2. Gröbner bases theory in design of experiments

1. Polynomials on finite set of points, and design of experiments

- First we overview the arguments of this topic by examples.

- Problem

  Show that there is a unique quadratic interpolating polynomial in x taking values y_i at $x = a_i$ $(i = 1, 2, 3)$ when a_1, a_2, a_3 are distinct points.

- Ans. Write the interpolating polynomial as

$$\beta_0 + \beta_1 x + \beta_2 x^2.$$

Then we have to show is that the simultaneous equation for the parameter

$$\begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} 1 & a_1 & a_1^2 \\ 1 & a_2 & a_2^2 \\ 1 & a_3 & a_3^2 \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{pmatrix} = M \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{pmatrix}$$

has the unique solution. In fact, the matrix M is the Vandermonde matrix and its determinant is

$$\det(M) = (a_3 - a_2)(a_3 - a_1)(a_2 - a_1).$$

When a_1, a_2, a_3 are distinct, $\det(M) \neq 0$ holds. □

We can also solve this problem using Gröbner basis theory.

- Ans. Let $f(x)$ be an arbitrary polynomial in $K[x]$ satisfying

$$f(a_i) = y_i, \quad i = 1, 2, 3.$$

From the division algorithm with respect to

$$d(x) = (x - a_1)(x - a_2)(x - a_3),$$

we have the expression

$$f(x) = q(x)d(x) + r(x),$$

where $\deg(r(x)) < \deg(d(x))$. Here, the remainder $r(x)$ is the interpolating polynomial because

$$y_i = f(a_i) = q(a_i)\underbrace{d(a_i)}_{=0} + r(a_i) = r(a_i), \quad i = 1, 2, 3.$$

Recall that the remainder is unique in the division algorithm for one variable polynomial ring $K[x]$. □

- Point:
  - The interpolating polynomial for given points is obtained as the remainder $r(x)$ of the standard form w.r.t. $d(x)$.
  - $d(x)$ is the polynomial with value 0 at the given points.

- We consider how to construct interpolating polynomials for given finite set of points.
- Here we consider functions defined on the given set of points D, $r: D \to \mathbb{R}^D$. We see this setting in design of experiments.

- Example (Development of instant coffee pack)

  Suppose we want to develop a new instant coffee pack. Each coffee pack includes “coffee”, “milk” and “suger”. Suppose the levels of each factor is “low” or “high”. We consider the optimal proportions of each factor by experiments.

  Observations: Score by each examinee. (10: highest score)

  Factors: coffee (x_1), sugar (x_2), milk(x_3), each with two levels.

Result of experiment:

x_1	x_2	x_3	Score
-1	-1	-1	3.9
-1	-1	1	6.1
-1	1	-1	6.8
-1	1	1	4.4
1	-1	-1	6.1
1	-1	1	8.0
1	1	-1	8.4
1	1	1	6.8

Each factor has levels

-1: low, 1: high

Score is the average for 14 examinees.

What is the optimal proportion of instant coffee pack?

- For the data obtained from designs of experiments, we regard the score y as the realization of the random variable Y and consider polynomial statistical models such as

$$Y = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + \varepsilon$$

or

$$Y = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + \theta_{12} x_1 x_2 + \theta_{13} x_1 x_3 + \theta_{23} x_2 x_3 + \varepsilon.$$

- The parameter is estimated from the data. The theory of Gröbner basis is used to characterize the polynomial models with estimable parameters.

Example of analysis.

x_1	x_2	x_3	Score
-1	-1	-1	3.9
-1	-1	1	6.1
-1	1	-1	6.8
-1	1	1	4.4
1	-1	-1	6.1
1	-1	1	8.0
1	1	-1	8.4
1	1	1	6.8

- The highest score is at $(1, 1, -1)$, "coffee and sugar is high level, milk is low level".
- However, the total for "milk: high"

$$6.1 + 4.4 + 8.0 + 6.8 = 25.3$$

is greater than the total for "milk: low"

$$3.9 + 6.8 + 6.1 + 8.4 = 25.2.$$

- This suggests the existence of the interaction effect.

The ANOVA table for the full two-factor interaction model

$$Y = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + \theta_{12} x_1 x_2 + \theta_{13} x_1 x_3 + \theta_{23} x_2 x_3 + \varepsilon$$

Factor	Sum. Sq.	df	Variance	F value	p value
x_1	8.2013	1	8.2013	54.2231	0.086
x_2	0.6613	1	0.6613	4.3719	0.284
x_3	0.0013	1	0.0013	0.0083	0.942
$x_1 \times x_2$	0.0013	1	0.0013	0.0083	0.942
$x_1 \times x_3$	0.0312	1	0.0312	0.2066	0.728
$x_2 \times x_3$	8.2013	1	8.2013	54.2231	0.086
Residual	0.1513	1	0.1513		
Total	17.2490	7			

- Parameter estimation: Least squares method.
  - Observation $\boldsymbol{y} = (y_1, \ldots, y_8)' = (3.9,\ \ldots,\ 6.8)'$
  - Parameter $\boldsymbol{\theta} = (\theta_0, \theta_1, \theta_2, \theta_3, \theta_{12}, \theta_{13}, \theta_{23})'$
  - Linear model $\boldsymbol{Y} = X\boldsymbol{\theta} + \boldsymbol{\varepsilon}$

$$X = \begin{pmatrix} 1 & -1 & -1 & -1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 \\ 1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & -1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}$$

- Least squares estimator of $\boldsymbol{\theta}$

$$\begin{aligned}
\hat{\boldsymbol{\theta}} &= \underset{\boldsymbol{\theta}}{\operatorname{argmin}} \|\boldsymbol{y} - X\boldsymbol{\theta}\|^2 \\
&= (X'X)^{-1}X'\boldsymbol{y} = \frac{1}{8}X'\boldsymbol{y} \\
&= (6.3125, 1.0125, 0.2875, 0.0125, -0.0125, 0.0625, -1.0125)'
\end{aligned}$$

- Point: Parameter is estimable because $X'X$ is nonsingular.

- In ANOVA table, the p value for $x_2 \times x_3$ is small. Then the polynomial model

$$Y = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + \theta_{23} x_2 x_3 + \varepsilon$$

seems better. The estimated parameter is

$$\begin{aligned}
\hat{\boldsymbol{\theta}} &= (\hat{\theta}_0, \hat{\theta}_1, \hat{\theta}_2, \hat{\theta}_3, \hat{\theta}_{23})' \\
&= (6.3125,\ 1.0125,\ 0.2875,\ 0.0125,\ -1.0125)'.
\end{aligned}$$

- An interpretation of the experiment:

  "Coffee" is better to be high level. "Sugar" and "Milk" are better to be opposite levels. It's better that "Sugar" is high level, "Milk" is low level.

- Now consider the interpolating polynomial on $D = \{-1, +1\}^3$. This is expressed as the saturated polynomial model

$$\begin{aligned} f(x_1, x_2, x_3) &= \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 \\ &\quad + \theta_{12} x_1 x_2 + \theta_{13} x_1 x_3 + \theta_{23} x_2 x_3 + \theta_{123} x_1 x_2 x_3. \end{aligned}$$

- This is also expressed as the linear model $\boldsymbol{Y} = X\boldsymbol{\theta}$ where

$$X = \begin{pmatrix} 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 \\ 1 & 1 & 1 & -1 & 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}$$

- Because $X'X$ is nonsingular, the parameter is estimable:

$$\begin{aligned} \hat{\boldsymbol{\theta}} &= (X'X)^{-1}X'\boldsymbol{y} = \frac{1}{8}X'\boldsymbol{y} \\ &= (6.3125, 1.0125, 0.2875, 0.0125, -0.0125, 0.0625, -1.0125, 0.1375)'. \end{aligned}$$

- This polynomial is obtained as the remainder of arbitrary interpolating polynomial $f \in \mathbb{R}[x_1, x_2, x_3]$ on D w.r.t.

$$x_1^2 - 1,\ x_2^2 - 1,\ x_3^2 - 1.$$

- We have also seen that for the polynomial model with the model matrix consisting of the columns of the model matrix for the interpolating polynomial, the parameter is estimable.

- Then, when does the parameter become non estimable?
  $\rightarrow$ Next consider fractional factorial designs.

- Example (cont.)

  In addition to “Coffee”, “Sugar” and “Milk”, we also consider “Grind type” with the levels -1: fine or $+1$: coarse. We want to fix the number of experiments as 8.

  What designs can we use?

  What polynomial model can we consider?

- Regular fractional factorial designs are natural choices.

D_1

x_1	x_2	x_3	x_4
-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	1	1

$x_2x_3x_4 = 1$

D_2

x_1	x_2	x_3	x_4
-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	1	1

$x_1x_2x_3x_4 = 1$

- What is an influence on the parameter estimation?

- For the design D_1 ($x_2x_3x_4 = 1$), the parameter of the polynomial model

$$Y = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + \theta_4 x_4 + \theta_{23} x_2 x_3 + \varepsilon$$

cannot be estimated simultaneously. Corresponding model matrix is as follows.

$$X = \begin{pmatrix} 1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 & -1 \\ 1 & -1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}$$

- From the defining relation $x_2x_3x_4 = 1$, the two-factor interaction effect $x_2 \times x_3$ and the main effect x_4 cannot be distinguished (i.e., they are confounded).
- In other words, x_4 and x_2x_3 are two elements of $\mathbb{R}[x_1, x_2, x_3, x_4]$ that cannot be distinguished on D_1.
- All the confounding relations:

$$
\begin{array}{lll}
1 = x_2x_3x_4, & & \\
x_1 = x_1x_2x_3x_4, & & \\
x_2 = x_3x_4, & x_3 = x_2x_4, & x_4 = x_2x_3, \\
x_1x_2 = x_1x_3x_4, & x_1x_3 = x_1x_2x_4, & x_1x_4 = x_1x_2x_3
\end{array}
$$

- The aim of this topic is to describe these confounding relation algebraically by the Gröbner basis theory.

2. Design and design ideal

- **Definition**

  A design D of n factors is a finite set of distinct m points in $\mathbb{Q}^n$. The size of a design D is $m = |D|$. Write the elements of D as

  $$D = \{\boldsymbol{d}_1, \ldots, \boldsymbol{d}_m\}, \ \boldsymbol{d}_i = (d_{i1}, \ldots, d_{in}) \in \mathbb{Q}^n, \ i = 1, \ldots, m,$$

  then the design matrix of the design D is an $m \times n$ matrix $X = (d_{ij}) \in \mathbb{Q}^{mn}$. For $j = 1, \ldots, n$, the level set A_j of the factor j is the set of the distinct elements of $\{d_{1j}, \ldots, d_{mj}\}$. The full factorial design is the direct product of the level set

  $$A_1 \times \cdots \times A_n.$$

  The fractional factorial design is a proper subset of the full factorial design.

- In general, for arbitrary subset V of K^n, the set of polynomials $f \in K[x_1, \ldots, x_n]$ that is zero on each point of V,

$$\mathbf{I}(V) = \{f(x_1, \ldots, x_n) \in K[x_1, \ldots, x_n] \mid \forall \boldsymbol{a} \in V, f(\boldsymbol{a}) = 0\},$$

  satisfies the definition of the ideal.
  This ideal is called an ideal of V.

- **Definition**

  The ideal of the design $D \subset \mathbb{Q}^n$, i.e., the ideal of the polynomial ring $\mathbb{Q}[x_1, \ldots, x_n]$ satisfying

  $$\mathbf{I}(D) = \{f(x_1, \ldots, x_n) \in \mathbb{Q}[x_1, \ldots, x_n] \mid \forall \boldsymbol{d} \in D, f(\boldsymbol{d}) = 0\}$$

  is called a design ideal of the design D.

- Example. The design ideal of the full factorial design of 3 factors with 2 levels $A = A_1 \times A_2 \times A_3,\ A_i = \{-1, +1\},\ i = 1, 2, 3$ is

$$\mathbf{I}(A) = \left\langle x_1^2 - 1,\ x_2^2 - 1,\ x_3^2 - 1 \right\rangle .$$

The design ideals of D_1 and D_2, the fractional factorial designs of 4 factors with 2 levels (size 8), are

$$\mathbf{I}(D_1) = \left\langle x_1^2 - 1,\ x_2^2 - 1,\ x_3^2 - 1,\ x_4^2 - 1,\ x_2x_3x_4 - 1 \right\rangle ,$$
$$\mathbf{I}(D_2) = \left\langle x_1^2 - 1,\ x_2^2 - 1,\ x_3^2 - 1,\ x_4^2 - 1,\ x_1x_2x_3x_4 - 1 \right\rangle .$$

- The design ideal is a fundamental tool to consider the designs algebraically.

- **Definition**

  For an ideal $I \subset K[x_1, \ldots, x_n]$,

  $$\mathbf{V}(I) = \{(a_1, \ldots, a_n) \in K^n \mid \forall f \in I,\ f(a_1, \ldots, a_n) = 0\}$$

  is called an affine variety of I.

  We call $V \subset K^n$ an affine variety if there exists an ideal I of $K[x_1, \ldots, x_n]$ satisfying $V = \mathbf{V}(I)$.

- In computational algebraic statistics, we consider the structure of the design ideal $\mathbf{I}(D)$ to consider the structure of the design D.
- Such an approach is justified because the mapping from the design to its ideal is injective, i.e,

$$\mathbf{V}(\mathbf{I}(V)) = V$$

holds.

Theorem

(i) A design $D \subset \mathbb{Q}^n$ is an affine variety.

(ii) $\mathbf{V}(\mathbf{I}(V)) = V$ holds for each affine variety $V \subset K^n$.

3. Examples of design ideals

- Full factorial designs
  - The 2^n full factorial designs $D = \{-1, +1\}^n$:

$$\mathbf{I}(D) = \left\langle x_1^2 - 1, \ldots, x_n^2 - 1 \right\rangle$$

  - The 2^n full factorial designs $D = \{0, 1\}^n$:

$$\mathbf{I}(D) = \langle x_1(x_1 - 1), \ldots, x_n(x_n - 1) \rangle$$

  - The 3^n full factorial designs $D = \{-1, 0, +1\}^n$:

$$\mathbf{I}(D) = \langle x_1(x_1 + 1)(x_1 - 1), \ldots, x_n(x_n + 1)(x_n - 1) \rangle$$

- For the general full factorial designs of m factors $D = A_1 \times \cdots \times A_m \subset \mathbb{Q}^m$,

$$A_j = \{a_{j1}, a_{j2}, \dots, a_{jr_j}\},\ j = 1, \dots, n,$$

the design ideal is

$$\mathbf{I}(D) = \langle f_1(x_1), \dots, f_n(x_n) \rangle ,$$

$$f_j(x_j) = (x_j - a_{j1})(x_j - a_{j2}) \cdots (x_j - a_{jr_j}).$$

- Regular fractional factorial designs
  - The 2^{4-1} design $D \subset \{-1, 1\}^4$ with $x_2 x_3 x_4 = 1$:

$$\mathbf{I}(D) = \left\langle x_1^2 - 1, \dots, x_4^2 - 1, x_2 x_3 x_4 - 1 \right\rangle$$

  - The 2^{4-1} design $D \subset \{-1, 1\}^4$ with $x_1 x_2 x_3 x_4 = 1$:

$$\mathbf{I}(D) = \left\langle x_1^2 - 1, \dots, x_4^2 - 1, x_1 x_2 x_3 x_4 - 1 \right\rangle$$

- The 2^{5-2} design $D \subset \{-1,1\}^5$ with $x_1x_2x_4 = x_1x_3x_5 = x_2x_3x_4x_5 = 1$:

x_1	x_2	x_3	x_4	x_5
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
−1	−1	1	1	−1
−1	−1	−1	1	1

$$\mathbf{I}(D) = \left\langle x_1^2 - 1, \ldots, x_5^2 - 1, x_1x_2x_4 - 1, x_1x_3x_5 - 1 \right\rangle$$

- The 3^{3-1} design $D \subset \{0,1,2\}^3$

x_1	x_2	x_3
0	0	0
0	1	2
0	2	1
1	0	2
1	1	1
1	2	0
2	0	1
2	1	0
2	2	2

with the defining relation

$$x_1 + x_2 + x_3 = 0 \pmod 3.$$

The defining relation

$$x_1 + x_2 + x_3 = 0 \pmod 3)$$

can be written as

$$x_1 + x_2 + x_3 = 0, 3, 6$$

because the levels are $\{0, 1, 2\}$. Therefore the simultaneous equations defining this design is

$$\begin{cases} x_1(x_1 - 1)(x_1 - 2) = 0 \\ x_2(x_2 - 1)(x_2 - 2) = 0 \\ x_3(x_3 - 1)(x_3 - 2) = 0 \\ (x_1 + x_2 + x_3)(x_1 + x_2 + x_3 - 3)(x_1 + x_2 + x_3 - 6) = 0. \end{cases}$$

$$\begin{aligned} \mathbf{I}(D) \quad = \quad & \langle x_1(x_1 - 1)(x_1 - 2),\ x_2(x_2 - 1)(x_2 - 2), x_3(x_3 - 1)(x_3 - 2), \\ & (x_1 + x_2 + x_3)(x_1 + x_2 + x_3 - 3)(x_1 + x_2 + x_3 - 6)\rangle \end{aligned}$$

- Consider a general design $D \subset \mathbb{Q}^n$ with the size m.

  D is the union of the affine varieties of each point in D.

  Therefore the design ideal of D is the intersection of the design ideals of each point in D.

$$D = \{\boldsymbol{d}_1, \ldots, \boldsymbol{d}_m\},\ \boldsymbol{d}_i = (d_{i1}, \ldots, d_{in}) \in \mathbb{Q}^n,\ i = 1, \ldots, m$$

$$\mathbf{I}(\{\boldsymbol{d}_i\}) = \langle x_1 - d_{i1},\ \ldots, x_n - d_{in} \rangle,\ i = 1, \ldots, m$$

$$\mathbf{I}(D) = \bigcap_{i=1}^{m} \mathbf{I}(\{\boldsymbol{d}_i\}) = \bigcap_{i=1}^{m} \langle x_1 - d_{i1},\ \ldots, x_n - d_{in} \rangle$$

<u>We need the computation of the intersection of ideals.</u>

- Let $I, J \subset K[x_1, \ldots, x_n]$ be ideals and

$$I \cap J = \{f \in K[x_1, \ldots, x_n] \mid f \in I, f \in J\}$$

be the intersection.

Define the ideals in $n+1$ variables polynomial ring $K[t, x_1, \ldots, x_n]$ as

$$tI = \langle \{tf \mid f \in I\} \rangle$$
$$(1-t)J = \langle \{(1-t)f \mid f \in J\} \rangle .$$

Lemma As ideals of $K[x_1, \ldots, x_n]$,

$$I \cap J = (tI + (1-t)J) \cap K[x_1, \ldots, x_n]$$

holds.

- From this lemma, for ideals of $K[x_1, \ldots, x_n]$,

$$I = \langle f_1, f_2, \ldots \rangle \text{ and } J = \langle g_1, g_2, \ldots \rangle,$$

the ideal $tI + (1-t)J \subset K[t, x_1, \ldots, x_n]$ is generated by

$$\{tf_1, tf_2, \ldots, (1-t)g_1, (1-t)g_2, \ldots\}.$$

The intersection $(tI + (1-t)J) \cap K[x_1, \ldots, x_n]$ is obtained by the elimination theory.

- It is easy to generalize the above result to the intersection of more than 2 ideals. For the design

$$D = \{\boldsymbol{d}_1, \ldots, \boldsymbol{d}_m\},\ \boldsymbol{d}_i = (d_{i1}, \ldots, d_{in}) \in \mathbb{Q}^n,\ i = 1, \ldots, m$$

and its design ideal

$$\mathbf{I}(D) \quad = \quad \bigcap_{i=1}^{m} \mathbf{I}(\{\boldsymbol{d}_i\}) = \bigcap_{i=1}^{m} \langle x_1 - d_{i1},\ \ldots, x_n - d_{in} \rangle\,,$$

consider the ideal

$$\langle t_i(x_1 - d_{i1}), \ldots, t_i(x_n - d_{in}),\ i = 1, \ldots, m,\ t_1 + \cdots + t_m - 1 \rangle$$

of $K[t_1, \ldots, t_m, x_1, \ldots, x_n]$. If G is the Gröbner basis of this ideal w.r.t. the pure lexicographic order $t_1 \succ \cdots \succ t_m \succ x_1 \succ \cdots \succ x_n$, then $G \cap K[x_1, \ldots, x_n]$ is the Gröbner basis of $\mathbf{I}(D)$ w.r.t. $\prec'$.

- Note: As for the elimination order, i.e., the monomial order that is used to elimination theory, the block order is more effective than the pure lexicographic order (in viewpoint of the computational time).

- **Definition**

  For the monomial orders $\prec_X$ on $K[x_1, \ldots, x_n]$ and $\prec_T$ on $K[t_1, \ldots, t_m]$, define the monomial order $\prec$ on $K[x_1, \ldots, x_n, t_1, \ldots, t_m]$ as follows:

  Let $u_T, v_T \in K[t_1, \ldots, t_m]$ and $u_X, v_X \in K[x_1, \ldots, x_n]$ are monomials,

  $$u_T u_X \prec v_T v_X \Leftrightarrow u_T \prec_T v_T \text{ or } (u_T = v_T \text{ and } u_X \prec_X v_X).$$

  Then $\prec$ is an elimination order on $K[x_1, \ldots, x_n, t_1, \ldots, t_m]$. This $\prec$ is called a block order with $\{t_1, \ldots, t_m\} \succ \{x_1, \ldots, x_n\}$.

- Example:

x_1	x_2	x_3	x_4
-1	-1	1	1
-1	1	-1	1
-1	1	1	-1
1	-1	-1	1
1	-1	1	-1
1	1	-1	-1

6 points from the 2^{4-1} design of $x_1x_2x_3x_4 = 1$.

The design ideal of this design is calculated as follows by free software `Macaulay2`.[a]

[a] See `macaulay2.com/` See also Macaulay2 online `web.macaulay2.com/`

```
i1 : R = QQ[t1,t2,t3,t4,t5,t6,x1,x2,x3,x4,MonomialOrder=>{6,4}];
i2 : I = ideal(t1*(x1+1),t1*(x2+1),t1*(x3-1),t1*(x4-1),
               t2*(x1+1),t2*(x2-1),t2*(x3+1),t2*(x4-1),
               t3*(x1+1),t3*(x2-1),t3*(x3-1),t3*(x4+1),
               t4*(x1-1),t4*(x2+1),t4*(x3+1),t4*(x4-1),
               t5*(x1-1),t5*(x2+1),t5*(x3-1),t5*(x4+1),
               t6*(x1-1),t6*(x2-1),t6*(x3+1),t6*(x4+1),
               t1+t2+t3+t4+t5+t6-1);
i3 : g = gens gb I
o3 = | x1+x2+x3+x4 x4^2-1 x3^2-1 x2x3+x2x4+x3x4+1 x2^2-1
     -------------------------------------------------------
     4t6-x3x4+x3+x4-1 4t5-x2x4+x2+x4-1 4t4+x2x4+x3x4+x2+x3
     -------------------------------------------------------
     4t3+x2x4+x3x4-x2-x3 4t2-x2x4-x2-x4-1 4t1-x3x4-x3-x4-1 |
     -------------------------------------------------------
             1       11
o3 : Matrix R  <--- R
```

```
i4 : selectInSubring(1,g)

o4 = | x1+x2+x3+x4 x4^2-1 x3^2-1 x2x3+x2x4+x3x4+1 x2^2-1 |

             1       5
o4 : Matrix R  <--- R
```

The reduced Gröbner basis of this design ideal is

$$\{x_1 + x_2 + x_3 + x_4,\ x_4^2 - 1,\ x_3^2 - 1,\ x_2x_3 + x_2x_4 + x_3x_4 + 1,\ x_2^2 - 1\}.$$

The next question:
What is the merit to obtain the Gröbner basis of the design ideal?

4. Polynomial functions and quotients by ideals

- Design with size m: $D \subset \mathbb{Q}^n$ (affine variety)
- The data (response) on D : $y_1, \ldots, y_m \in K$ can be viewed as a function Φ (called a response function)

$$\begin{array}{cccc} \Phi : & D & \rightarrow & K \\ & (d_1, \ldots, d_n) & \mapsto & y = \Phi(d_1, \ldots, d_n) \end{array}$$

- Definition: A function Φ is a polynomial function if

$$\exists f \in K[x_1, \ldots, x_n],\ \forall (d_1, \ldots, d_n) \in D,$$
$$\Phi(d_1, \ldots, d_n) = f(d_1, \ldots, d_n).$$

The polynomial f is said to represent Φ. The polynomials that represent the same Φ are said to be confounded over D.

- Note that two polynomials $f, g \in K[x_1, \ldots, x_m]$ represent the same polynomial function on D if and only if $f - g \in \mathbf{I}(D)$.
- **Definition**
  The collection of polynomial function over D is denoted by $K[D]$.
- In the textbook of the design of experiments, $K[D]$ is called the response space on D.

  Now consider the structure of $K[D]$.

- $K[D]$ is an Abelian ring with the following operations:

$$(\Phi + \Psi)(\boldsymbol{d}) = \Phi(\boldsymbol{d}) + \Psi(\boldsymbol{d}),$$
$$(\Phi \cdot \Psi)(\boldsymbol{d}) = \Phi(\boldsymbol{d}) \cdot \Psi(\boldsymbol{d})$$

  where $\boldsymbol{d} \in D$ and $\Phi, \Psi \in K[D]$. Moreover, if $f \in K[x_1, \ldots, x_n]$ represents Φ and $g \in K[x_1, \ldots, x_n]$ represents Ψ, then $f + g$ represents $\Phi + \Psi$ and $f \cdot g$ represents $\Phi \cdot \Psi$.

- Definition

  Let $I \subset K[x_1, \ldots, x_n]$ be an ideal and $f, g \in K[x_1, \ldots, x_n]$. Then f and g are said to be congruent modulo I if $f - g \in I$. In this case, we write

$$f \equiv g \bmod I.$$

- Proposition

  Let $I \subset K[x_1, \ldots, x_n]$ be an ideal. Then the congruent relation modulo I is an equivalence relation on $K[x_1, \ldots, x_n]$.

- For the case of $I = \mathbf{I}(D)$, $f \equiv g \bmod \mathbf{I}(D)$ if and only if f and g represent the same function on D, i.e., "f and g are confounded on D".

- Definition

  Let I be an ideal in $K[x_1, \ldots, x_n]$. The quotient of $K[x_1, \ldots, x_n]$ modulo I is defined as

  $$K[x_1, \ldots, x_n]/I = \{[f] \mid f \in K[x_1, \ldots, x_n]\},$$

  where we define

  $$[f] = \{g \in K[x_1, \ldots, x_n] \mid f - g \in I\}.$$

- Now consider the structure of $K[x_1, \ldots, x_n]/I$.

- We define the sum and the product of two equivalence classes $[f], [g] \in K[x_1, \ldots, x_n]/I$ as the corresponding sum and product of $f, g \in K[x_1, \ldots, x_n]$,

$$[f] + [g] = [f + g], \quad [f] \cdot [g] = [f \cdot g].$$

- **Proposition** The above sum and product are well-defined.
- From Proposition, it is shown that $K[x_1, \ldots, x_n]/I$ is a commutative ring.

- Now, for the design D, we have two rings $K[D]$ and $K[x_1, \ldots, x_n]/\mathbf{I}(D)$, the set of polynomial functions on D and the quotient of $K[x_1, \ldots, x_n]$ modulo $\mathbf{I}(D)$.
- These two rings are essentially the same in the following sense.

  Theorem

  The sets $K[D]$ and $K[x_1, \ldots, x_n]/\mathbf{I}(D)$ are isomorphic.

5. Standard monomials and Macaulay'2 theorem

- We see that
  - $K[D]$, the response space on D, and the quotient ring $K[x_1, \ldots, x_n]/\mathbf{I}(D)$ are isomorphic, and
  - $f, g \in K[x_1, \ldots, x_n]$ are confounded on D if and only if f, g are in the same equivalence class of $K[x_1, \ldots, x_n]/\mathbf{I}(D)$.
- We consider the structure of $K[x_1, \ldots, x_n]/\mathbf{I}(D)$, (i.e., dimension and basis) using Gröbner basis theory.

- **Theorem** Fix a monomial order $\prec$ on M_n. Let $I \subset K[x_1, \ldots, x_n]$ be an ideal.

  (i) Each $f \in K[x_1, \ldots, x_n]$ is congruent to the polynomial r modulo I, where r is a K-linear combination of the monomials not included in $\mathrm{in}_\prec(I)$, and is unique.

  (ii) The set $\{u \in M_n \mid u \notin \mathrm{in}_\prec(I)\}$ is linearly independent modulo I, i.e.,

$$\sum_\alpha c_\alpha u_\alpha \equiv 0 \bmod I$$

  yields $c_\alpha = 0$ for $\forall \alpha$, where $\{u_\alpha\}$ is the set of monomials satisfying $u_\alpha \notin \mathrm{in}_\prec(I)$.

- Consequently, the quotient ring $K[x_1, \ldots, x_n]/\mathbf{I}(D)$ and the K-vector space spanned by the monomials $\{u \in M_n \mid u \notin \mathrm{in}_{\prec}(I)\}$ are isomorphic. In other words, the set $\{u \in M_n \mid u \notin \mathrm{in}_{\prec}(I)\}$ is a K-basis of the vector space $K[x_1, \ldots, x_n]/\mathbf{I}(D)$ over K.

  This is called a Macaulay's theorem on initial ideals.

- We write

$$\mathrm{Est}_{\prec}(D) \quad = \quad \{u \mid u \in M_n \notin \mathrm{in}_{\prec}(\mathbf{I}(D))\}.$$

- Each element of $\mathrm{Est}_{\prec}(D)$ is called a standard monomial.

- Examples of standard monomials
  - 2^3 design $D = \{-1, 1\}^3$:

$$\mathbf{I}(D) = \left\langle x_1^2 - 1,\ x_2^2 - 1,\ x_3^2 - 1 \right\rangle$$

    This is Gröbner basis (for any monomial order).

$$\mathrm{Est}_{\prec}(D) = \{1,\ x_1,\ x_2,\ x_3,\ x_1x_2,\ x_1x_3,\ x_2x_3,\ x_1x_2x_3\}$$

  - Regular 2^{4-1} design D with $x_1x_2x_3x_4 = 1$:

$$\mathbf{I}(D) = \left\langle x_1^2 - 1,\ x_2^2 - 1,\ x_3^2 - 1,\ x_4^2 - 1,\ x_1x_2x_3x_4 - 1 \right\rangle$$

    This is not a Gröbner basis. We need to compute Gröbner basis to obtain the standard monomials.

Pure Lexicographic order ($x_1 \succ_{\text{purelex}} \cdots \succ_{\text{purelex}} x_4$)

```
i1 : R = QQ[x1,x2,x3,x4,MonomialOrder=>Lex];
i2 : I = ideal(x1^2-1,x2^2-1,x3^2-1,x4^2-1,x1*x2*x3*x4-1);
o2 : Ideal of R
i3 : gens gb I
o3 = | x4^2-1 x3^2-1 x2^2-1 x1-x2x3x4 |
             1       4
o3 : Matrix R  <--- R
```

Gröbner basis:

$$\{x_4^2 - 1,\ x_3^2 - 1,\ x_2^2 - 1,\ x_1 - x_2x_3x_4\}$$

$$\text{Est}_{\prec_{\text{purelex}}}(D) = \{1,\ x_2,\ x_3,\ x_4,\ x_2x_3,\ x_2x_4,\ x_3x_4,\ x_2x_3x_4\}$$

Reverse lexicographic order ($x_1 \succ_{\text{rec}} \cdots \succ_{\text{rev}} x_4$)

```
i4 : R2 = QQ[x1,x2,x3,x4];
i5 : use R2;
i6 : I2=(map(R2,R))(I);
o6 : Ideal of R2
i7 : gens gb I2
o7 = | x4^2-1 x3^2-1 x2x3-x1x4 x1x3-x2x4 x2^2-1 x1x2-x3x4 x1^2-1 |
              1        7
o7 : Matrix R2  <--- R2
```

Gröbner basis:

$$\{x_4^2 - 1, x_3^2 - 1, x_2x_3 - x_1x_4, x_1x_3 - x_2x_4, x_2^2 - 1, x_1x_2 - x_3x_4, x_1^2 - 1\}$$

$$\text{Est}_{\prec_{\text{rev}}}(D) = \{1,\ x_1,\ x_2,\ x_3,\ x_4,\ x_1x_4,\ x_2x_4,\ x_3x_4\}$$

The cardinality of $\text{Est}_{\prec}(D)$ is the same to the size of D.

∘ 3^{3-1} design D with $x_1 + x_2 + x_3 = 0$ (mod) 3:

```
i1 : R = QQ[x1,x2,x3];
i2 : I = ideal(x1*(x1-1)*(x1-2),x2*(x2-1)*(x2-2),x3*(x3-1)*(x3-2),
               (x1+x2+x3)*(x1+x2+x3-3)*(x1+x2+x3-6));
o2 : Ideal of R
i3 : g = gens gb I
o3 = | x1x2+x2^2-x1x3-x3^2-3x2+3x3 x1^2-x2^2+x1x3-x2x3-3x1+3x2
     -----------------------------------------------------------
       x3^3-3x3^2+2x3 x1x3^2+x2x3^2-2x1x3-2x2x3-2x3^2+4x3
     -----------------------------------------------------------
     3x2^2x3+3x2x3^2-3x2^2-12x2x3-3x3^2-2x1+7x2+7x3 x2^3-3x2^2+2x2 |
             1       6
o3 : Matrix R  <--- R
i4 : J = ideal leadTerm I; S = R/J; basis S
o4 : Ideal of R
o6 = | 1 x1 x1x3 x2 x2^2 x2x3 x2x3^2 x3 x3^2 |
             1       9
o6 : Matrix S  <--- S
```

Gröbner basis w.r.t. $\prec_{\mathrm{rev}}$:

$$\begin{aligned}
&\underline{x_1x_2} + x_2^2 - x_1x_3 - x_3^2 - 3x_2 + 3x_3,\\
&\underline{x_1^2} - x_2^2 + x_1x_3 - x_2x_3 - 3x_1 + 3x_2,\\
&\underline{x_3^3} - 3x_3^2 + 2x_3,\\
&\underline{x_1x_3^2} + x_2x_3^2 - 2x_1x_3 - 2x_2x_3 - 2x_3^2 + 4x_3,\\
&3\underline{x_2^2x_3} + 3x_2x_3^2 - 3x_2^2 - 12x_2x_3 - 3x_3^2 - 2x_1 + 7x_2 + 7x_3,\\
&\underline{x_2^3} - 3x_2^2 + 2x_2
\end{aligned}$$

$$\mathrm{Est}_{\prec_{\mathrm{rev}}}(D) = \{1,\ x_1,\ x_1x_3,\ x_2,\ x_2^2,\ x_2x_3,\ x_2x_3^2,\ x_3,\ x_3^2\}$$

- The interpolating polynomial on D is constructed by the standard monomials.
- Write $\mathrm{Est}_{\prec}(D)$ as

$$\mathrm{Est}_{\prec}(D) = \{x^a = x_1^{a_1} \cdots x_n^{a_n} \mid a = (a_1, \ldots, a_n) \in L\}.$$

For example,

$$\mathrm{Est}_{\prec_{\mathrm{rev}}}(D) = \{1,\ x_1,\ x_2,\ x_3,\ x_4,\ x_1x_4,\ x_2x_4,\ x_3x_4\}$$

$$\begin{aligned} \Rightarrow L \quad = \quad & \{(0,0,0,0),\ (1,0,0,0),\ (0,1,0,0),\ (0,0,1,0), \\ & (0,0,0,1),\ (1,0,0,1),\ (0,1,0,1),\ (0,0,1,1)\} \end{aligned}$$

- **Theorem** Fix a monomial order $\prec$.

$$D = (\boldsymbol{d}_1, \ldots, \boldsymbol{d}_m),\ \ \boldsymbol{d}_i = (d_{i1}, \ldots, d_{in}) \in \mathbb{Q}^n,\ \ i = 1, \ldots, m.$$

$\mathrm{Est}_{\prec}(D) = \{x^a \mid a \in L\}$ is the set of the standard monomials. Then the following holds.

(i) $|L| = m$

(ii) The model matrix $X = [\boldsymbol{d}_i^a]_{i=1,\ldots,m;\ a\in L}$ is nonsingular

(iii) Let $f:\ D \to \mathbb{R}$ be a response function on D, and let $\boldsymbol{y} = (f(\boldsymbol{d}_1), \ldots, f(\boldsymbol{d}_m)) \in \mathbb{R}^m$ be a response. Then the interpolating polynomial is

$$f(x_1, \ldots, x_n) = \sum_{a\in L} \theta_a x^a,$$

where $\boldsymbol{\theta} = [\theta_a]_{a\in L}$ is a column vector defined by $\boldsymbol{\theta} = X^{-1}\boldsymbol{y}$.

- Note that the matrix X is "the model matrix for the saturated polynomial model" we have seen in the slide page 14.

  The coefficient vector $\boldsymbol{\theta} = X^{-1}\boldsymbol{y}$ corresponds to the least square estimator for the saturated model

$$\hat{\boldsymbol{\theta}} = (X'X)^{-1}X'\boldsymbol{y} = X^{-1}\boldsymbol{y}.$$

- Example: 2^{4-1} design with $x_1x_2x_3x_4 = 1$:

x_1	x_2	x_3	x_4	y
1	1	1	1	y_1
1	1	−1	−1	y_2
1	−1	1	−1	y_3
1	−1	−1	1	y_4
−1	1	1	−1	y_5
−1	1	−1	1	y_6
−1	−1	1	1	y_7
−1	−1	−1	−1	y_8

$\Rightarrow$

$x_1 \quad x_2 \quad x_3 \quad x_4$	y
$\boldsymbol{d}_1$	y_1
$\boldsymbol{d}_2$	y_2
$\boldsymbol{d}_3$	y_3
$\boldsymbol{d}_4$	y_4
$\boldsymbol{d}_5$	y_5
$\boldsymbol{d}_6$	y_6
$\boldsymbol{d}_7$	y_7
$\boldsymbol{d}_8$	y_8

$$\mathrm{Est}_{\prec_{\mathrm{rev}}}(D) = \{1,\ x_1,\ x_2,\ x_3,\ x_4,\ x_1x_4,\ x_2x_4,\ x_3x_4\}$$

The model matrix $X = [\boldsymbol{d}_i^a]_{i=1,\ldots,m;\ a\in L}$

$X =$

	1	x_1	x_2	x_3	x_4	x_1x_4	x_2x_4	x_3x_4
$\boldsymbol{d}_1$	1	1	1	1	1	1	1	1
$\boldsymbol{d}_2$	1	1	1	−1	−1	−1	−1	1
$\boldsymbol{d}_3$	1	1	−1	1	−1	−1	1	−1
$\boldsymbol{d}_4$	1	1	−1	−1	1	1	−1	−1
$\boldsymbol{d}_5$	1	−1	1	1	−1	1	−1	−1
$\boldsymbol{d}_6$	1	−1	1	−1	1	−1	1	−1
$\boldsymbol{d}_7$	1	−1	−1	1	1	−1	−1	1
$\boldsymbol{d}_8$	1	−1	−1	−1	−1	1	1	1

$$\boldsymbol{\theta} = [\theta_a]_{a \in L} = X^{-1}\boldsymbol{y}$$

$$\begin{pmatrix} \theta_{0000} \\ \theta_{1000} \\ \theta_{0100} \\ \theta_{0010} \\ \theta_{0001} \\ \theta_{1001} \\ \theta_{0101} \\ \theta_{0011} \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \end{pmatrix}$$

The interpolating polynomial on D: $f(x_1, \ldots, x_8) = \sum_{a \in L} \theta_a x^a$

$$\begin{aligned} f(x_1, \ldots, x_8) &= \theta_{0000} + \theta_{1000}x_1 + \theta_{0100}x_2 + \theta_{0010}x_3 + \theta_{0001}x_4 \\ &\quad + \theta_{1001}x_1x_4 + \theta_{0101}x_2x_4 + \theta_{0011}x_3x_4 \end{aligned}$$

- Example: 3^{3-1} design with $x_1 + x_2 + x_3 = 0 \pmod 3$

$$\mathrm{Est}_{\prec_{\mathrm{rev}}}(D) = \{1,\ x_1,\ x_1x_3,\ x_2,\ x_2^2,\ x_2x_3,\ x_2x_3^2,\ x_3,\ x_3^2\}$$

x_1	x_2	x_3
0	0	0
0	1	2
0	2	1
1	0	2
1	1	1
1	2	0
2	0	1
2	1	0
2	2	2

$\Rightarrow X =$

1	x_1	x_1x_3	x_2	x_2^2	x_2x_3	$x_2x_3^2$	x_3	x_3^2
1	0	0	0	0	0	0	0	0
1	0	0	1	1	2	4	2	4
1	0	0	2	4	2	2	1	1
1	1	2	0	0	0	0	2	4
1	1	1	1	1	1	1	1	1
1	1	0	2	4	0	0	0	0
1	2	2	0	0	0	0	1	1
1	2	0	1	1	0	0	0	0
1	2	4	2	4	4	8	2	4

$$\begin{aligned} f(x_1, x_2, x_3) &= \theta_{000} + \theta_{100}x_1 + \theta_{101}x_1x_3 + \theta_{010}x_2 + \theta_{020}x_2^2 \\ &\quad + \theta_{011}x_2x_3 + \theta_{012}x_2x_3^2 + \theta_{001}x_3 + \theta_{002}x_3^2 \end{aligned}$$

6. The identifiability of the polynomial model

- As we have seen, the parameter of the interpolating polynomial is estimable. The parameter of any submodel of the interpolating polynomial is also estimable.
- For a given polynomial, the parameter estimability is judged from the standard form w.r.t. the Gröbner basis.

- **Theorem**

For a subset $M \subset M_n$, let

$$f = \sum_{\boldsymbol{x}^{\boldsymbol{a}} \in M} \theta_a \boldsymbol{x}^{\boldsymbol{a}}$$

be a polynomial on $D \subset \mathbb{Q}^n$. Fix a monomial order $\prec$ on M_n. Let $G_\prec$ be the Gröbner basis of $\mathbf{I}(D)$ w.r.t. $\prec$ and

$$\mathrm{Est}_\prec(D) = \{\boldsymbol{x}^{\boldsymbol{a}} \mid \boldsymbol{a} \in L\}.$$

Let the remainder of f w.r.t. $G_\prec$ be

$$r = \sum_{\boldsymbol{a} \in \tilde{L} \subset L} \mu_{\boldsymbol{a}} \boldsymbol{x}^{\boldsymbol{a}}$$

Then the parameter of f is estimable when the map $\{\theta_{\boldsymbol{a}}\} \mapsto \{\mu_{\boldsymbol{a}}\}$ is injective. In this case, f is identifiable.

- Example: 2^{4-1} design with $x_1x_2x_3x_4 = 1$:

  Gröbner basis:

$$x_4^2 - 1,\ x_3^2 - 1,\ x_2^2 - 1,\ x_1^2 - 1,$$
$$x_2x_3 - x_1x_4,\quad x_1x_3 - x_2x_4,\quad x_1x_2 - x_3x_4$$

  Therefore it is easy to see that

$$x_1x_2 - x_3x_4 \in \mathbf{I}(D),$$

  i.e., two-factor interaction $x_1 \times x_2$ and $x_3 \times x_4$ are confounded.

For the full two-factor interaction model

$$
\begin{aligned}
f(x_1, x_2, x_3, x_4) \quad &= \quad \theta_{0000} + \theta_{1000}x_1 + \theta_{0100}x_2 + \theta_{0010}x_3 + \theta_{0001}x_4 \\
&\quad +\theta_{1100}x_1x_2 + \theta_{1010}x_1x_3 + \theta_{1001}x_1x_4 \\
&\quad +\theta_{0110}x_2x_3 + \theta_{0101}x_2x_4 + \theta_{0011}x_3x_4,
\end{aligned}
$$

the remainder r is

$$
\begin{aligned}
r \quad &= \quad \theta_{0000} + \theta_{1000}x_1 + \theta_{0100}x_2 + \theta_{0010}x_3 + \theta_{0001}x_4 \\
&\quad +(\theta_{1001} + \theta_{0110})x_1x_4 + (\theta_{0101} + \theta_{1010})x_2x_4 + (\theta_{0011} + \theta_{1100})x_3x_4
\end{aligned}
$$

$f(x_1, x_2, x_3, x_4)$ and r are confounded on D.
The parameter $\theta_{1001}, \theta_{0110}$ can be estimated only in the form $\theta_{1001} + \theta_{0110}$.

- Example: 2^2 design $D = \{0,1\}^2$
  Gröbner basis: $G = \{x_1^2 - x_1,\ x_2^2 - x_2\}$

$$\mathrm{Est}(D) = \{1,\ x_1,\ x_2,\ x_1x_2\}$$

  - $f(x_1, x_2) = \theta_{20}x_1^2 + \theta_{02}x_2^2 + \theta_{12}x_1x_2$
    $\rightarrow r = \theta_{20}x_1 + \theta_{02}x_2 + \theta_{12}x_1x_2 \Rightarrow f$ is identifiable.
  - $f(x_1, x_2) = \theta_{30}x_1^3 + \theta_{03}x_2^3 + \theta_{21}x_1^2x_2 + \theta_{12}x_1x_2^2$
    $\rightarrow r = \theta_{30}x_1 + \theta_{03}x_2 + (\theta_{21} + \theta_{12})x_1x_2 \Rightarrow \theta_{21}, \theta_{12}$ are confounded.

- Example: 2^2 design $D = \{-1,1\}^2$
  Gröbner basis: $G = \{x_1^2 - 1,\ x_2^2 - 1\}$

$$\mathrm{Est}(D) = \{1,\ x_1,\ x_2,\ x_1x_2\}$$

  - $f(x_1, x_2) = \theta_{20}x_1^2 + \theta_{02}x_2^2 + \theta_{12}x_1x_2$
    $\rightarrow r = (\theta_{20} + \theta_{02}) + \theta_{12}x_1x_2 \Rightarrow \theta_{20}, \theta_{02}$ are confounded.

- Problem Box-Behnken design of 3 factors.

x_1	x_2	x_3
1	1	0
1	−1	0
−1	1	0
−1	−1	0
1	0	1
1	0	−1
−1	0	1
−1	0	−1
0	1	1
0	1	−1
0	−1	1
0	−1	−1
0	0	0

In the response surface methods, this design is used for degree 2 response surface model i.e., the polynomial model

$$Y = \theta_{000} + \theta_{100}x_1 + \theta_{010}x_2 + \theta_{001}x_3 + \theta_{200}x_1^2 + \theta_{020}x_2^2 + \theta_{002}x_3^2 + \theta_{110}x_1x_2 + \theta_{101}x_1x_3 + \theta_{011}x_2x_3$$

is considered.

Show that the above polynomial model is identifiable.

Derive 3 more terms that can be added to the above polynomial model.

```
i1 : R=QQ[t1,t2,t3,t4,t5,t6,t7,t8,t9,t10,t11,t12,t13,x1,x2,x3,
     MonomialOrder=>{13,3}];
i2 : I=ideal(t1*(x1-1),t1*(x2-1),t1*x3,t2*(x1-1),t2*(x2+1),t2*x3,
        t3*(x1+1),t3*(x2-1),t3*x3,t4*(x1+1),t4*(x2+1),t4*x3,
        t5*(x1-1),t5*x2,t5*(x3-1),t6*(x1-1),t6*x2,t6*(x3+1),
        t7*(x1+1),t7*x2,t7*(x3-1),t8*(x1+1),t8*x2,t8*(x3+1),
        t9*x1,t9*(x2-1),t9*(x3-1),t10*x1,t10*(x2-1),t10*(x3+1),
        t11*x1,t11*(x2+1),t11*(x3-1),t12*x1,t12*(x2+1),t12*(x3+1),
        t13*x1,t13*x2,t13*x3,
        t1+t2+t3+t4+t5+t6+t7+t8+t9+t10+t11+t12+t13-1);
o2 : Ideal of R
i3 : G = gb I; g = gens G
o4 = | x3^3-x3 x1x2x3 x1^2x3+x2^2x3-x3 x2^3-x2 x1x2^2+x1x3^2-x1
     -----------------------------------------------------------
     (output omitted)
     -----------------------------------------------------------
     8t1+2x1x3^2+2x2x3^2-x1^2-2x1x2-x2^2+x3^2-2x1-2x2 |
             1       21
o4 : Matrix R  <--- R
i5 : h = selectInSubring(1,g)
```

```
o5 = | x3^3-x3 x1x2x3 x1^2x3+x2^2x3-x3 x2^3-x2 x1x2^2+x1x3^2-x1
     -----------------------------------------------------------
     x1^2x2+x2x3^2-x2 x1^3-x1 2x2^2x3^2+x1^2-x2^2-x3^2 |
             1       8
o5 : Matrix R  <--- R
i6 : S = QQ[x1,x2,x3];
i7 : J = (map(S,R))(ideal(h));
o7 : Ideal of S
i8 : Jlt = ideal leadTerm J; U = S / Jlt; basis U
o8 : Ideal of S
o10 = | 1 x1 x1^2 x1x2 x1x3 x1x3^2 x2 x2^2 x2^2x3 x2x3 x2x3^2 x3 x3^2 |
              1       13
o10 : Matrix U  <--- U
```

The set of the standard monomial w.r.t. $\prec_{\text{rev}}$ is

$$\{1,\ x_1,\ x_2,\ x_3,\ x_1^2,\ x_2^2,\ x_3^2,\ x_1x_2,\ x_1x_3,\ x_2x_3\ x_1x_3^2,\ x_2^2x_3,\ x_2x_3^2\},$$

then we see that the degree 2 response surface model is identifiable.
Adding 3 terms to it,

$$\begin{aligned} f = \quad & \theta_{000} + \theta_{100}x_1 + \theta_{010}x_2 + \theta_{001}x_3 + \theta_{200}x_1^2 + \theta_{020}x_2^2 + \theta_{002}x_3^2 \\ & + \theta_{110}x_1x_2 + \theta_{101}x_1x_3 + \theta_{011}x_2x_3 + \theta_{102}x_1x_3^2 + \theta_{021}x_2^2x_3 + \theta_{012}x_2x_3^2 \end{aligned}$$

is also an identifiable (interpolating) polynomial model.