Some results on minimality and invariance of Markov bases

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Items

1. **Introduction (two-way and three-way tables)**
2. **Markov bases and Gröbner bases**
3. **Minimality and invariance of Markov bases**

Purpose of the talk : give a general introduction to Markov bases, with some emphasis on minimality and invariance.

1. Introduction (two-way and three-way contingency tables)

- **Contingency table is still a rich source of problems for algebraic statistics.**
- **We begin with two-way tables for introduction. However we are really interested in tables with more factors.**
- **In particular the no-three-factor interaction model for three-way tables is surprisingly difficult.**

- **For four-way or more, almost all models are difficult in view of Markov bases. The exception is the decomposable model.**
- **General $I \times J$ two-way table**

Factor 1\ Factor 2	1	...	J	row sum
1	x_{11}	...	x_{1J}	x_{1+}
⋮		...		⋮
I	x_{I1}	...	x_{IJ}	x_{I+}
column sum	x_{+1}	...	x_{+J}	n

- x_{i+}, x_{+j} **: marginal frequency,** n**: total**

sample size

- **Hypothesis of independence**

$$H_0: \; p_{ij} = \alpha_i \beta_j, \qquad \forall i, j \tag{1}$$

p_{ij} is the cell probability.
$\alpha_i = p_{i+}$, $\beta_j = p_{+j}$ is the marginal probability

- **Exact test: evaluated the P-values based on the hypergeometric distribution over the set of contingency tables with the same row sums and the column sums as the observed table.**

Example: 3×3 case

- **Marginal frequencies:**
  $\boldsymbol{b} = (x_{1+}, x_{2+}, x_{3+}, x_{+1}, x_{+2}, x_{+3})$
- **Joint frequencies:** $\boldsymbol{x} = (x_{11}, x_{12}, \ldots, x_{33})^t$

- “configuration”

$$\boldsymbol{A} = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \boldsymbol{E}_3 \otimes \mathbf{1}_3^t \\ \mathbf{1}_3^t \otimes \boldsymbol{E}_3 \end{pmatrix},$$

$\boldsymbol{E}_k$: identity matrix, $\mathbf{1}_k$:vector will all 1’s.

- The relation between marginal frequencies and joint frequencies.

$$\boldsymbol{b} = \boldsymbol{A}\boldsymbol{x}$$

- **Fiber**: the set of contingency tables sharing the set of marginal frequencies

$$\mathcal{F}_{\boldsymbol{b}} = \{\boldsymbol{x} \in \mathbb{N}^{I \times J} \mid \boldsymbol{b} = \boldsymbol{A}\boldsymbol{x}\}, \quad \mathbb{N} = \{0, 1, \dots\}$$

- We use MCMC for sampling from the fiber
- basic move: choose the following "basic move"

z randomly and add to the current table.

	j	j'
i	$+1$	-1
i'	-1	$+1$

- **$0 = Az$: marginals do not change.**
- **When we have a negative cell, discard the move and choose another one.**
- **Question: Can we move all over the fiber with the basic moves only?**
- **YES for two-way tables (irrespective of I, J)**

Three-way tables (no-three-factor interaction model)

x_{111}	$\cdots$	x_{11K}		x_{I11}	$\cdots$	x_{I1K}
$\vdots$		$\vdots$	$\cdots$	$\vdots$		$\vdots$
x_{1J1}	$\cdots$	x_{1JK}		x_{IJ1}	$\cdots$	x_{IJK}

- **We consider fixing two-factor marginals**

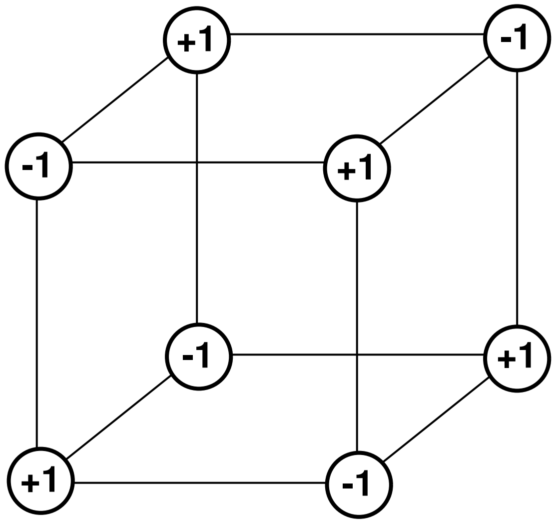
$$x_{ij+} = \sum_k x_{ijk}, \qquad (x_{i+k}, x_{+jk} \text{ similarly defined})$$

- **The fiber of contingency tables sharing all the two-factor marginals with the observed table $x^o = \{x^o_{ijk}\}$**

$$\mathcal{F}_b = \{x = (x_{ijk}) \mid x_{ijk} \in \mathbb{N}, x_{ij+} = x^o_{ij+}, \\ x_{i+k} = x^o_{i+k}, x_{+jk} = x^o_{+jk}, \ \forall i, \forall j, \forall k\}$$

- **Structure of the fiber becomes immensely difficult as I, J, K become large.**

- **Basic move for this case**



- **However not every fiber is connected by these moves.**

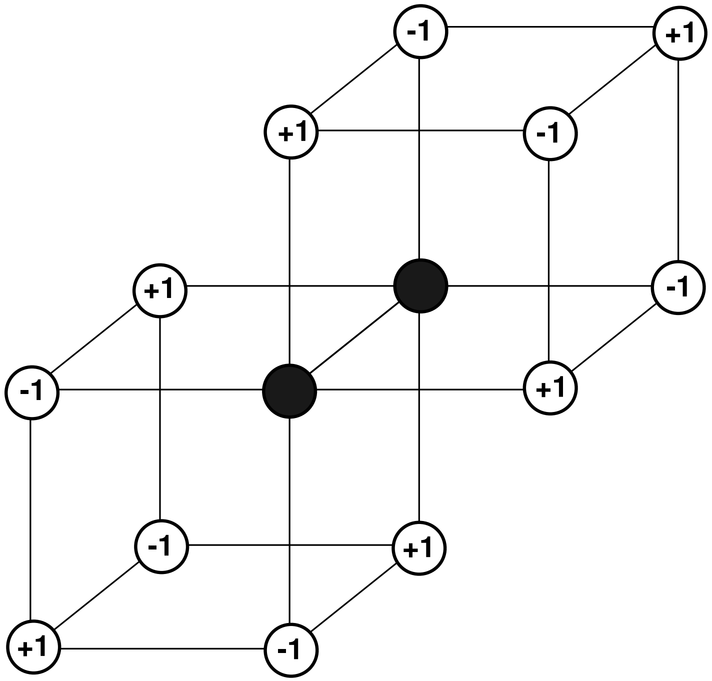
- **Example:** $I = J = K = 3$

$$\mathcal{F} = \{x = (x_{ijk}) \mid x_{ijk} \in \mathbb{N},$$
$$a = x_{ij+} = x_{i+k} = x_{+jk},\ 1 \le i,j,k \le 3\}$$

- **The following element of this fiber is isolated**

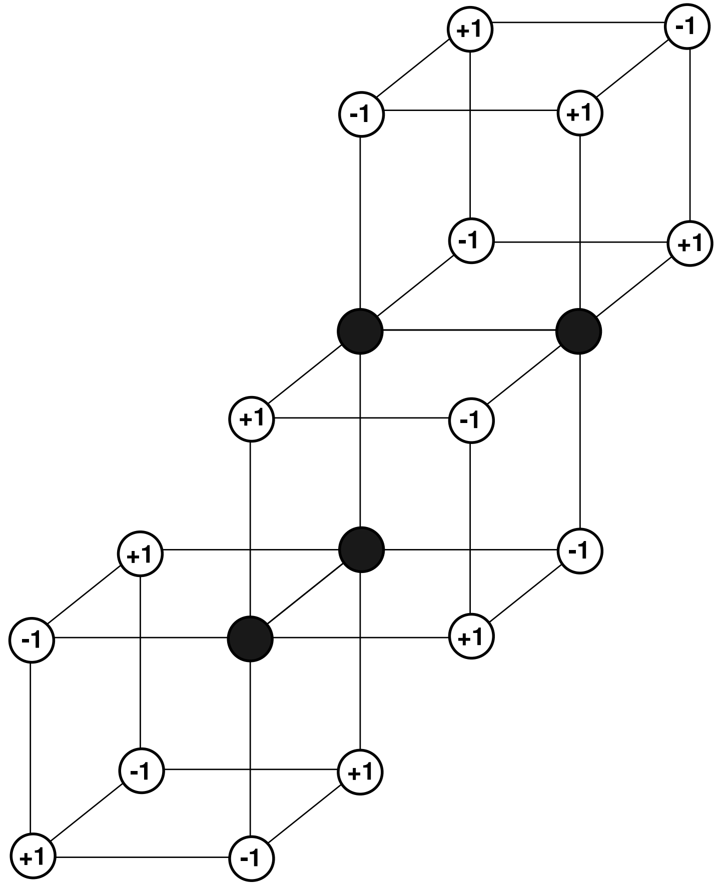
$$\boxed{\begin{matrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & a \end{matrix}} \qquad \boxed{\begin{matrix} 0 & a & 0 \\ 0 & 0 & a \\ a & 0 & 0 \end{matrix}} \qquad \boxed{\begin{matrix} 0 & 0 & a \\ a & 0 & 0 \\ 0 & a & 0 \end{matrix}}$$

- **For $3 \times 3 \times 3$ it suffices to add the following "degree 6" moves:**

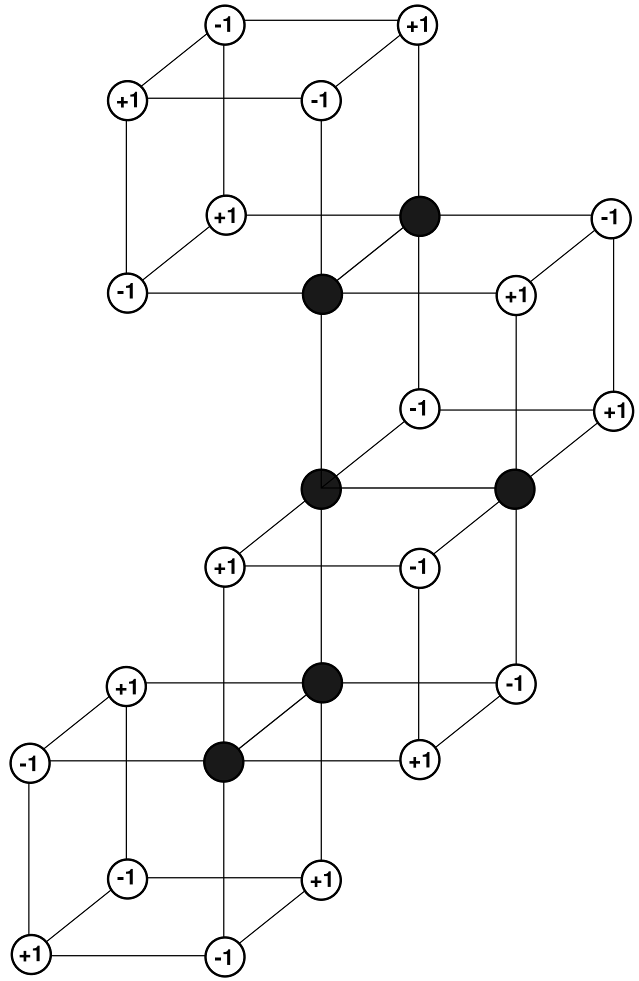


(Every fiber becomes connected).

- **We additionally need the following degree 8 move for $3 \times 3 \times 4$ tables:**



- **Additionally need the following degree 10 move for $3 \times 3 \times 5$ tables:**



But these are enough!

- **For $3 \times 3 \times K$, $K \geq 5$, we only need the above moves for connecting every fiber. (generalized by Santos and Sturmfels.)**

- **However if we also increase I and J, then we need more and more complicated moves for connectivity of the fibers. It is known that the fibers get arbitrarily complicated (De Loera and Onn).**

3. Markov bases and Gröbner bases

Formulation

- A: $d \times q$ non-negative integer matrix. "Configuration" Let $\mathcal{I}$ denote the set of columns ("cells") of A.
- Technical assumption: $(1, \ldots, 1)$ belongs to the row space of A.
- Fiber:

$$\mathcal{F}_b = \{x \in \mathbb{N}^q \mid b = Ax\}$$

- move: an integer vector z belonging to the

kernel of A:

$$0 = Az$$

- **If z is a move, then**

$$A(x + z) = Ax$$

  and we stay in the same fiber, provided that there is no negative element in $x + z$.

- **Write $z = z^+ - z^-$, where z^+ is the positive part and z^- is the negative part of z. z^+ and z^- belong to the same fiber.**

- **A finite set of moves $\mathcal{B} = \{z_1, \ldots, z_L\}$ makes each fiber an undirected graph:**

– **An edge between $x, y \in \mathcal{F}_b$ if there exists $z \in \mathcal{B}$ such that**

$$x = y + z \text{ or } y = x + z.$$

- **Definition of Markov basis**

> **A finite set of moves $\mathcal{B}$ is a Markov basis for the configuration A if every fiber becomes a connected graph by $\mathcal{B}$.**

- **BASIC FACT** (Diaconis and Sturmfels (1998))

A finite set of moves is a Markov basis for A if and only if it corresponds to a system of generators of the toric ideal I_A.

  - k: a filed
  - $\mathrm{k}(p_1, \ldots, p_q)$: polynomial ring for the column
  - $\mathrm{k}(v_1, \ldots, v_d)$: polynomial ring for the rows
  - $\pi_A : p_i \mapsto \prod_{j=1}^{d} v_j^{a_{ji}}$: homomorphism
  - $I_A = \mathrm{Ker}(\pi_A)$: a toric ideal

An algebraic look at probability models

- **Two-way independence model**

$$p_{ij} = \alpha_i \beta_j$$

- **Joint probability function of $x = (x_{11}, \ldots, x_{IJ})$:**

$$(\text{mult.coeff.}) \times \prod_{i,j} p_{ij}^{x_{ij}}$$

- **Look at $\{p_{ij}\}$ as "indeterminates" and x_{ij} as "powers". Then $p^x = \prod_{i,j} p_{ij}^{x_{ij}}$ is a monomial.**
- **k($\{p_{ij}\}$) : polynomial ring in indeterminates $\{p_{ij}\}$.**

- **Also look at $\{\alpha_i\} \cup \{\beta_j\}$ as indeterminates.**
- **Homomorphism. Define**
  $\pi : \mathrm{k}(\{p_{ij}\}) \longrightarrow \mathrm{k}(\{\alpha_i\} \cup \{\beta_j\})$ **by**

$$\pi : p_{ij} \mapsto \alpha_i \beta_j$$

- $I_A = \mathrm{Ker}(\pi)$ **is the toric ideal for the configuration**

$$A = \begin{pmatrix} E_I \otimes 1_J^t \\ 1_I^t \otimes E_J \end{pmatrix}$$

- **Example**

$$\begin{aligned}\pi(p_{11}p_{22} - p_{12}p_{21}) &= \pi(p_{11})\pi(p_{22}) - \pi(p_{12})\pi(p_{21}) \\ &= \alpha_1\beta_1\alpha_2\beta_2 - \alpha_1\beta_2\alpha_2\beta_1 \\ &= 0.\end{aligned}$$

- **Similarly** $p_{ij}p_{i'j'} - p_{ij'}p_{i'j} \in I_A$. **These correspond exactly to the basic move:** $\begin{matrix} +1 & -1 \\ -1 & +1 \end{matrix}$

In general

- **Every toric ideal I_A has a system of generators consisting of binomials, i.e. I_A is generated by finite number of binomials $p^y - p^x$.**

- **$p^y - p^x$ belongs to I_A if and if $z = y - x = z^+ - z^-$ is a move.**

- **This equivalence yields the BASIC FACT.**

- **Gröbner basis is a nice system of generators with some additional properties. Also it is tractable by algorithms.**

Gröbner base for the $3 \times 3 \times 3$ case (revlex term order)

In addition to the basic moves and degree 6 moves, it contains the following moves:

- **28 moves of degree 7:**

$$\boxed{\begin{array}{ccc} 0 & 0 & 0 \\ 0 & -1 & +1 \\ 0 & +1 & -1 \end{array}} \quad \boxed{\begin{array}{ccc} +1 & 0 & -1 \\ -1 & +1 & 0 \\ 0 & -1 & +1 \end{array}} \quad \boxed{\begin{array}{ccc} -1 & 0 & +1 \\ +1 & 0 & -1 \\ 0 & 0 & 0 \end{array}}$$

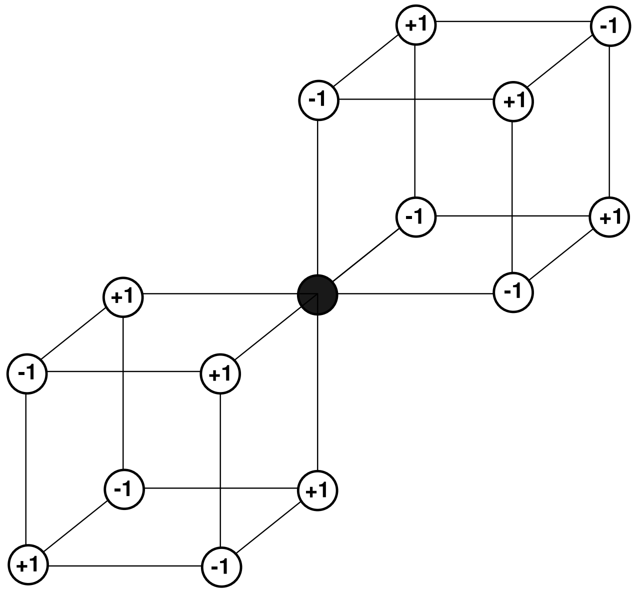
- **Just one move of degree 9:**

$\color{blue}{-2}$	$+1$	$+1$
$+1$	0	-1
$+1$	-1	0

$+1$	0	-1
0	0	0
-1	0	$+1$

$+1$	-1	0
-1	0	$+1$
0	$+1$	-1

- **Picture of the degree 7 move**



- **Actually we do not need degree 7 moves and degree 9 moves for connectivity.**
- **As a matter of fact, for the $3 \times 3 \times 3$ case, the set of basic moves and degree 6 moves forms a unique minimal Markov basis.**

4. Minimality and invariance of Markov bases

- **Motivation: The reduced Gröbner basis is not necessarily minimal as a set of generators of a toric ideal. Also sometimes it does not reflect the symmetry inherent in the configuration A.**
- **A system of generators $\mathcal{B} = \{z_1, \ldots, z_L\}$ is minimal if no proper subset is a system of generators.**
- **A move (or a binomial) z is indispensable if z**

(or $-z$) belongs to every system of generators.

- **Fact: A minimal system of generators is unique if and only if the set of indispensable binomials is a system of generators.**

- **z is indispensable if and only if the fiber $\mathcal{F}_{Az^+}$ consists of just two elements $\{z^+, z^-\}$:**

$$\mathcal{F}_{Az^+} = \{z^+, z^-\}$$

- **"The $4 \times 4 \times 4$ challenge"**
  Hemmecke and Malkin (2006). One week of computation. The unique minimal basis consists of 148,968 moves. By symmetry, they are classified into 15 types of moves.

  1. $p_{111}p_{144}p_{414}p_{441} - p_{114}p_{141}p_{411}p_{444}$
  2. $p_{111}p_{144}p_{334}p_{341}p_{414}p_{431} - p_{114}p_{141}p_{331}p_{344}p_{411}p_{434}$
  3. $p_{111}p_{122}p_{134}p_{143}p_{414}p_{423}p_{432}p_{441} -$
     $p_{114}p_{123}p_{132}p_{141}p_{411}p_{422}p_{434}p_{443}$
  4. $p_{111}p_{144}p_{324}p_{333}p_{341}p_{414}p_{423}p_{431} -$
     $p_{114}p_{141}p_{323}p_{331}p_{344}p_{411}p_{424}p_{433}$
  5. $p_{111}p_{144}p_{234}p_{243}p_{323}p_{341}p_{414}p_{421}p_{433} -$
     $p_{114}p_{141}p_{233}p_{244}p_{321}p_{343}p_{411}p_{423}p_{434}$
  6. $p_{111}p_{122}p_{133}p_{144}p_{324}p_{332}p_{341}p_{414}p_{423}p_{431} -$
     $p_{114}p_{123}p_{132}p_{141}p_{322}p_{331}p_{344}p_{411}p_{424}p_{433}$

7. $p_{111}p_{144}p_{222}p_{234}p_{243}p_{323}p_{341}p_{414}p_{421}p_{432} -$
$p_{114}p_{141}p_{223}p_{232}p_{244}p_{321}p_{343}p_{411}p_{422}p_{434}$

8. $p_{111}p_{144}p_{222}p_{233}p_{324}p_{332}p_{341}p_{414}p_{423}p_{431} -$
$p_{114}p_{141}p_{223}p_{232}p_{322}p_{331}p_{344}p_{411}p_{424}p_{433}$

9. $p_{111}p_{112}p_{133}p_{144}p_{223}p_{224}p_{232}p_{241}p_{314}p_{322}p_{413}p_{421} -$
$p_{113}p_{114}p_{132}p_{141}p_{221}p_{222}p_{233}p_{244}p_{312}p_{324}p_{411}p_{423}$

10. $p_{111}p_{112}p_{133}p_{144}p_{224}p_{232}p_{243}p_{313}p_{322}p_{341}p_{414}p_{421} -$
$p_{113}p_{114}p_{132}p_{141}p_{222}p_{233}p_{244}p_{312}p_{321}p_{343}p_{411}p_{424}$

11. $p_{111}p_{134}p_{143}p_{222}p_{233}p_{241}p_{314}p_{323}p_{342}p_{412}p_{424}p_{431} -$
$p_{114}p_{133}p_{141}p_{223}p_{231}p_{242}p_{312}p_{324}p_{343}p_{411}p_{422}p_{434}$

12. $p_{111}p_{134}p_{143}p_{224}p_{232}p_{241}p_{314}p_{323}p_{342}p_{412}p_{421}p_{433} -$
$p_{114}p_{133}p_{141}p_{221}p_{234}p_{242}p_{312}p_{324}p_{343}p_{411}p_{423}p_{432}$

13. $p_{111}^2p_{124}p_{133}p_{144}p_{214}p_{223}p_{242}p_{313}p_{332}p_{341}p_{414}p_{424}p_{431} -$
$p_{114}^2p_{123}p_{131}p_{141}p_{213}p_{222}p_{244}p_{311}p_{333}p_{342}p_{411}p_{424}p_{432}$

14. $p_{111}^2p_{124}p_{133}p_{144}p_{214}p_{232}p_{243}p_{312}p_{323}p_{341}p_{414}p_{422}p_{431} -$
$p_{114}^2p_{123}p_{131}p_{141}p_{212}p_{233}p_{244}p_{311}p_{322}p_{343}p_{411}p_{424}p_{432}$

15. $p_{111}^2p_{133}p_{144}p_{223}p_{224}p_{232}p_{242}p_{313}p_{322}p_{341}p_{414}p_{422}p_{431} -$
$p_{113}p_{114}p_{131}p_{141}p_{222}^2p_{233}p_{244}p_{311}p_{323}p_{342}p_{411}p_{424}p_{432}$

All these relations are derived by elimination of α_{ij}', β_{ik}'s and γ_{jk}'s from the relation

$$p_{ijk} = \alpha_{ij}\beta_{ik}\gamma_{jk}, \ 1 \leq i, j, k \leq 4,$$

Symmetry of the system of generators

- **Symmetry of $3 \times 3 \times 3$ tables (or $4 \times 4 \times 4$ tables)**
  - **Interchange of levels for each factor**
  - **Interchange of factors**
  - **Example: $4 \times 4 \times 4$ case. A direct product $S_4 \times S_4 \times S_4 \times S_3$ acts on the set of cells as permutations.**
  - **The above list shows representative elements from the orbits of the action.**

- **How to define the symmetry of A for a general configuration $A : d \times q$?**

- **$S_q = S_{|\mathcal{I}|}$ acts on the q-dimensional rational linear space $\mathbb{Q}^q$ by permutation of cells.**

- **For a subspace $L \subset \mathbb{Q}^q$, denote the setwise stabilizer of S_q w.r.t. L by**

$$G_L = \{g \in S_{|\mathcal{I}|} \mid gL = L\}$$

(invariant as a subspace)

Definition of the invariance group for A.

- **We call the setwise stabilizer $G_{\mathrm{Ker}(A)}$ of S_q w.r.t. Ker(A) the group of invariance for the configuration A.**
- **The invariance group is the set of permutations of the cells, which leaves the set of moves invariant.**
- **A Markov basis $\mathcal{B}$ is invariant if it is invariant with respect to the permutations in $G_{\mathrm{Ker}(A)}$.**
- **Many bases such as Graver bases or universal Gröbner bases, which does not depend on the term orders are invariant.**

- **Configurations A for statistical models are often highly symmetric. Exploiting this symmetry, we can concisely express invariant Markov bases by a list of representative elements of the orbits.**

- **It is an important (but difficult) topic to exploit symmetry inherent in the configuration in algebraic algorithms.**

Summary of the talk

- **We discussed performing exact tests for two-way tables and three-way tables by MCMC.**

- **We defined Markov bases and explained one-to-one correspondences between moves and binomials of toric ideals.**

- **For three-way tables, we saw that Gröbner basis does not correspond to a minimal system of generators.**

- **We defined the notion of indispensable moves**

and its relation to uniqueness of minimal Markov basis

- **We defined symmetry inherent in a configuration $\boldsymbol{A}$.**

We wrote a review paper in Japanese. An English translation will appear in "Sugaku Expositions". Just ask me for the translation.