Minimality properties of Markov bases and normality of semigroups

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Introduction and Notation

Introduction and Notation

- In this talk, we look at various properties of moves in a Markov basis from the viewpoint of minimality.
- Mainly a summary of past papers of me and coauthors (Aoki, Hara, Yoshida, Ohsugi, Hibi)
- We are also interested in "normality" of semigroups and its relation to Markov bases.
- As always, we start with a small two-way table (3×3):

alge.\ stat.	A	B	C	total
A	7	5	1	13
B	5	10	6	21
C	2	6	8	16
total	14	21	15	50

Introduction and Notation

- The relation between the joint frequencies and the marginal frequencies is written as

$$\begin{pmatrix} 13 \\ 21 \\ 16 \\ 14 \\ 21 \\ 15 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 7 \\ 5 \\ 1 \\ 5 \\ 10 \\ 6 \\ 2 \\ 6 \\ 8 \end{pmatrix}$$

- Write this as

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

Introduction and Notation

- A ($d \times q$): "configuration"
  - For simplicity assume that the elements of A are nonnegative.
  - Also assume that A is "homogeneous", in the sense that $(1, 1, \dots, 1)$ is in the row-space of A.
- $\boldsymbol{x} \geq 0$: joint frequency vector
- $\boldsymbol{b}$: marginal frequency vector
- Move: an integer vector $\boldsymbol{z}$ such that $A\boldsymbol{z} = 0$. Then

$$A(\boldsymbol{x} + \boldsymbol{z}) = A\boldsymbol{x}$$

(We do not change the marginal frequencies.)

Introduction and Notation

- $$\begin{pmatrix} 7 & 5 & 1 \\ 5 & 10 & 6 \\ 2 & 6 & 8 \end{pmatrix} + \begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 8 & 4 & 1 \\ 4 & 11 & 6 \\ 2 & 6 & 8 \end{pmatrix}$$
- This way we move around the set ("fiber") of contingency tables with common marginal frequencies.
- Fiber:
$$\mathcal{F}_{\boldsymbol{b}} = \{\boldsymbol{x} \geq 0 \mid \boldsymbol{b} = A\boldsymbol{x}\}$$
- Markov basis: a finite set of moves, by which we can reach every table of every fiber.

Introduction and Notation

- FACT: for $I \times J$ two-way tables, the set of moves of the form

$$\begin{array}{ccccc} & \vdots & & \vdots & \\ \dots & 1 & \dots & -1 & \dots \\ & \vdots & & \vdots & \\ \dots & -1 & \dots & 1 & \dots \\ & \vdots & & \vdots & \end{array}$$

forms a Markov basis. Call it a "basic move".

Introduction and Notation

- A simple proof by "distance reducing argument" (TA2005Bernoulli)
- Suppose we have two different tables $\boldsymbol{x}, \boldsymbol{y}$ in the same fiber.
- Let

$$d(\boldsymbol{x}, \boldsymbol{y}) = |\boldsymbol{x} - \boldsymbol{y}| = \sum_{i,j} |\boldsymbol{x}(i,j) - \boldsymbol{y}(i,j)|$$

  denote the L_1-distance between $\boldsymbol{x}$ and $\boldsymbol{y}$. (In this talk $|\cdot|$ denote the L_1 norm.)
- Because $\boldsymbol{x} \neq \boldsymbol{y}$, there exists a cell such that

$$\boldsymbol{x}(i,j) < \boldsymbol{y}(i,j)$$

  (total sample size n is common to $\boldsymbol{x}$ and $\boldsymbol{y}$.)

Introduction and Notation

- Therefore there exists a sign pattern of $\boldsymbol{x} - \boldsymbol{y}$:

$$
\begin{array}{cccccccc}
 & & j & & j' & \\
 & & \vdots & & \vdots & \\
i & \dots & - & \dots & + & \dots \\
 & & \vdots & & \vdots & \\
i' & \dots & + & \dots & ? & \dots \\
 & & \vdots & & \vdots &
\end{array}
$$

- In particular $\boldsymbol{x}(i', j) > 0, \boldsymbol{x}(i, j') > 0$ and we can subtract "1" from both cells of $\boldsymbol{x}$. We can always add 1 to $\boldsymbol{x}(i, j)$ and $\boldsymbol{x}(i', j')$.
- Irrespective of the sign of "?", we can reduce $d(\boldsymbol{x}, \boldsymbol{y})$ by 2 or 4.

Introduction and Notation

- Are all the basic moves necessary?
  - Consider the fiber:

			1
			1
			0
1	1	0	2

  - There are only two tables in the fiber:

1	0	0
0	1	0
0	0	0

or

0	1	0
1	0	0
0	0	0

  - To move from one table to another, we need a basic move.

Introduction and Notation

- Observation: difference of two tables in a two-element fiber is always needed in a Markov basis.
- We call it an "indispensable move". (TA2004AISM)
- We saw that for two-way tables the basic moves form a Markov basis. Furthermore each basic move is indispensable.

Minimal Markov bases

Minimal Markov bases

- In this section we formalize observations in the previous slides on indispensable moves.
- Then we give a characterization of minimal Markov bases.
- Positive part and negative part of a move $\boldsymbol{z}$:

$$\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^-$$

  $\boldsymbol{z}^+$ and $\boldsymbol{z}^-$ have disjoint supports.
- $0 = A\boldsymbol{z} \Rightarrow A\boldsymbol{z}^+ = A\boldsymbol{z}^-$. Therefore $\boldsymbol{z}^+$ and $\boldsymbol{z}^-$ belong to the same fiber.

Minimal Markov bases

- Conversely the difference of two elements of the same fiber is a move.
- Indispensable move: we saw that the difference of two elements of a two-element fiber has to belong to every Markov basis:

  Definition: $\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^-$ is an indispensable move if $\{\boldsymbol{z}^+, \boldsymbol{z}^-\} = \mathcal{F}_{A\boldsymbol{z}^+}$ is a two-element fiber.

- On the other hand, suppose that a fiber has more than two elements. Say $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{u}$. Then we can go from $\boldsymbol{x}$ to $\boldsymbol{y}$ via $\boldsymbol{u}$.
- If $\mathrm{supp}(\boldsymbol{x}) \cap \mathrm{supp}(\boldsymbol{y}) = \emptyset$, then the move $\boldsymbol{x} - \boldsymbol{y}$ can be replaced by $\boldsymbol{x} - \boldsymbol{u}$ and $\boldsymbol{u} - \boldsymbol{y}$.

Minimal Markov bases

- Consequence 1: A move z belongs to every Markov basis if and only if z is indispensable. (This can be taken as a definition now.)
- Consequence 2: The minimal Markov basis is unique if and only if the set of indispensable moves forms a Markov basis.

Minimal Markov bases

- We now consider structure of minimal Markov bases, when they are not unique.
- Let $\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^-$ be a move. The total sample size

$$n = |\boldsymbol{z}^+| = |\boldsymbol{z}^-| = \deg \boldsymbol{z}$$

  is the degree of $\boldsymbol{z}$.
- Let $\boldsymbol{x}$ be a contingency table and $\boldsymbol{z}$ be a move. Consider the case that

$$\boldsymbol{x} + \boldsymbol{z} = (\boldsymbol{x} - \boldsymbol{z}^-) + \boldsymbol{z}^+$$

  does not produce a negative cell ("$\boldsymbol{z}$ is applicable to $\boldsymbol{x}$").

Minimal Markov bases

- This holds if and only if

$$\boldsymbol{x} \geq \boldsymbol{z}^- \qquad \text{(elementwise)}$$

  And in this case $\boldsymbol{x} \neq \boldsymbol{z}^-$ if and only if $|\boldsymbol{x}| > |\boldsymbol{z}^-|$.

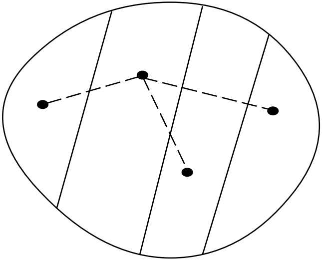
- The key notion: replace a move $\boldsymbol{x} - \boldsymbol{y}$ by a sequence of moves of lower degree.

- Consider a fiber $\mathcal{F}_{\boldsymbol{b}}$ and let n be the sample size of the fiber. Write $\boldsymbol{x} \sim \boldsymbol{y}$ if we can reach $\boldsymbol{y}$ from $\boldsymbol{x}$ by a sequence of moves of degree less than n.

- $\mathcal{F}_{\boldsymbol{b}}$ is partitioned into equivalence classes by the mutual reachability by lower degree moves.

Minimal Markov bases

- If $\mathcal{F}_{\boldsymbol{b}}$ contains more than one equivalence classes, we choose representative elements from each equivalence class and connect them by a tree.
- Moves corresponding to the edges of the tree are elements of a minimal Markov basis.



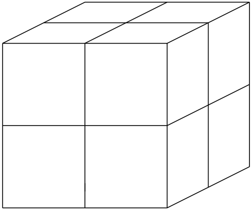
Minimal Markov bases

- $z = z^+ - z^-$ is "non-replaceable by lower degree moves" if z can not be replaced by a sequence moves with degree $< \deg z$ (i.e., we can not go from z^+ to z^- by a sequence of lower degree moves.) (AT2005Bernoulli)
- Conversely $z = z^+ - z^-$ is "redundant" (Ohsugi and Hibi) if it can be replaced by lower degree moves.
- The set of moves not replaceable by lower degree moves is the union of all minimal Markov basis. ("The minimum fiber MB" TA2005Bernoulli)

Indispensable monomials

Indispensable monomial

- An example: independence model of $2 \times 2 \times 2$ three-way table.
- Consider the fiber with all one-dimensional marginals equal to 1.



1	0
0	0

Only one 1 in each two-dimensional slice

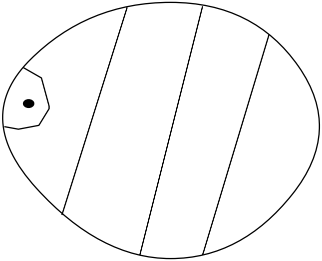
- There are 4 tables in the fiber. Each has two 1's in the "diagonal position".

Indispensable monomial

- It is a 4-element fiber. Therefore differences of the elements are dispensable moves.
- However each table has to be connected to at least one of the other 3 tables by a move.
- Each table has to appear as a monomial (i.e., the positive part or the negative part) of some move. This holds for every Markov basis.
- Definition: x is an indispensable monomial if x appears as a monomial in every Markov basis. (ATY2008JSC).
- Each part of an indispensable move is an indispensable monomial. But not conversely.

Indispensable monomial

- An alternative definition: $\boldsymbol{x} \in \mathcal{F}_{\boldsymbol{b}}$ is an indispensable monomial iff $\{\boldsymbol{x}\}$ is a singleton equivalence class of $\mathcal{F}_{\boldsymbol{b}}$ by the lower degree moves than $|\boldsymbol{x}|$.



- Yet another definition: $\boldsymbol{x}$ is indispensable iff $\{\boldsymbol{x} - \boldsymbol{e}_i\}$ is a one-element fiber for every $i \in \mathrm{supp}(\boldsymbol{x})$, where $\boldsymbol{e}_i = (0, \ldots, 0, 1, \ldots, 0)$ with 1 at the i-th position.

Indispensable monomial

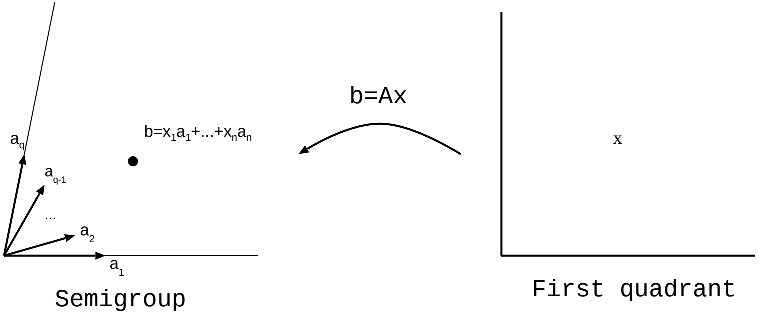
- If there exists $\boldsymbol{u} \neq \boldsymbol{x} - \boldsymbol{e}_i$ such that $A(\boldsymbol{x} - \boldsymbol{e}_i) = A\boldsymbol{u}$, then

$$A\boldsymbol{x} = A(\boldsymbol{u} + \boldsymbol{e}_i)$$

  $\boldsymbol{x}$ and $\boldsymbol{u} + \boldsymbol{e}_i$ has a common support at i and they are different. Therefore $\boldsymbol{x}$ is not a singleton.
- Therefore indispensable monomials are located "just above one-element fibers".

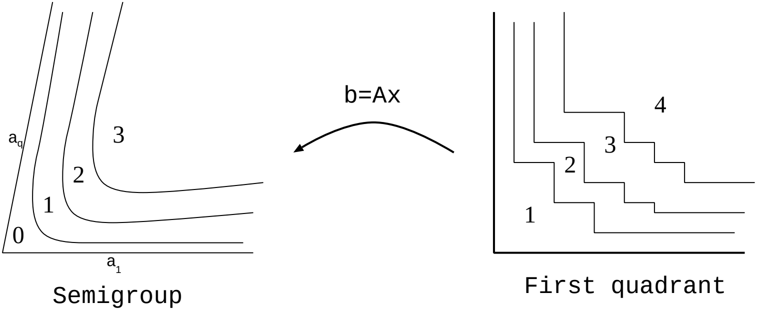
Indispensable monomial

- The first quadrant is mapped to the semigroup generated by the columns of A:



Indispensable monomial

- Zero-element fibers ("holes"), one-element fibers, two-element fibers, . . ., are nested in the semigroup.



Indispensable monomial

- Suppose that $\mathcal{F}_{\boldsymbol{b}} = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_k\}$ is a k-element fiber. Then for each $\boldsymbol{a}_i = A\boldsymbol{e}_i$,

$$\mathcal{F}_{\boldsymbol{b}+\boldsymbol{a}_i} \supset \{\boldsymbol{x}_1 + \boldsymbol{e}_i, \dots, \boldsymbol{x}_k + \boldsymbol{e}_i\}$$

  and $\mathcal{F}_{\boldsymbol{b}+\boldsymbol{a}_i}$ has at least k elements.

- Consider the inverse image of the set of fibers with at least k-elements:

$$M_k = \{\boldsymbol{x} \mid \mathcal{F}_{\boldsymbol{b}} \text{ has at least } k \text{ elements}\}$$

Indispensable monomial

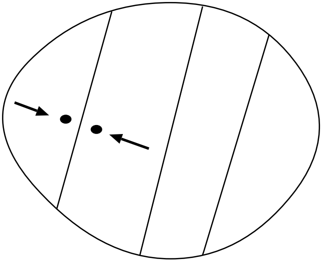
- M_k is a "monomial ideal", i.e. $\boldsymbol{x} \in M_k \Rightarrow \boldsymbol{x} + \boldsymbol{e}_i \in M_k$ for every i.
- Yet another characterization of indispensable monomials is given by Charalambous, Katsabekis and Thoma (2007). Proc. Amer. Math. Soc.

  Indispensable monomials are the minimal elements (generators) of M_2.
- So indispensable monomials are just above one-element fibers.

Distance reduction technique

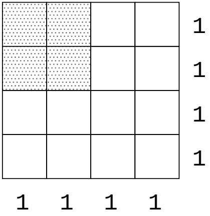
Distance reduction technique

- We have seen that distance reduction technique is useful in deriving a Markov basis.
- Basically it is useful for finding a move which is non-replaceable by lower degree moves.
- We often find closest elements from two equivalence classes:



Distance reduction technique

- In the case of two-way tables, we saw that we can always reduce the distance by a basic move (in one step).
- There is some problem, where a minimal Markov basis does not have this property.
- One example: subtable sum problem (HTY2009JPAA).



Row sums are 1

Column sums are 1

Sum of upper 2x2 cells is 1

Distance reduction technique

- Consider the following two tables in the fiber. We can show that they are connected by basic moves.

a)

1			
		1	
	1		
			1

b)

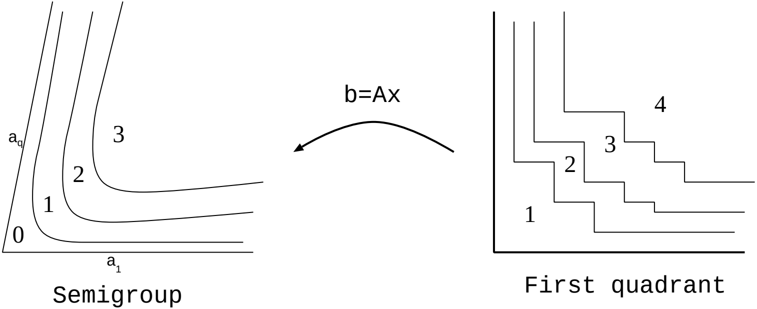
			1
	1		
		1	
1			

- However we can not decrease the distance at this point. We have to go around several states, without decreasing the distance for a while.
- In our recent manuscript on multiple logistic regression (HTYarXiv:0810.1793v1) we found an even harder example, where a fiber is connected, but we have to go "further away" initially.

Normality of semigroups

Normality of semigroups

- We now consider zero-element fibers in the figure



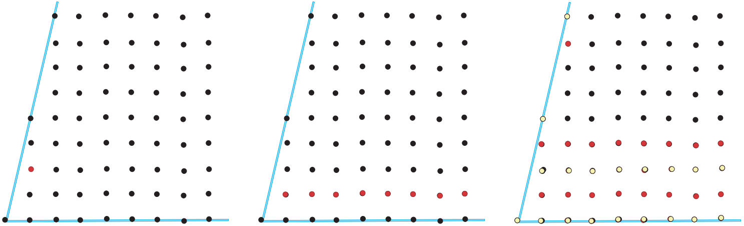
- $Q(A) = A\mathbb{N}^q = \{A\boldsymbol{x} \mid \boldsymbol{x} \geq 0, \text{integral}\}$: the semigroup.

Normality of semigroups

- We call
$$\boldsymbol{b} \in (\mathrm{cone}(A) \cap A\mathbb{Z}^q) \setminus Q(A) \quad \text{a hole.}$$
- $Q(A)$ is "normal" if there is no hole.
- $Q(A)$ is "very ample" if there are only finitely many holes.
- In TY2008DiscOptim we have discussed how to determine whether the number of holes is finite or infinite.

Normality of semigroups

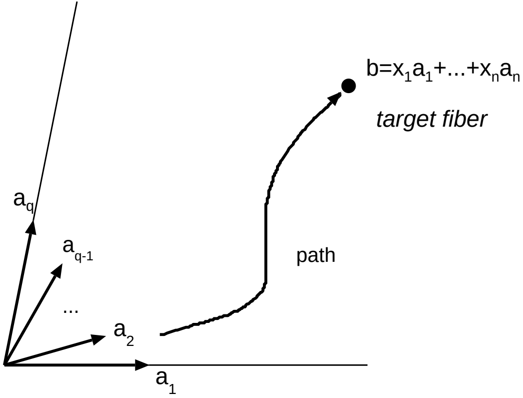
- Simple examples



$$A = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 3 & 4 \end{pmatrix} \quad A = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 2 & 3 & 4 \end{pmatrix} \quad A = \begin{pmatrix} 1 & 1 & 2 & 1 \\ 0 & 2 & 5 & 4 \end{pmatrix}$$

Normality of semigroups

- Why are we interested in holes? $\Leftarrow$ its relation to sequential importance sampling.



Normality of semigroups

- A path corresponds to a contingency table (ignoring the order of sampling).
- In SIS, we start from the origin and try to reach the target fiber.
- With a Markov basis, we subtract z^- and add z^+. Therefore we move very locally around the target fiber.
- These are extreme cases. We can go half the way to the origin and come back again.
- A hole seems to cause a difficulty in SIS: suppose that we are already close to the target fiber. If the target fiber is a hole when looked from the current fiber, then we need to retreat (or simply abandon the path).

Normality of semigroups

Two results by Ohsugi and Hibi on the relation between holes and non-square-free moves.

Result 1. Suppose that $\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^-$ is non-replaceable by lower degree moves and both parts of $\boldsymbol{z}$ are non-square-free:

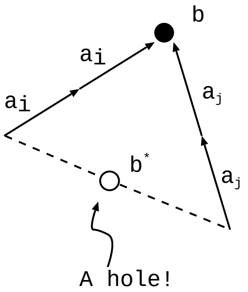
$$\boldsymbol{z}^+ = \boldsymbol{x} + 2\boldsymbol{e}_i, \quad \boldsymbol{z}^- = \boldsymbol{y} + 2\boldsymbol{e}_j$$

Then

$$\boldsymbol{b}^* = A\left(\frac{\boldsymbol{x}+\boldsymbol{y}}{2}\right)$$

is a hole.

Normality of semigroups



Proof.

- Since $\boldsymbol{x}$ and $\boldsymbol{y}$ are non-negative, $\boldsymbol{b}^* = A(\boldsymbol{x}+\boldsymbol{y})/2$ belongs to $\mathrm{cone}(A)$.
- Since $\boldsymbol{b}^* = \boldsymbol{b} - \boldsymbol{a}_i - \boldsymbol{a}_j$, $\boldsymbol{b}^*$ belongs to $A\mathbb{Z}^q$.

Normality of semigroups

- If there exists a non-negative integer vector $\boldsymbol{u}$ such that $\boldsymbol{b}^* = A\boldsymbol{u}$, then $\boldsymbol{w} = \boldsymbol{u} + \boldsymbol{e}_i + \boldsymbol{e}_j \in \mathcal{F}_b$ and

$$\boldsymbol{z} = (\boldsymbol{z}^+ - \boldsymbol{w}) + (\boldsymbol{w} - \boldsymbol{z}^-)$$

- Since $i \in \mathrm{supp}(\boldsymbol{z}^+) \cap \mathrm{supp}(\boldsymbol{w})$ and $j \in \mathrm{supp}(\boldsymbol{z}^-) \cap \mathrm{supp}(\boldsymbol{w})$, the right-hand side is a sum of two moves of degree less than $\deg \boldsymbol{z}$. This is a contradiction. (Q.E.D.)

- In 2003, Aoki found an indispensable (actually a "fundamental") move whose both parts are non-square-free for no-three-factor interaction model of $6 \times 4 \times 3$ tables.

- The above construction gives the well known hole by Vlach (1986).

Normality of semigroups

For the case that $\boldsymbol{z}$ is fundamental, there is a stronger result.
$\boldsymbol{z}^* = \boldsymbol{z}^{*+} - \boldsymbol{z}^{*-}$ is called fundamental if

$$\begin{aligned} &\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^- \text{ is move and } \mathrm{supp}(A\boldsymbol{z}) \subset \mathrm{supp}(A\boldsymbol{z}^*) \\ &\Rightarrow \ \boldsymbol{z} = c\boldsymbol{z}^*, \qquad c : \text{integer}. \end{aligned}$$

Result 2. (Presented in Kyoto December 2008!)
Assume that $\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^-$ is fundamental in Result 1. Then $Q(A)$ is not very ample (i.e. there exist infinitely many holes in $Q(A)$.

Concluding remarks

Concluding remarks

- We discussed indispensable moves and indispensable monomials.
- We presented some cases, where Markov basis is not distance-reducing in one step.
- On normality of semigroups, we showed relations between holes and non-square-free indispensable moves.

Questions:

- Is there an algorithm to obtain representative elements of the equivalence classes by mutual reachability by lower degree moves?
- Are there more relations between holes, finiteness of holes, and moves?

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Thank you for your attention!