Indispensable Monomials of Toric Ideals and Markov Bases

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What is a Markov Basis??

Suppose $P = \{x \in \mathbb{R}^d | Ax = b,\, x \geq 0\} \neq \emptyset$ and let M be a finite set such that $M \subset \{x \in \mathbb{Z}^d | Ax = 0\}$.

We define the graph G_b such that:

- Nodes of G_b are the lattice points inside P.
- We draw an undirected edge between a node u and a node v iff $u - v \in M$.

Definition :

M is called a **Markov basis** if G_b is a connected graph for all b with $P \neq \emptyset$.

Example

				Total
	? ? ?	? ? ?	? ? ?	6
	? ? ?	? ? ?	? ? ?	6
Total	4	4	4	

Table 1: 2×3 tables with 1-marginals.

There are 19 tables with these marginals.

$$\pm \begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \end{pmatrix} \qquad \pm \begin{pmatrix} 0 & 1 & -1 \\ 0 & -1 & 1 \end{pmatrix}$$

$$\pm \begin{pmatrix} 1 & 0 & -1 \\ -1 & 0 & 1 \end{pmatrix}$$

There are 3 elements in a Markov basis modulo signs.

4	0	2
0	4	2

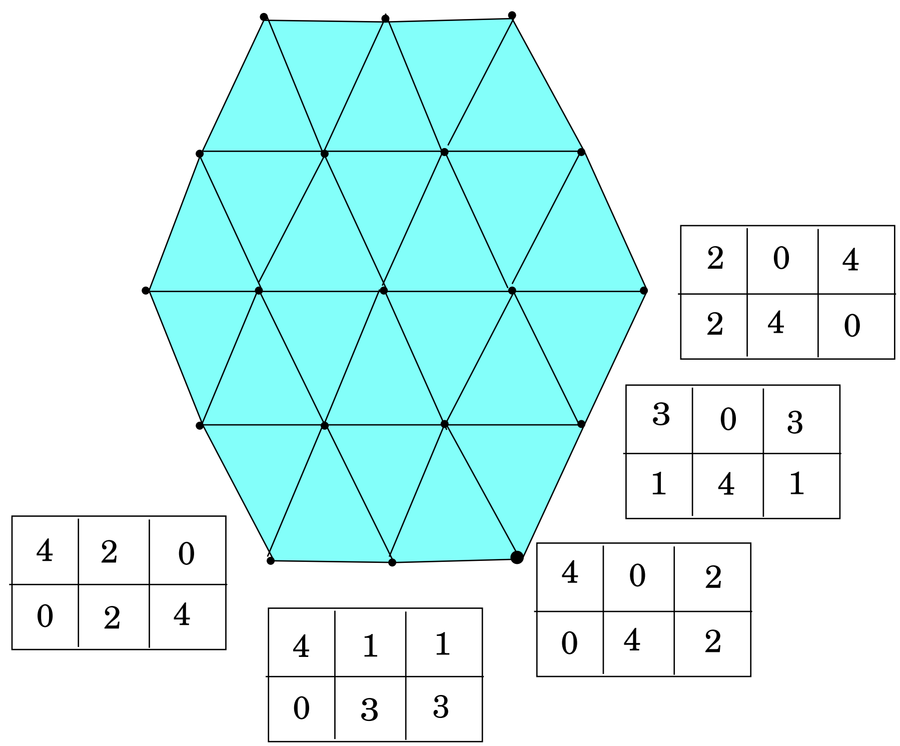
+

-1	0	1
1	0	-1

=

3	0	3
1	4	1

A table with the marginals plus an element of a Markov basis is also a table with the given marginals.



A Markov basis for 2×3 tables. An element of the Markov basis is a undirected edge between integral points in the polytope.

What is a Gröbner basis??

Let $P = \{x \in \mathbb{R}^d : Ax = b, x \geq 0\} \neq \emptyset$, where $A \in \mathbb{Z}^{n \times d}$ and $b \in \mathbb{Z}^n$. Let M be a finite set such that $M \subset \{x \in \mathbb{Z}^d : Ax = 0\}$ and let $\prec$ be any term order on $\mathbb{N}^d$. Then we define the graph G_b such that:

- Nodes of G_b are lattice points inside P.
- Draw a directed edge from a node v to a node u if and only if $u \prec v$ for $u - v \in M$.

If G_b is acyclic and has a unique sink for all b with $P \neq \emptyset$, then M is a **Gröbner basis** for a toric ideal associate with a matrix A with respect to $\prec$.

Note: A Gröbner basis of a toric idea I_A associate to a matrix A with any term order is a Markov basis associate to a matrix A. So one can compute a Markov basis from a Gröbner basis of I_A with any term order.

Note: A minimal Markov basis associate to a matrix A is not unique in general while the minimal Gröbner basis of I_A with the given term order is unique.

Note: The number of elements in a Gröbner basis of I_A is exponentially in term of the number of indeterminates.

Problem: Want to decide whether a minimal Markov basis associate to A is unique or not and if it is unique, want to find some alternative way to find elements in the minimal Markov basis.

A key element to solve this problem is to study **indispensable** moves in a Markov basis.

Indispensable Moves

Definition: A **fiber** of b, $\mathcal{F}_b$, is the preimage of the linear map $f_A : Z_+^d \to Z^n$, $x \mapsto b = Ax$.

Definition: A move $z = z^+ - z^-$ is called **indispensable** if z^+ and z^- constitute a two-element fiber, i.e., the fiber $\mathcal{F}_{Az^+} (= \mathcal{F}_{Az^-})$ is written as $\mathcal{F}_{Az^+} = \{z^+, z^-\}$.

Example: All moves in the minimal Markov basis for 2×3 tables are indispensable moves.

Definition: A binomial $u^z = u^{z^+} - u^{z^-}$ is **indispensable** if every system of binomial generators of I_A contains u^z or $-u^z$.

Note: A binomial u^z is indispensable if and only if a move z is indispensable.

Background

Theorem [Takemura and Aoki (2004)]:

The unique minimal Markov basis exists if and only if the set of indispensable moves forms a Markov basis. In this case, the set of indispensable moves is the unique minimal Markov basis.

Theorem [Ohsugi and Hibi (2005)]:

A binomial u^z is indispensable if and only if either u^z or $-u^z$ belongs to the reduced Gröbner basis of I_A for any lexicographical term order on $k[u]$.

Note: The set of indispensable binomials is characterized as the intersection of binomials in reduced Gröbner bases with respect to any lexicographical term orders.

Indispensable Monomials

Definition: A monomial u^x is **indispensable** if every system of binomial generators of I_A contains a binomial f such that u^x is a term of f.

Note: Both terms of an indispensable binomial $u^{z^+} - u^{z^-}$ are indispensable monomials, but the converse does not hold in general.

We want to study indispensable monomials so that we might be able to enumerate all moves in the minimal Markov basis if it is unique (or one can determine it is not unique).

First we mimic Ohsugi and Hibi's Theorem in term of indispensable monomials.

Theorem [Aoki, Takemura, and Y. (2005)]:

Let $<_{\text{lex}}$ be any lexicographic $<_{\text{lex}}$. A monomial u^x is indispensable if the reduced Gröbner basis with respect to $<_{\text{lex}}$ contains u^x.

Note: We can characterize the set of indispensable monomials as the intersection of monomials in reduced Gröbner bases with respect to all the lexicographical term orders.

Question: Is there a way to enumerate all indispensable monomials without computing reduced Gröbner bases with respect to all the lexicographical term orders?

Minimal Multi-element

Definition: x is a **minimal multi-element** if $|\mathcal{F}_{Ax}| \geq 2$ and $|\mathcal{F}_{A(x-e_i)}| = 1$ for every $i \in \mathrm{supp}(x)$.

Definition: x is a **minimal i-lacking 1-element** if $|\mathcal{F}_{Ax}| = 1$, $|\mathcal{F}_{A(x+e_i)}| \geq 2$ and $|\mathcal{F}_{A(x+e_i-e_j)}| = 1$ for each $j \in \mathrm{supp}(x)$.

Lemma [Aoki, Takemura, and Y. (2005)]:

u^x is an indispensable monomial if and only if x is a minimal multi-element.

We will study indispensable monomials using minimal multi-elements and minimal i-lacking 1-elements.

Main Theorem

Theorem [Aoki, Takemura, and Y. (2005)]:

The following three conditions are equivalent:

1. u^x is an indispensable monomial,
2. for each $i \in \mathrm{supp}(x)$, $x - e_i$ is a minimal i-lacking 1-element,
3. for some $i \in \mathrm{supp}(x)$, $x - e_i$ is a minimal i-lacking 1-element.

Computing Indispensable Monomials

Note: Let $\mathcal{M} = (m+1)(d-m)D(A)$, where $D(A)$ is the absolute value of the biggest $m \times m$ subdeterminant. Each of the exponents of an element in reduced Gröbner bases is bounded by $\mathcal{M}$ (Sturmfels, (1994)).

Using the main theorem, one can compute indispensable monomials as:

Step 1: Find any 1-element x. Randomly choose $1 \leq i \leq d$ and check whether $x + e_i$ remains to be a 1-element.

Step 2: Once $|\mathcal{F}_{A(x+e_i)}| \geq 2$, then subtract e_j's, $j \neq i$, one by one from x check whether it becomes a minimal i-lacking 1-element.

Step 3: We stop the procedure if an exponent of a monomial becomes $\mathcal{M}$.

$2 \times 2 \times 2$ **Tables**

We will illustrate computing indispensable monomials with an example of a $2 \times 2 \times 2$ contingency table with 2-marginals.

Consider the following matrix A given as:

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \end{pmatrix} .$$

We start with the monomial $u^x = u_{111}$ and consider $x + e_i, i \in \mathcal{I}$. Then we have:

- $u_{111}^2, u_{111}u_{112}, u_{111}u_{121}, u_{111}u_{211}$ are 1-elements,
- $u_{111}u_{122}, u_{111}u_{212}, u_{111}u_{221}$ are 2-elements and
- $u_{111}u_{222}$ is a 4-element.

We found four indispensable monomials, $u_{111}u_{122}, u_{111}u_{212}, u_{111}u_{221}$ and $u_{111}u_{222}$, since each of $u_{122}, u_{212}, u_{221}, u_{222}$ is a 1-element.

Similarly, we can find the following list of indispensable monomials,

- $u_{111}u_{122}, u_{111}u_{212}, u_{111}u_{221}, u_{112}u_{121}, u_{112}u_{211}, u_{112}u_{222}, u_{121}u_{222}, u_{121}u_{211}, u_{122}u_{221}, u_{122}u_{212}, u_{211}u_{222}, u_{212}u_{221}$, each of which is a 2-element monomial, and
- $u_{111}u_{222}, u_{112}u_{221}, u_{121}u_{212}, u_{122}u_{211}$, each of which is a 4-element monomial.

Consider the newly produced 1-element monomials, $u_{111}^2, u_{111}u_{112}, u_{111}u_{121}, u_{111}u_{211}$ etc. and consider adding $e_i, i \in \mathcal{I}$ one by one, checking whether they are multi-element or not.

To find all the indispensable monomials for this problem, we have to repeat the above procedure for monomials of degree $4, 5, \ldots$.

Note: This procedure never stops since there are infinite 1-element monomials, such as

$$u_{111}^{n},\ u_{111}^{n}u_{112}^{m}, \ldots$$

for arbitrary n, m.

Thus we will stop when one of exponents of a monomial becomes bigger than $\mathcal{M}$.

Future Work

- We would like to have a nice system to compute all 1-elements using generating functions.
- We would like to have a nice system to compute all minimal multi-elements using generating functions.
- We would like to have a nice system to compute all minimal i-lacking 1-elements using generating functions.
- We are currently investigating the semi-group of A and the saturation of the semi-group to see if there is anyway to compute minimal i-lacking 1-elements from them.

Questions??

Thank you....

The paper is available at arXiv:math.ST/0511290.