Markov basis for design of experiments with three-level factors

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Conditional tests for fractional factorial designs

- **Example: Wave-solder experiment (seven factors, each at two levels)**

  A: prebake condition

  B: flux density

  C: conveyer speed

  D: preheat condition

  E: cooling time

  F: ultrasonic solder agitator

  G: solder temperature

  Observations: number of solder defects

L. W. Condra, *Reliability Improvement with Design of Experiments*, **1993.**

- **Aim of this experiment: decide which levels for each factors are desirable to reduce solder defects**

- **full factorial design needs $2^7 = 128$ runs (high cost!)**

- **perform $\frac{1}{8}$ fraction of 128 runs**

  $\underline{2^{7-3}\ \textbf{fractional factorial design}}$

- **design and observation**

run	A	B	C	D	E	F	G	y
1	+1	+1	+1	+1	+1	+1	+1	$y_1 = 69$
2	+1	+1	+1	−1	−1	−1	−1	$y_2 = 31$
3	+1	+1	−1	+1	+1	−1	−1	$y_3 = 55$
4	+1	+1	−1	−1	−1	+1	+1	$y_4 = 149$
5	+1	−1	+1	+1	−1	+1	−1	$y_5 = 46$
6	+1	−1	+1	−1	+1	−1	+1	$y_6 = 43$
7	+1	−1	−1	+1	−1	−1	+1	$y_7 = 118$
8	+1	−1	−1	−1	+1	+1	−1	$y_8 = 30$
9	−1	+1	+1	+1	−1	−1	+1	$y_9 = 43$
10	−1	+1	+1	−1	+1	+1	−1	$y_{10} = 45$
11	−1	+1	−1	+1	−1	+1	−1	$y_{11} = 71$
12	−1	+1	−1	−1	+1	−1	+1	$y_{12} = 380$
13	−1	−1	+1	+1	+1	−1	−1	$y_{13} = 37$
14	−1	−1	+1	−1	−1	+1	+1	$y_{14} = 36$
15	−1	−1	−1	+1	+1	+1	+1	$y_{15} = 212$
16	−1	−1	−1	−1	−1	−1	−1	$y_{16} = 52$

aliasing relation

$$\mathrm{ABDE} = \mathrm{ACDF} = \mathrm{BCDG} = \mathrm{I}$$

- *Design matrix (orthogonal array)*

$$D = \begin{pmatrix} +1 & +1 & +1 & +1 & +1 & +1 & +1 \\ +1 & +1 & +1 & -1 & -1 & -1 & -1 \\ +1 & +1 & -1 & +1 & +1 & -1 & -1 \\ +1 & +1 & -1 & -1 & -1 & +1 & +1 \\ +1 & -1 & +1 & +1 & -1 & +1 & -1 \\ +1 & -1 & +1 & -1 & +1 & -1 & +1 \\ +1 & -1 & -1 & +1 & -1 & -1 & +1 \\ +1 & -1 & -1 & -1 & +1 & +1 & -1 \\ -1 & +1 & +1 & +1 & -1 & -1 & +1 \\ -1 & +1 & +1 & -1 & +1 & +1 & -1 \\ & & & \vdots & & & \\ -1 & -1 & -1 & +1 & +1 & +1 & +1 \\ -1 & -1 & -1 & -1 & -1 & -1 & -1 \end{pmatrix}$$

- **In the theory of designed experiments, the observations are usually assumed to be normally distributed. However, $y_1, \ldots, y_{16}$ are *NOT* normally distributed (${y_i}$'s are discrete observations) .**

- **Statistical Model (short review of the theory of** *generalized linear models***):**
  - $y_i \sim \mathrm{Po}(\mu_i)$**,** $i = 1, \ldots, k$**, i.i.d.**
  - **systematic part:**

$$\log \mu_i = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_{\nu-1} x_{i\nu-1}, \ \ i = 1, \ldots, k,$$

$x_{i1}, \ldots, x_{i\nu-1}$**:** *covariates***.**

- **ν-dimensional parameter β:**

$$\beta = (\beta_0, \beta_1, \ldots, \beta_{\nu-1})'$$

- **covariate matrix X:**

$$X = \begin{pmatrix} 1 & x_{11} & \cdots & x_{1\nu-1} \\ \vdots & \vdots & & \vdots \\ 1 & x_{k1} & \cdots & x_{k\nu-1} \end{pmatrix} : \quad k \times \nu \quad \text{matrix}$$

- **observation vector $\mathbf{y}$:**

$$\mathbf{y} = (y_1, \ldots, y_k)'$$

- **Likelihood function:**

$$\prod_{i=1}^{k} \frac{\mu_i^{y_i}}{y_i!} e^{-\mu_i} = \left(\prod_{i=1}^{k} \frac{e^{-\mu_i}}{y_i!} \right) \exp \left(\sum_{i=1}^{k} y_i \log \mu_i \right)$$

$$= \left(\prod_{i=1}^{k} \frac{e^{-\mu_i}}{y_i!} \right) \exp \left(\beta' X' \mathbf{y} \right)$$

(X'y is the sufficient statistic for β.)

- **How to define X ?**

  The matrix X is constructed from the design matrix D to reflect the effects of the factors and their interactions which we intend to measure.

- **For example, the simplest main effects model is given by**

$$X = \begin{pmatrix} 1 & x_{11} & \cdots & x_{1\nu-1} \\ \vdots & \vdots & & \vdots \\ 1 & x_{k1} & \cdots & x_{k\nu-1} \end{pmatrix} = \begin{pmatrix} 1 & \\ \vdots & D \\ 1 & \end{pmatrix}.$$

$$D = \begin{array}{c} \begin{array}{ccccccc} \mathrm{A} & \mathrm{B} & \mathrm{C} & \mathrm{D} & \mathrm{E} & \mathrm{F} & \mathrm{G} \end{array} \\ \left(\begin{array}{ccccccc}
+1 & +1 & +1 & +1 & +1 & +1 & +1 \\
+1 & +1 & +1 & -1 & -1 & -1 & -1 \\
+1 & +1 & -1 & +1 & +1 & -1 & -1 \\
+1 & +1 & -1 & -1 & -1 & +1 & +1 \\
+1 & -1 & +1 & +1 & -1 & +1 & -1 \\
+1 & -1 & +1 & -1 & +1 & -1 & +1 \\
+1 & -1 & -1 & +1 & -1 & -1 & +1 \\
+1 & -1 & -1 & -1 & +1 & +1 & -1 \\
-1 & +1 & +1 & +1 & -1 & -1 & +1 \\
-1 & +1 & +1 & -1 & +1 & +1 & -1 \\
 & & & \vdots & & & \\
-1 & -1 & -1 & +1 & +1 & +1 & +1 \\
-1 & -1 & -1 & -1 & -1 & -1 & -1
\end{array}\right) \end{array}$$

- **We can consider more complicated models containing various interaction effects, under the condition that it is consistent with the aliasing relations,**

$$\mathrm{ABDE} = \mathrm{ACDF} = \mathrm{BCDG} = \mathrm{I}.$$

i.e., we may consider appropriate models where all the parameters are estimable.

- **For example, the model of seven main effects and two two-factor interaction effects,** $\mathrm{A} \times \mathrm{B}, \mathrm{D} \times \mathrm{E}$**, is NOT estimable since** AB **and** DE **are confounded from the aliasing relation**

$$\mathrm{ABDE} = \mathrm{I}$$

since we have

$$\mathrm{AB} = \mathrm{DE}.$$

- **On the other hand, the model of seven main effects and two two-factor interaction effects,** $\mathrm{A} \times \mathrm{C}, \mathrm{B} \times \mathrm{D}$**, is estimable since** AC **and** BD **are not confounded.**

- **Relation to the work by Pistone and Wynn**

  The aliasing relations are more elegantly expressed as a set of polynomials defining and ideal in a polynomial ring.

  - **Consider** $\mathrm{A}, \mathrm{B}, \ldots, \mathrm{G}$ **as indeterminates.**
  - $\mathbb{C}(\mathrm{A}, \mathrm{B}, \ldots, \mathrm{G})$**: The ring of polynomials in** $\mathrm{A}, \mathrm{B}, \ldots, \mathrm{G}$ **with complex coefficients.**

Then the ideal

$$\langle \mathrm{A}^2-1, \mathrm{B}^2-1, \ldots, \mathrm{G}^2-1, \mathrm{ABDE}-1, \mathrm{ACDF}-1, \mathrm{BCDG}-1 \rangle$$

determines the aliasing relations.

Two interaction effects are aliased with each other *if and only if their difference belongs to the ideal***.**

- **Consider the model of seven main effects and two two-factor inter.** A × C, B × D.

○ **The covariate matrix:**

$$X = \begin{array}{cccc} & & \text{AC} & \text{BD} \\ \left(\begin{array}{c} 1 \\ 1 \\ \vdots \\ 1 \\ 1 \end{array} \right. & D & \begin{array}{c} 1 \\ 1 \\ \vdots \\ 1 \\ 1 \end{array} & \left. \begin{array}{c} 1 \\ -1 \\ \vdots \\ -1 \\ 1 \end{array} \right) \end{array}$$

○ **Likelihood function:**

$$\prod_{i=1}^{k} \frac{\mu_i^{y_i}}{y_i!} e^{-\mu_i} \quad = \quad \left(\prod_{i=1}^{k} \frac{e^{-\mu_i}}{y_i!} \right) \exp\left(\beta' X' \mathbf{y}\right)$$

- **The conditional distribution of y given the sufficient statistics:**

$$f(\mathbf{y} \mid X'\mathbf{y} = X'\mathbf{y}^o) = \text{Const.} \times \prod_{i=1}^{k} \frac{1}{y_i!},$$

$\mathbf{y}^o$: observed data,

$$\mathcal{F}(X'\mathbf{y}^o) = \{\mathbf{y} \mid X'\mathbf{y} = X'\mathbf{y}^o,\ \mathbf{y} \in \{0,1,2,\ldots\}^k\}$$

The set of y with the same sufficient statistics to $\mathbf{y}^o$. (We call $\mathcal{F}(X'\mathbf{y}^o)$ a fiber).

- **Note: by sufficiency the conditional distribution does not depend on the values of the nuisance parameters.**
- **Based on this conditional distribution, we can consider various conditional tests for the parameter β.**

See our paper, Aoki and Takemura (2007), for detail.

- **Next we consider three-level designs.**

  Example: 3^{4-2} **fractional factorial design**

	Factor				y
Run	A	B	C	D	
1	**0**	**0**	**0**	**0**	y_1
2	**0**	**1**	**1**	**2**	y_2
3	**0**	**2**	**2**	**1**	y_3
4	**1**	**0**	**1**	**1**	y_4
5	**1**	**1**	**2**	**0**	y_5
6	**1**	**2**	**0**	**2**	y_6
7	**2**	**0**	**2**	**2**	y_7
8	**2**	**1**	**0**	**1**	y_8
9	**2**	**2**	**1**	**0**	y_9

- **This design is given by**

$$\begin{cases} a + b + 2c = 0 \pmod 3 \\ a + 2b + 2d = 0 \pmod 3 \end{cases}$$

or, equivalently,

$$\begin{cases} c = a + b \pmod 3 \\ d = a + 2b \pmod 3). \end{cases}$$

This relation is expressed as the *aliasing relation*

$$\mathrm{C} = \mathrm{AB}, \quad \mathrm{D} = \mathrm{AB}^2$$

- **In the three-level designs, each n-factor interaction effect has 2^n degree of freedom.**

  For example, $\mathrm{A} \times \mathrm{B}$ **interaction effect is decomposed to two components denoted by** AB **and** AB^2**, where** AB **represents the contrasts**

  $$a + b = 0, 1, 2 \pmod 3,$$

  and AB^2 **represents the contrasts**

  $$a + 2b = 0, 1, 2 \pmod 3,$$

  respectively.

Similarly, the three-factor interaction $\mathrm{A} \times \mathrm{B} \times \mathrm{C}$ **is decomposed to the** 4 **components**

$$\mathrm{ABC},\ \ \mathrm{ABC}^2,\ \ \mathrm{AB}^2\mathrm{C},\ \ \mathrm{AB}^2\mathrm{C}^2,$$

and the four-factor interaction $\mathrm{A} \times \mathrm{B} \times \mathrm{C} \times \mathrm{D}$ **is decomposed to the** 8 **components**

$$\mathrm{ABCD},\ \ \mathrm{ABCD}^2,\ \ \mathrm{ABC}^2\mathrm{D},\ \ \mathrm{ABC}^2\mathrm{D}^2,$$
$$\mathrm{AB}^2\mathrm{CD},\ \ \mathrm{AB}^2\mathrm{CD}^2,\ \ \mathrm{AB}^2\mathrm{C}^2\mathrm{D},\ \ \mathrm{AB}^2\mathrm{C}^2\mathrm{D}^2.$$

We use the notation convention that *the coefficient for the first nonzero factor is* 1 **to avoid ambiguity. (Wu and Hamada, 2000)**

- **Another example:** 3^{4-1} **fractional factorial design given by** D = ABC**.**

  By the *modulus 3 calculus***, we can derive all the aliasing relations as follows.**

$$\begin{array}{ll}
I = ABCD^2 & \\
A = BCD^2 = AB^2C^2D & B = ACD^2 = AB^2CD^2 \\
C = ABD^2 = ABC^2D^2 & D = ABC = ABCD \\
AB = CD^2 = ABC^2D & AB^2 = AC^2D = BC^2D \\
AC = BD^2 = AB^2CD & AC^2 = AB^2D = BC^2D^2 \\
AD = AB^2C^2 = BCD & AD^2 = BC = AB^2C^2D^2 \\
BC^2 = AB^2D^2 = AC^2D^2 & BD = AB^2C = ACD \\
CD = ABC^2 = ABD &
\end{array}$$

- **From the relation, we can clarify the models where all the effects are estimable. For example,**
  - **the model of the main effects and the interaction effects $\mathrm{A} \times \mathrm{B}$, $\mathrm{A} \times \mathrm{C}$ is estimable.**

    AB, AB^2, AC, AC^2 **are not confounded to any main effect, nor not confounded in each other.**
  - **the model of the main effects and the interaction effects $\mathrm{A} \times \mathrm{B}$, $\mathrm{C} \times \mathrm{D}$ is NOT estimable.**

    AB **and** CD^2 **are confounded.**

- **Relation to the work by Pistone and Wynn**

  The aliasing relations are more elegantly expressed as a set of polynomials defining and ideal in a polynomial ring.

  Here, we must fully write down the aliasing relation as

$$
\begin{aligned}
&\mathrm{I} = \mathrm{ABCD}^2, \\
&\mathrm{A} = \mathrm{B}^2\mathrm{C}^2\mathrm{D} = \mathrm{A}^2\mathrm{BCD}^2, \quad \mathrm{A}^2 = \mathrm{BCD}^2 = \mathrm{AB}^2\mathrm{C}^2\mathrm{D}, \\
&\qquad\qquad\qquad\vdots \\
&\mathrm{AB} = \mathrm{C}^2\mathrm{D} = \mathrm{A}^2\mathrm{B}^2\mathrm{CD}^2, \quad \mathrm{AB}^2 = \mathrm{A}^2\mathrm{CD}^2 = \mathrm{BC}^2\mathrm{D}, \\
&\mathrm{A}^2\mathrm{B} = \mathrm{AC}^2\mathrm{D} = \mathrm{B}^2\mathrm{CD}^2, \quad \mathrm{A}^2\mathrm{B}^2 = \mathrm{CD}^2 = \mathrm{ABC}^2\mathrm{D}\ .
\end{aligned}
$$

Then the ideal

$$\langle \mathrm{A}^3 - 1, \mathrm{B}^3 - 1, \mathrm{C}^3 - 1, \mathrm{D}^3 - 1, \mathrm{D} - \mathrm{ABC} \rangle$$

determines the aliasing relations, i.e., two interaction effects are aliased if and only if their difference belongs to the ideal.

For example, A **and** $\mathrm{B}^2\mathrm{C}^2\mathrm{D}$ **are aliased since**

$$\begin{aligned} & \mathrm{A} - \mathrm{B}^2\mathrm{C}^2\mathrm{D} \\ & = (\mathrm{B}^2\mathrm{C}^2\mathrm{D} - \mathrm{A})(\mathrm{A}^3 - 1) - \mathrm{A}^4\mathrm{C}^3(\mathrm{B}^3 - 1) - \mathrm{A}^4(\mathrm{C}^3 - 1) - \mathrm{A}^3\mathrm{B}^2\mathrm{C}^2(\mathrm{D} - \mathrm{ABC}) \\ & \in \langle \mathrm{A}^3 - 1, \mathrm{B}^3 - 1, \mathrm{C}^3 - 1, \mathrm{D}^3 - 1, \mathrm{D} - \mathrm{ABC} \rangle \ . \end{aligned}$$

- **How to define X ?**

  The matrix X is constructed to include the main and the interaction effects *with two columns for each component of two degrees*.

Example: full model for 3^{4-2} fractional factorial design

		A×B	
A	B	AB	AB^2
0	**0**	**0**	**0**
0	**1**	**1**	**2**
0	**2**	**2**	**1**
1	**0**	**1**	**1**
1	**1**	**2**	**0**
1	**2**	**0**	**2**
2	**0**	**2**	**2**
2	**1**	**0**	**1**
2	**2**	**1**	**0**

⇒

					A×B			
	A		B		AB		AB^2	
1	**1**	**0**	**1**	**0**	**1**	**0**	**1**	**0**
1	**1**	**0**	**0**	**1**	**0**	**1**	**0**	**0**
1	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**1**
1	**0**	**1**	**1**	**0**	**0**	**1**	**0**	**1**
1	**0**	**1**	**0**	**1**	**0**	**0**	**1**	**0**
1	**0**	**1**	**0**	**0**	**1**	**0**	**0**	**0**
1	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**
1	**0**	**0**	**0**	**1**	**1**	**0**	**0**	**1**
1	**0**	**0**	**0**	**0**	**0**	**1**	**1**	**0**

Markov chain Monte Carlo tests for the designed experiments

- **Strategy to calculate p values for conditional tests (for discrete responses):**

1. **Traditional large-sample approximations**

   $\cdots$ **The adequacy of the approximation becomes poor for the data containing both small and large expected frequencies.**

2. **Exact calculations**

   $\cdots$ **become infeasible if the sample size is moderate size.**

3. **Monte Carlo procedure**

- **We consider a Monte Carlo method to evaluate p values, assuming that the exact calculation of p values is not feasible.**
- **Monte Carlo procedure to calculate p values: Generate samples from $f(\mathbf{y} \mid X'\mathbf{y} = X'\mathbf{y}^o)$.**

- **The closed form expression of $f(\mathbf{y} \mid X'\mathbf{y} = X'\mathbf{y}^o)$ cannot be obtained.**

  $\longrightarrow$ Markov chain Monte Carlo approach is valuable

- **If a connected Markov chain over $\mathcal{F}(X'\mathbf{y}^o)$ is constructed, the chain can be modified to give a connected and aperiodic Markov chain with stationary distribution $f(\mathbf{y} \mid X'\mathbf{y} = X'\mathbf{y}^o)$ by the usual Metropolis procedure.**

- **To construct a connected chain, a frequently used approach is to prepare a *Markov basis* (Diaconis and Sturmfels, 1998).**
- **If we obtain a Markov basis, we can easily construct a connected chain by adding elements of the Markov basis one by one.**
- **To derive a Markov basis, in applications, it is most convenient to rely on algebraic computational packages such as 4ti2.**

Markov bases and corresponding models for 3^{p-q} contingency tables

- **We investigate relationships between contingency tables and fractional factorial designs with 3^{p-q} runs.**
- **Basic fact: hierarchical models for the controllable factors in the 3^p full factorial design corresponds to the hierarchical models for the 3^p contingency table completely.**

- **Example: 3^2 full factorial design**

Run	A	B	AB	AB^2	**y**
1	0	0	0	0	y_1
2	0	1	1	2	y_2
3	0	2	2	1	y_3
4	1	0	1	1	y_4
5	1	1	2	0	y_5
6	1	2	0	2	y_6
7	2	0	2	2	y_7
8	2	1	0	1	y_8
9	2	2	1	0	y_9

$$\Rightarrow \boxed{\begin{array}{c} y_{11} \\ y_{12} \\ y_{13} \\ y_{21} \\ y_{22} \\ y_{23} \\ y_{31} \\ y_{32} \\ y_{33} \end{array}}$$

  - ○ **The sufficient statistic for the parameter of the total mean is expressed as $y_{\cdot\cdot}$.**
  - ○ **The sufficient statistic for the parameter of the main effects of A and B are expressed as $y_{i\cdot}$ and $y_{\cdot j}$.**

- **Fact. (Aoki and Takemura, 2007)**
  For 3^p full factorial design, write observations as $\mathbf{y} = (y_{i_1 \cdots i_p})$. Then the necessary and the sufficient condition that the $\{i_1, \ldots, i_n\}$-marginal n-dimensional table $(n \le p)$ is uniquely determined from $X'\mathbf{y}$ is that the covariate matrix X includes the contrasts for all the components of m-factor interaction effects $\mathrm{A}_{j_1} \times \mathrm{A}_{j_2} \times \cdots \times \mathrm{A}_{j_m}$ for all $\{j_1, \ldots, j_m\} \subset \{i_1, \ldots, i_n\}, m \le n$.

- **We also consider 3^{p-q} fractional factorial designs.**
- **Key point : write $k(=p-q)$ observations $\mathbf{y}=(y_1,\ldots,y_k)'$ as if they are the frequencies of 3^{p-q} contingency tables, i.e.,**

$$\mathbf{y}=(y_{i_1\cdots i_{p-q}})$$

- **An interesting observation: Many three-element fibers arise for constructing a connected chain.**

- **Example: main effects model for the** 3^{3-1} **fractional factorial design** C = AB

Run	A	B	C	**y**
1	**0**	**0**	**0**	y_{11}
2	**0**	**1**	**1**	y_{12}
3	**0**	**2**	**2**	y_{13}
4	**1**	**0**	**1**	y_{21}
5	**1**	**1**	**2**	y_{22}
6	**1**	**2**	**0**	y_{23}
7	**2**	**0**	**2**	y_{31}
8	**2**	**1**	**0**	y_{32}
9	**2**	**2**	**1**	y_{33}

$$\Rightarrow \quad X = \begin{array}{|c|cc|cc|cc|}
\multicolumn{1}{c}{} & \multicolumn{2}{c}{\mathrm{A}} & \multicolumn{2}{c}{\mathrm{B}} & \multicolumn{2}{c}{\mathrm{C}} \\
\hline
\mathbf{1} & \mathbf{1} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{1} & \mathbf{0} \\
\mathbf{1} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{1} \\
\mathbf{1} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\
\mathbf{1} & \mathbf{0} & \mathbf{1} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{1} \\
\mathbf{1} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} \\
\mathbf{1} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} \\
\mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\
\mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{1} & \mathbf{0} \\
\mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{1} \\
\hline
\end{array}$$

- **The sufficient statistic $X'\mathbf{y}$:**

$$\{y_{i\cdot}\},\ \{y_{\cdot j}\},$$

$$y_{11} + y_{23} + y_{32},\ y_{12} + y_{21} + y_{33},\ y_{13} + y_{22} + y_{31}$$

$$\begin{array}{|ccc|}\hline 0 & 1 & 2 \\ 1 & 2 & 0 \\ 2 & 0 & 1 \\ \hline\end{array}$$

- **Minimal Markov basis is constructed by the moves connecting the three-elements fiber**

$$\left\{ \boxed{\begin{array}{ccc} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{array}}, \boxed{\begin{array}{ccc} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{array}}, \boxed{\begin{array}{ccc} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{array}} \right\}.$$

Therefore any two moves from the set

$$\left\{ \boxed{\begin{array}{ccc} +1 & -1 & 0 \\ 0 & +1 & -1 \\ -1 & 0 & +1 \end{array}}, \boxed{\begin{array}{ccc} +1 & 0 & -1 \\ -1 & +1 & 0 \\ 0 & -1 & +1 \end{array}}, \boxed{\begin{array}{ccc} 0 & +1 & -1 \\ -1 & 0 & +1 \\ +1 & -1 & 0 \end{array}} \right\}$$

is a minimal Markov basis.

- **Similarly, we calculate minimal Markov bases by 4ti2 and investigate their uniqueness for various hierarchical models of** 27 **runs designs:**
  - ◦ 3^{4-1}_{IV} **design** $\mathrm{D} = \mathrm{ABC}$
  - ◦ 3^{5-2}_{III} **design** $\mathrm{D} = \mathrm{AB}, \mathrm{E} = \mathrm{AB^2C}$
  - ◦ 3^{5-2}_{III} **design** $\mathrm{D} = \mathrm{AB}, \mathrm{E} = \mathrm{AB^2}$
- **For some models, the minimal Markov bases is unique. For the other models, three-elements fibers arise and the minimal Markov bases are not unique.**

Discussion

- We investigate a Markov basis arising from the fractional factorial designs with three-level factors.
- Though we suppose that the observations are counts, our arguments can also be applied to the case that the observations are the ratio of counts. In this case, we consider the logistic link function instead of the logit link, and investigate the relation between 3^{p-q} fractional factorial designs to the 3^{p-q+1} contingency tables.

- **Interesting observations: many three-elements fibers arise in considering minimal Markov bases.**

  In fact, in all the examples considered today, all the dispensable moves of minimal Markov bases are needed for connecting three-elements fibers, where each element of the fibers does not share supports in each other.

  This shows that the every positive and the negative part of the dispensable moves is a indispensable. See notion of the *indispensable monomial* **(Aoki, Takemura and Yoshida, 2007).**

- **Future works: designs other than fractional factorial designs, such as the Plackett-Burman designs or the balanced incomplete block designs.**

- **Models for** 3^{4-1}_{IV} **design** $\mathrm{D} = \mathrm{ABC}$
  - **unique minimal MB exists**
    - **main effects + inter. effects** $\mathrm{A} \times \mathrm{B}, \mathrm{A} \times \mathrm{C}, \mathrm{B} \times \mathrm{C}$
  - **unique minimal MB does not exist**
    - **main effects**
    - **main effects + inter. effects** $\mathrm{A} \times \mathrm{B}$
    - **main effects + inter. effects** $\mathrm{A} \times \mathrm{B}, \mathrm{A} \times \mathrm{C}$
    - **main effects + inter. effects** $\mathrm{A} \times \mathrm{B}, \mathrm{A} \times \mathrm{C}, \mathrm{A} \times \mathrm{D}$

- **Models for** 3^{5-2}_{III} **design** $\mathrm{D} = \mathrm{AB}, \mathrm{E} = \mathrm{AB}^2\mathrm{C}$
  - **unique minimal MB exists**
    - **main effects** + **inter. effect** $\mathrm{C} \times \mathrm{E}$
    - **main effects** + **inter. effects** $\mathrm{A} \times \mathrm{C}, \mathrm{B} \times \mathrm{C}$
    - **main effects** + **inter. effects** $\mathrm{A} \times \mathrm{C}, \mathrm{C} \times \mathrm{E}$
    - **main effects** + **inter. effects** $\mathrm{A} \times \mathrm{C}, \mathrm{A} \times \mathrm{E}, \mathrm{C} \times \mathrm{E}$
    - **main effects** + **inter. effects** $\mathrm{A} \times \mathrm{C}, \mathrm{B} \times \mathrm{C}, \mathrm{C} \times \mathrm{D}$
    - **main effects** + **inter. effects** $\mathrm{A} \times \mathrm{C}, \mathrm{B} \times \mathrm{C}, \mathrm{C} \times \mathrm{E}$
  - **unique minimal MB does not exist**
    - **main effects**
    - **main effects** + **inter. effect** $\mathrm{A} \times \mathrm{C}$
    - **main effects** + **inter. effects** $\mathrm{A} \times \mathrm{C}, \mathrm{A} \times \mathrm{E}$

- **Models for** 3^{5-2}_{III} **design** $\mathrm{D} = \mathrm{AB}, \mathrm{E} = \mathrm{AB}^2$
  - **Unique minimal Markov basis exists for all the hierarchical models**
    - **main effects**
    - **main effects + inter. effect** $\mathrm{A} \times \mathrm{C}$
    - **main effects + inter. effects** $\mathrm{A} \times \mathrm{C}, \mathrm{B} \times \mathrm{C}$
    - **main effects + inter. effects** $\mathrm{A} \times \mathrm{C}, \mathrm{B} \times \mathrm{C}, \mathrm{C} \times \mathrm{D}$