomials of the same degree are functions well defined on the affine cone of a mixture design.

Example 12. Consider the three points \( P_1 = (1, 0, 0), P_2 = (0, 1, 0), P_3 = (0, 0, 1) \) and the lines \( L_i \) through \( P_i \) and the origin \((0, 0, 0)\). The cone over the points \( P_1, P_2, P_3 \) is equal to \( L_1 \cup L_2 \cup L_3 \). Let \( F \) be the function which assumes the value \( i \) on \( L_i, i = 1, 2, 3 \). First, we show that \( F \) cannot be represented as a polynomial. In fact, if \( f \) is a polynomial such that \( f(x, 0, 0) = 1 \) for each \( x \neq 0 \), then \( f = 1 + f_1(y, z) \). But, \( f(0, y, 0) = 1 + f_1(y, 0) = 2 \) for every \( y \neq 0 \), and so \( f = 2 + f_2(z) \). Hence, \( f(x, 0, 0) = 2 \), and so \( F \) cannot be represented by a polynomial. Next, note that \( x + 2y + 3z \) represents \( F \) on the considered cone.

The above leads to the following definition, which specializes the ideal of indicator function to mixture designs. The larger design \( \mathcal{D} \) could be any mixture design, i.e. a simple lattice, see [Scheffé (1958)] or a simple centroid design, see [Scheffé (1963)]. Example 12 shows that we need to consider ratios of polynomials of the same degree to define a function on \( \mathcal{C}_\mathcal{D} \) and not simply a polynomial, see Definition 2.12 and 2.11 below. Furthermore, the notion of separator as introduced is for consistency with algebraic standard, and takes zero value in \( \mathcal{D} \setminus \mathcal{F} \).
Definition 2. Let $\mathcal{F} \subseteq \mathcal{D} \subset k^m$ be designs for a mixture experiment.

A1) A separator of $\zeta \in \mathcal{F}$ is any homogeneous polynomial $S_\zeta$ such that $S_\zeta \notin I(\mathcal{C}_\mathcal{F})$ and $S_\zeta \in I(\mathcal{C}_{\mathcal{D}\setminus\mathcal{F}})$.

A2) The separator function of $\zeta \in \mathcal{F}$ is $S_\zeta = \frac{S_\zeta}{(\sum_{i=1}^{\deg} x_i)^{s_\zeta}}$ where $s_\zeta$ is the degree of $S_\zeta$.

B1) A separator of $\mathcal{F} \subset \mathcal{D}$ is any homogeneous polynomial $S_\mathcal{F}$ such that $S_\mathcal{F} \notin I(\mathcal{C}_\mathcal{F})$ and $S_\mathcal{F} \in I(\mathcal{C}_{\mathcal{D}\setminus\mathcal{F}})$.

B2) The separator function of $\mathcal{F} \subset \mathcal{D}$ is $SF_\mathcal{F} = \frac{S_\mathcal{F}}{(\sum_{i=1}^{\deg} x_i)^{s_\mathcal{F}}} = \sum_{\zeta \in \mathcal{F}} S_\zeta$ where $s_\mathcal{F}$ is the degree of $S_\mathcal{F}$.

Example 13. The cone generated by $\mathcal{F}_P = \{(0, 0, 1), (0, 1, 0), (1, 0, 0), (1/3, 1/3, 1/3)\} \subset \mathcal{F}_P$ is the same as the cone generated by $\mathcal{F} = \{(0, 0, 1), (0, 1, 0), (1, 0, 0), (1, 1, 1)\} \subset \mathcal{D}$ where $\mathcal{D} \setminus \mathcal{F} = \{(1, 1, 0), (1, 0, 1), (0, 1, 1)\}$. We have

$$SF_\mathcal{F} = \frac{x_1^6 - 2x_1x_2^5 + 732x_1x_2x_3^4 - 2x_1x_2^5 + x_3^6 - 2x_2x_3^5 + x_3^6}{(x_1 + x_2 + x_3)^6},$$

indeed $S_\mathcal{F}(\zeta) = 1$ if $\zeta \in \mathcal{F}$ or if $\zeta \in \mathcal{F}_P$ and $S_\mathcal{F}(\zeta) = 0$ if $\zeta \notin \mathcal{D} \setminus \mathcal{F}$ or $\zeta \notin \mathcal{F}_P \setminus \mathcal{F}_P$. In Example 14 we shall compute a lower degree separator for the same fraction. This shows that there exist different ways of writing in polynomial form the separators for the same fraction.

We are now ready to name the two polynomial representations of a design.

Definition 3. Let $\succ$ be a term ordering on $k$, $\mathcal{F} \subseteq \mathcal{D} \subset k^m$ two designs.

1. The Gröbner representation of $\mathcal{F}$ with respect to $\succ$ is the reduced Gröbner basis of $I(\mathcal{F})$ with respect to $\succ$.

2. Let $\{d_1, \ldots, d_p\} \subset R$ be the reduced $\succ$-Gröbner basis of $I(\mathcal{D})$ and $F$ the indicator function of $\mathcal{F}$ in $\mathcal{D}$. The indicator representation of $\mathcal{F} \subset \mathcal{D}$ with respect to $\succ$ is $\{d_1, \ldots, d_p, F - 1\}$.

Suppose now that $\mathcal{F}$ and $\mathcal{D}$ are designs for mixture experiments.

1. The homogeneous Gröbner representation of $\mathcal{F}$ with respect to $\succ$ is the reduced Gröbner basis of $I(\mathcal{C}_\mathcal{F})$ with respect to $\succ$.

2. Let $\{d_1, \ldots, d_p\} \subset R$ be the reduced $\succ$-Gröbner basis of $I(\mathcal{C}_\mathcal{D})$ and $S_{\mathcal{D}\setminus\mathcal{F}}$ the separator of $\mathcal{D} \setminus \mathcal{F}$ in $\mathcal{D}$. The homogeneous indicator representation of $\mathcal{F} \subset \mathcal{D}$ with respect to $\succ$ is $\{d_1, \ldots, d_p, S_{\mathcal{D}\setminus\mathcal{F}}\}$.

As a mixture design is in particular a design, it admits both the homogenous representation and the non-homogeneous representation. Of course, when using the non-homogeneous one we loose the advantages introduced with the design cone.

While in the non mixture case $\{d_1, \ldots, d_p, F - 1\}$ is a generating set of $I(\mathcal{F})$, in the mixture case the ideal $I(\mathcal{C}_\mathcal{F})$ is the saturation of the ideal $\langle d_1, \ldots, d_p, S_{\mathcal{D}\setminus\mathcal{F}} \rangle$. The saturation $I^{sat}$ of a homogeneous ideal $I \subset R$ contains all the homogeneous polynomials $f$ such that $f x_{1}^{m_1} \in I$ for some $m_i \in \mathbb{Z}_{\geq 0}$ and every $i = 1, \ldots, m$. In fact, the given generators are homogeneous and so they span only homogeneous polynomials of degree not smaller than the degrees of the generators, while in the saturation we obtain also polynomials of degree smaller than the degree of the generators. For example, the ideals $\langle x \rangle$ and $\langle x^2, xy \rangle$ in $R = k[x, y]$ have the cone over $P = (0, 1)$ as zero set. Furthermore, $I(\mathcal{C}_P) = \langle x \rangle = \langle x^2, xy \rangle^{sat}$. For more on saturation see Cox et al. (2005) and Kreuzer and Robbiano (2000).

We could substitute the requirement of reduced Gröbner bases with that of generating sets. Uniqueness of representations will be lost, while there will be no longer dependence on a term-ordering.
3 Changing representation

Let $F$ be the indicator function of $F$ in $D \subset k^m$, $I(D) = \langle d_1, \ldots, d_p \rangle$ and $I(F) = \langle d_1, \ldots, d_p, g_1, \ldots, g_q \rangle$. Note that usually the generator set $\{d_1, \ldots, d_p\}$ is known and has an easy structure, often being $D$ a full factorial design and hence $d_j$ a polynomial in $x_j$ for $j = 1, \ldots, m$, or a simplex lattice design in the mixture case. The difficulty and interest are related to $F$. Then,

1. $I(F) = \langle d_1, \ldots, d_p, F - 1 \rangle$. This means that once $F$ is known, a Gröbner basis of $I(F)$ is obtained by applying the Buchberger algorithm to $\{d_1, \ldots, d_p, F - 1\}$. 

2. Vice versa, the lexicographic Gröbner basis (see Example 7) for $h \succ f \succ x$ of the ideal

$$\langle d_1, \ldots, d_p, (1 - f) - \sum_j h_j g_j, fg_1, \ldots, fg_q \rangle$$

contains a unique polynomial of the form $p(f)$ where $p$ is a polynomial in the $x$ indeterminates only. Then the evaluation function $F : D \rightarrow \{0, 1\}$ defined as $F(d) = p(d)$ for $d \in D$, is the indicator function of $F$ in $D$. See (Pistone et al., 2007, Ch. 6, Th. 2 and 3).

Items 1. and 2. above provide algorithms to switch from indicator function representation to Gröbner basis representation and vice versa. While the passage from the indicator function to the Gröbner representation is relatively easy as it consists of the union of polynomials, equivalently a sum of ideals, the computation of the lexicographic Gröbner basis required for the passage to the indicator function representation can be computationally expensive and often the computation does not terminate. In Section 4 we describe a faster algorithm for this.

Items 1. and 2. are easily adapted to the mixture/homogeneous case by considering the cone ideal and the (rational) separator function, i.e. ideals generated by homogenous polynomials, for example, $F - 1$ has to be substituted with $S_F - (\sum x_i)^s$ where $s = \deg(S_F)$. Moreover, each time we define an ideal, we must saturate it, to compute generators of small degree. See Item 2 of the Appendix for a GoGGA algorithm.

4 An efficient algorithm

In this section, we present a different and more efficient algorithm to switch from the Gröbner representation to the indicator one for a fraction $F$ of a design $D$. The algorithm is based on the following remark: a polynomial $f$ interpolating the indicator function $F$ of $F$ belongs to $I(D \setminus F)$ because of the definition of design ideal. Moreover, $1 - f$ belongs to $I(F)$ for the same argument. If $G = \{g_1, \ldots, g_q\}$ is a Gröbner basis of $I(F)$ then the second remark says that $1 - f = \sum_{i=1}^q h_i g_i$, for some $h_1, \ldots, h_q \in R$. Hence, $f = 1 - \sum_{i=1}^q h_i g_i$ has normal form $0$ in $R/I(D \setminus F)$.

The problem now is to efficiently choose $h_1, \ldots, h_q$. If $D$ has cardinality $N$ and $F$ has cardinality $n$, then we want $h_1, \ldots, h_q$ to depend by $N - n$ parameters because $f = 0$ in $R/I(D \setminus F)$ and the dimension of $R/I(D \setminus F)$ as vector space is $N - n$, written as $\dim R/I(D \setminus F) = N - n$. Moreover, we would like to compute $h_1, \ldots, h_q$ with linear algebra techniques, because they usually have smaller computational complexity than Gröbner bases based algorithms.

Lemma 1 and Theorem 1 describe how to chose efficiently $h_1, \ldots, h_q$.

**Lemma 1.** Let $\text{Est}_D$ (resp. $\text{Est}_F$) be a monomial basis of $R/I(D)$ (resp. $R/I(F)$) computed by using the previously described procedure Gbasis/LT. Then $\text{Est}_F \subset \text{Est}_D$.

**Proof.** $F$ is a fraction of $D$, i.e. $F \subset D$ and $I(D) \subset I(F)$. We prove the equivalent statement: if $x^\alpha \notin \text{Est}_D$ then $x^\alpha \notin \text{Est}_F$. Let $x^\alpha \notin \text{Est}_D$ then there exists a polynomial in $I(D)$ whose leading term is $x^\alpha$. The inclusion between the ideals shows that $x^\alpha \notin \text{Est}_F$, and the statement holds. □

Let $x^{\alpha_1}, \ldots, x^{\alpha_{N-n}}$ be the monomials in $\text{Est}_D \setminus \text{Est}_F$. For each $j = 1, \ldots, N - n$ there exists $g_{i(j)}$ in the Gröbner basis $G$ of $I(F)$ such that $x^{\alpha_j} = m_j \text{LT}(g_{i(j)})$ for some monomial $m_j$, because of the construction of the monomial basis of a quotient ring.
Theorem 1. With the notation as above, the classes of \(m_1g_{i(1)}, \ldots, m_{N-n}g_{i(N-n)}\) are a basis of \(R/I(D \setminus F)\).

PROOF. It is sufficient to prove that they are linearly independent. Let \(a_1, \ldots, a_{N-n} \in k\) be elements of the ground field such that

\[
a_1m_1g_{i(1)} + \cdots + a_{N-n}m_{N-n}g_{i(N-n)}
\]

is the zero class in \(R/I(D \setminus F)\), that is to say, it belongs to \(I(D \setminus F)\) because of the definition of the quotient ring. Hence, we have that \(a_1m_1g_{i(1)} + \cdots + a_{N-n}m_{N-n}g_{i(N-n)} \in I(D)\) because it vanishes also on the points in \(F\) being a combination of elements in a Gröbner basis of \(I(F)\). By construction, the leading terms of \(m_jg_{i(j)}\) are all different and so the leading term of \(a_1m_1g_{i(1)} + \cdots + a_{N-n}m_{N-n}g_{i(N-n)}\), say \(m_1LT(g_{i(1)})\), is in \(Est_D\). This is not possible, and so \(a_1 = 0\). By iterating the argument a finite number of times, we obtain that \(a_1 = \cdots = a_{N-n} = 0\) and the claim follows. \(\Box\)

We know that \(f = 1 - \sum_{i=1}^{N} h_i g_i\) and so we have that the indicator polynomial \(f\) can have the form \(f = 1 - a_1m_1g_{i(1)} + \cdots + a_{N-n}m_{N-n}g_{i(N-n)} \in I(D \setminus F)\). Hence, if we compute the normal form \(N F(f)\) of \(f\) in the ring \(R/I(D \setminus F)\), it must be 0. In general, \(N F(f)\) is a polynomial with monomials in \(Est_D\setminus F\) and linear combinations of \(a_1, \ldots, a_{N-n}\) as coefficients. Therefore, we obtain a linear system in the unknowns \(a_1, \ldots, a_{N-n}\) which has a unique solution by Theorem 1. The resulting algorithm is implemented in Maple in Item 3(a) of the Appendix.

A few modifications are needed to adapt the algorithm to mixture designs. First, we consider homogeneous polynomials of a fixed degree. To speed up computations, we work with polynomials of degree \(s\) where

\[
s = \min \left\{ t \in \mathbb{Z}_{>0} | \dim_{\mathbb{R}} \left( \frac{R}{I(D)} \right)_t = N \right\}.
\]

The integer \(s\) can be easily computed by using the Hilbert function of \(R/I(D)\) that calculates the dimension as vector space of the degree \(t\) polynomials in \(R/I(D)\) for every \(t \in \mathbb{Z}_{\geq 0}\). Second, we compute monomial bases \(Est_{D,s}\) and \(Est_{x,s}\) of the degree \(s\) pieces of the quotient rings \((R/I(D))_s\) and \((R/I(F))_s\), respectively. Third, the indicator function is now a ratio \(F = \frac{f}{(x_1 + \cdots + x_n)^s}\) where \(\text{deg}(f) = s\) with the constraints \(f \in I(D \setminus F)\) and \((x_1 + \cdots + x_n)^s - f \in I(F)\). Hence, the changes are straightforward and the result follows also in this case. See Item 3(b) of the Appendix for a Maple algorithm.

Example 14 (Continuation of Example 11). The set \(\{x_1^3, x_2^2, x_2x_3^2, x_3^3\} \subset Est_{F}\), is identified by the fraction \(F = \frac{f}{(x_1 + x_2 + x_3)^3}\) where \(f(x_1, x_2, x_3)\) is the numerator.

The following Maple script performs the computation using the algorithm in Item 3(b) of the Appendix.

```maple
var:= [x,y,z] -- we change x,1, x,2, x,3 to x, y, z, respectively
EstX:= \{x^3, y^2, y^3, x*y*x, x*z^2, y*z^2, z^3\} -- monomial basis of \((R/I(F_P))_3\)
EstY:= \{x^3, y^z, z^2, z^3\} -- monomial basis of \((R/I(F))_3\)
GY:= \{(z*(x-y)), (x-z) + y*z, (y-z)\}
GXMinusY:= \{z*(x-y-z), y*(x-y-z), x^2-y^2+2+y*z-z^2, y+z*(y-z)\}
G_to_F_homo(GY, GXMinusY, EstX, EstY, var, t)
```

The following Maple script performs the computation using the algorithm in Item 3(b) of the Appendix.

\[
SF_F = \frac{x_1^3 + 3x_2^2x_2 + 3x_1^3x_3 - 5x_1x_2^2 + 30x_1x_2x_3 - 5x_1x_3^2 + x_3^3 + 11x_2^2x_3 - 13x_2x_3^2 + x_3^3}{(x_1 + x_2 + x_3)^3}
\]
5 Example

The simplex centroid design is defined in [1] and used for experiments with mixtures. In $k$ factors it has $2^k - 1$ points. Fractions of the simple centroid design with many less points are defined in [2] and used to screen for significant factors. Their definition depends on an integer parameter $p$ and the double interactions are completely aliased over any such fraction in sets of size $p$. A typical example is $F_{MC}$ below

$$F_{MC} = \{(1,0,0,0,0,0,0,0), (0,1,0,0,0,0,0,0), (0,0,1,0,0,0,0,0),$$
$$ (0,0,0,1,0,0,0,0), (0,0,0,0,1,0,0,0), (0,0,0,0,0,1,0,0),$$
$$ (0,0,0,0,0,1,0,0), (0,0,0,0,0,0,1,0), (0,0,0,0,0,0,0,1),$$
$$ (1/3,1/3,1/3,0,0,0,0,0), (1/3,0,1/3,0,0,0,1/3), (0,1/3,0,0,1/3,0,0,1/3),$$
$$ (0,0,1/3,0,1/3,1/3,0,0,0), (0,0,0,1/3,1/3,1/3,0,0,0), (0,1/3,0,1/3,0,0,1/3,0),$$
$$ (0,0,1/3,0,1/3,0,1/3), (1/3,0,0,0,0,1/3,0,0,1/3), (0,0,0,0,0,0,1/3,1/3,1/3),$$
$$ (1/3,0,0,0,1/3,0,1/3,0,0), (0,1/3,0,0,1/3,0,1/3,0,1/3), (0,0,1/3,1/3,0,0,0,1/3)\} .$$

The design $F_{MC}$ can be seen as a subset of the simple centroid design in 9 factors $D_1$ and also as a fraction of the simplex centroid which includes the corner points of the simplex and the points with coordinates equal to zero or 1/3, call it $D_2$.

IdealOfPoints($F_{MC}$) with respect to the default term ordering in CoCoA is generated by 43 polynomials, while IdealOfProjectivePoints($F_{MC}$) is generated by 42 ones. See [3] for a discussion of these results.

The indicator functions of $F_{MC}$ in $D_1$ and of $F_{MC}$ in $D_2$, and the separator of $F_{MC}$ in $D_2$ have been computed by using the Maple algorithm in the Appendix in less than 10 sec. the first one, and in less than 1 sec. the last two. The indicator functions of $F_{MC}$ in $D_1$ is a combination of 444 terms, in $D_2$ is a combination of 70 terms, and the separator of $F_{MC}$ in $D_2$ is a combination of 165 terms.

6 Discussion

This note regards two polynomial representations of an experimental design $F$ one of which uses the indicator function of $F$ in $D$ and the other one uses Gröbner bases which does not require to think of $F$ as a fraction of the larger design $D$. The Gröbner representation depends on a technical object: a term ordering, while the indicator function is most informative with a complex coding of the factor levels. In applied work term orderings have been used to the advantage of the statistical analysis, see [4]. In [5] it is shown that the real part of the complex response retains most of the properties of the full complex response while having a clearer physical interpretation. Moreover, notice that most of the properties discussed in Section 2.1 depend intrinsically on the level coding. A trivial example is that the $2^2$ full factorial design with levels ±1 is orthogonal for $\{1, x_1, x_2, x_1x_2\}$ while with levels $\{0, 1\}$ it is not.

Both representations can be used to identify alias relations imposed by $F$ on Est$_D$, which is a finite set, or on some other sets of monomials, possible all the infinite set of monomials. Furthermore, both provide a vector-space basis of the response space. This is hierarchical for the Gröbner basis representation.

The choice as to which representation to use should be made in the light of the interests of the practitioner. If the responses have been collected and standard or slower techniques have not returned a satisfactory statistical analysis or are not implementable (maybe because there are missing values with respect to the planned experiment), then it seems convenient to apply the GBasis/LT procedure. This returns an identifiable hierarchical regression model and the alias relations in the Gröbner basis can be used to change model terms with more significant or interpretable model interactions. Instead, prior to data collection, the indicator function seems a useful tool to select a design with relevant properties by working on the coefficients of the indicator functions. Two issues have to be considered: 1. the need of a complex coding for some properties and 2. the need to solve a system of polynomial equations to obtain...
Two polynomial representations of experimental design

the point coordinates. Point 1 has been discussed above. In most practical cases Point 2 can be easily addressed by
computing a Gröbner basis with respect to a lexicographic ordering. Generally the joint use of the two represent-
ations seems advisable, also in the light of the switching algorithms in Sections 3 and 4. Indeed, if one representa-
tion is known then the other one can be computed using techniques of linear algebra. This is possible because designs
are zero dimensional varieties. The complexity of the algorithms in the Appendix is essentially the complexity of the
computation of the normal form of a polynomial w.r.t. a Gröbner basis. In fact the last step of the algorithm consists in
solving a linear system which has a smaller computational complexity. For the large designs of Section 5 the algorithm
gave the solutions in just a few seconds, as previously mentioned.

Finally, we wanted to have in the public domain a complete set of computer functions to perform the computations
in the diagram of the Introduction.

Appendix

1. The CoCoA code for the indicator function of $F_A$ in Example 6

Use $S:=\mathbb{Q}[x[1..2]]$;
Define $\text{InFu}(\text{Points}, D)$; $\text{ND}:=\text{Len}(D)$; $\text{PA}:=\text{NewList}(\text{ND}, 0)$; $P:=\text{NewList}(\text{ND})$
For $H:=1$ To $\text{Len}(\text{Points})$ Do
  For $K:=1$ To $\text{Len}(\text{PA})$ Do If $\text{Points}[H]=\text{D}[K]$ Then $\text{PA}[K]:=1$ End; End;
End;
$\text{IdD}:=\text{IdealAndSeparatorsOfPoints}(D)$;
For $K:=1$ To $\text{Len}(\text{PA})$ Do $P[K]:=\text{PA}[K]*\text{IdD}.\text{Separators}[K]$ End;
$F:=$Sum($P$); Return $F$;
End;

$D:=\text{Tuples}([-1, 0, 1], \text{NumIndets}())$; $\text{PointsF}:=\{[1, 0], [-1, 0], [0, 1], [0, -1]\}$;
$\text{InFu}(\text{Points}, D)$;

2. The CoCoA code for $S_F$ of Example 13 with the algorithm described in Item 2 of Section 3

Use $T:=\mathbb{Q}[f h x[1..3]]$, Lex;
Set Indentation;
$D:=\{x[2]^2x[3] - x[2]x[3]^2, x[1]^2x[3] - x[1]x[3]^2, x[1]^2x[2] - x[1]x[2]^2\}$; -- simplex lattice
$G:=\{x[1]x[3] - x[2]x[3], -x[1]x[2]+x[2]x[3]\}$; -- (0,0,1), (0,1,0), (1,0,0), (1,1,1)
$P:=(x[1]+x[2]+x[3])^3$; $S:=\{\}$;
For $I:=1$ To $\text{Len}(G)$ Do
  $L:=\text{ConcatLists}(\{D, [P-hG[I], fG[I]]\})$;
  $\text{Id}:=\text{Saturation}(\text{Ideal}(L), \text{Ideal}(x[1], x[2], x[3]));$
  $\text{GB}:=\text{ReducedGBasis}(\text{Id});$ $S:=\text{Concat}(\{f-\text{GB}[1]\}, S)$;
EndFor;
$\text{SF}:=\text{NF}(\text{Product}(S), \text{Ideal}(D));$ $\text{SF}$;

3. The Maple code of the procedure described in Section 4 to compute the indicator functions of $Y \subset X$ where
$Y$ and $X$ are sets of points. The affine and the projective cases are considered. Notice that all computations are
with respect to the tdeg term ordering of var. This can be changed by the user.

(a) Affine case. In input the procedure requires:

$GY = \text{Gröbner basis of } I(Y)$,
$GXMMinusY = \text{Gröbner basis of } I(X \setminus Y)$,
$\text{EstX} = \text{standard basis of } R/I(X)$,
$\text{EstY} = \text{standard basis of } R/I(Y)$,
$\text{var} = \text{list of indeterminates}$

The Output is the polynomial representation of the indicator function in $R/I_X$. 
\begin{verbatim}
G_to_F := proc(GY, GXMinusY, EstX, EstY, var)
local E, InY, ly, L, flag, tt, F, i, m, l, v, CC, VV;
with(Groebner);
  v := op(var);
  E := 'minus'(EstX, EstY);
  InY := [seq(leadterm(GY[i], tdeg(v)), i = 1 .. nops(GY))];
  ly := nops(InY);
  L := [];
  for m in E while true do
    flag := 0;
    while flag = 0 do
      for i to ly do
        if gcd(InY[i], m) = InY[i] then flag := 1; tt := i end if
      end do;
    end do;
    L := [op(L), GY[tt] * m / leadterm(GY[tt], tdeg(v))]
  end do;
  F := 0; i := 0;
  for l in L while true do
    i := i + 1; F := F + a[i] * l
  end do;
  CC := coeffs(normalf(1 - F, GXMinusY, tdeg(v)), [v]);
  VV := solve({CC});
  expand(subs(VV, F + 1))
end proc;

(b) Projective case. In input the procedure requires:
  GY = \text{Gröbner basis of } I(Y), which is an homogeneous ideal,
  GXMinusY = \text{Gröbner basis of } I(X \setminus Y), which is an homogeneous ideal,
  EstX = \text{standard basis of degree } t \text{ of } R/I(X)
  EstY = \text{standard basis of degree } t \text{ of } R/I(Y),
  var = \text{list of indeterminates},

here \( t \) is the minimal degree for which \((R/I_X)_t\) as a vector space has the same dimension as the number of points in \( X \).

The Output is the numerator of the ratio of polynomials giving the separator function of \( Y \) in \( X \). Its denominator is the \( t \)-power of the sum of the variables.

G_to_F_homo:=proc(GY, GXMinusY, EstX, EstY, var, t)
local E, InY, ly, L, flag, tt, F, i, m, l, v, CC, VV, S;
with(Groebner):
  v := op(var);
  E := EstX minus EstY;
  InY := {seq(leadterm(GY[i], tdeg(v)), i = 1 .. nops(GY))};
  ly := nops(InY);
  L := [];
  for m in E do
    flag := 0;
    while flag = 0 do
      for i from 1 to ly do
        if gcd(InY[i], m) = InY[i] then flag := 1; tt := i end if
      end do;
    end do;
    L := [op(L), GY[tt] * m / leadterm(GY[tt], tdeg(v))]
  end do;
  F := 0; i := 0;
  for l in L do
    i := i + 1; F := F + a[i] * l
  end do;
  S := sum('v[k]', k = 1 .. nops(var));
  CC := coeffs(normalf(S \text{ } t - F, GXMinusY, tdeg(v)), [v]);
  VV := solve({CC});
  expand(subs(VV, S \text{ } t - F))
end proc;
\end{verbatim}
References

Char, B., Geddes, K., Gonnet, G., Leong, B., Monogan, M., Watt, S., 1991. MAPLE V Library Reference Manual. Springer-Verlag, New York.

Cheng, S.-W., Ye, K. Q., 2004. Geometric isomorphism and minimum aberration for factorial designs with quantitative factors. The Annals of Statistics 32 (5), 2168–2185.

CoCoATeam, 2005. GoCoA: a system for doing Computations in Commutative Algebra. Available at http://cocoa.dima.unige.it

Cox, D., Little, J., O’Shea, D., 2005. Using algebraic geometry, 2nd Edition. Springer-Verlag, New York.

Cox, D. A., Little, J. B., O’Shea, D., 1997. Ideals, Varieties, and Algorithms, 2nd Edition. Springer-Verlag, New York.

Draper, N. R., Pukelsheim, F., 1998. Mixture models based on homogeneous polynomials. J. Statist. Plann. Inference 71 (1-2), 303–311.

Fontana, R., Pistone, G., Rogantin, M.-P., 1997. Algebraic analysis and generation of two-levels designs. Statistica Applicata 9 (1), 15–29.

Fontana, R., Pistone, G., Rogantin, M. P., 2000. Classification of two-level factorial fractions. J. Statist. Plann. Inference 87 (1), 149–172.

Holliday, T., Pistone, G., Riccomagno, E., Wynn, H. P., 1999. The application of computational algebraic geometry to the analysis of designed experiments: a case study. Comput. Statist. 14 (2), 213–231.

Kreuzer, M., Robbiano, L., 2000. Computational Commutative Algebra 1. Springer, Berlin-Heidelberg.

Kreuzer, M., Robbiano, L., 2005. Computational Commutative Algebra 2. Springer, Berlin-Heidelberg.

Maruri-Aguilar, H., Notari, R., Riccomagno, E., 2007. On the description and identifiability analysis of mixture designs. Statistica Sinica (accepted for publication).

McConkey, B., Mezey, P., Dixon, D., Grenberg, B., 2000. Fractional simplex designs for interaction screening in complex mixtures. Biometrics 56, 824–832.

Mora, T., Robbiano, L., 1988. The Gröbner fan of an ideal. Journal of Symbolic Computation 6, 183–208.

Pistone, G., Riccomagno, E., Rogantin, M., 2007. In Search for Optimality in Design and Statistics: Algebraic and Dynamical System Methods. Ch. Methods in Algebraic Statistics for the Design of Experiments, pp. 97–132.

Pistone, G., Riccomagno, E., Wynn, H. P., 2001. Algebraic Statistics: Computational Commutative Algebra in Statistics. Chapman&Hall, Boca Raton.

Pistone, G., Rogantin, M., 2007a. Algebraic statistics of level codings for fractional factorial designs. J. Statist. Plann. Inference (in press).

Pistone, G., Rogantin, M., 2007b. Indicator function and complex coding for mixed fractional factorial designs. J. Statist. Plann. Inference (in press).

Pistone, G., Wynn, H. P., 1996. Generalised confounding with Gröbner bases. Biometrika 83 (3), 653–666.

Scheffé, H., 1958. Experiments with mixtures. J. Roy. Statist. Soc. Ser. B 20, 344–360.
Scheffé, H., 1963. The simplex-centroid design for experiments with mixtures. J. Roy. Statist. Soc. Ser. B 25, 235–263.

Tang, B., Deng, L. Y., 1999. Minimum $G_2$-aberration for nonregular fractional factorial designs. The Annals of Statistics 27 (6), 1914–1926.

Ye, K. Q., 2003. Indicator function and its application in two-level factorial designs. The Annals of Statistics 31 (3), 984–994.