## Markov bases of lattice ideals

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Applications to algebraic statistics

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## Lattice ideals

Let  $L \subset \mathbb{Z}^n$  be a lattice. The lattice ideal  $I_L \subset K[x_1, \ldots, x_n]$  is

$$I_L := \langle \mathbf{x}^{\mathbf{u}} - \mathbf{x}^{\mathbf{v}} : \mathbf{u} - \mathbf{v} \in L \rangle = \langle \mathbf{x}^{\mathbf{w}^+} - \mathbf{x}^{\mathbf{w}^-} : \mathbf{w} \in L \rangle$$

#### Definition

If *L* is such that  $L \cap \mathbb{N}^n = \{\mathbf{0}\}$  (repectively  $L \cap \mathbb{N}^n \neq \{\mathbf{0}\}$ ) we say that *L* is *positively graded* (*not positively graded*). Let *L*<sub>pure</sub> be the sublattice of *L* generated by  $L \cap \mathbb{N}^n$ .

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# Minimal generating sets of lattice ideals

#### Definition

A set *S* is a Markov basis for  $I_L$  if *S* consists of binomials and *S* is a minimal generating set of  $I_L$  of minimal cardinality.

For counting purposes, a binomial B is the same as -B.

- How many "different" Markov bases are there?
- Can we compute the cardinality of a Markov basis?
- Can we compute all Markov bases?
- Is there a characteristic shared by different Markov bases?

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## Degrees and fibers

Let  $\mathcal{A}$  be the subsemigroup of  $\mathbb{Z}^n/L$  generated by the elements  $\{\mathbf{a}_i = \mathbf{e}_i + L : 1 \le i \le n\}$ , where  $\{\mathbf{e}_i : 1 \le i \le n\}$  is the canonical basis of  $\mathbb{Z}^n$  and set

$$\deg_{\mathcal{A}}(\mathbf{x}^{\mathbf{v}}) := v_1 \mathbf{a}_1 + \cdots + v_n \mathbf{a}_n \in \mathcal{A}$$

where  $\mathbf{x}^{\mathbf{v}} = x_1^{v_1} \cdots x_n^{v_n}$ . It follows that

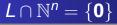
$$\textit{I}_{\textit{L}} = \langle \textbf{x}^{\textbf{u}} - \textbf{x}^{\textbf{v}} : \; \textsf{deg}_{\mathcal{A}}(\textbf{x}^{\textbf{u}}) = \textsf{deg}_{\mathcal{A}}(\textbf{x}^{\textbf{v}}) \; \rangle$$

and that  $I_L$  is  $\mathcal{A}$ -graded.

#### Definition

Let  $\text{deg}_{\mathcal{A}}(\mathbf{x}^u) = \mathbf{b}$ . The fiber of u is the following set of monomials:

$$\mathcal{F}_{\mathbf{x}^{\mathbf{u}}} = \deg_{\mathcal{A}}^{-1}(\mathbf{b}) = \{\mathbf{x}^{\mathbf{w}} \mid \deg_{\mathcal{A}}(\mathbf{x}^{\mathbf{w}}) = \mathbf{b}\} = \{\mathbf{x}^{\mathbf{w}} : \mathbf{x}^{\mathbf{u}} - \mathbf{x}^{\mathbf{w}} \in I_{L}\}$$



• The semigroup  $\mathcal{A}$  is partially ordered:

 $\textbf{c} \geq \textbf{d} \Longleftrightarrow \ \text{there is } \textbf{e} \in \mathcal{A} \ \text{such that } \textbf{c} = \textbf{d} + \textbf{e} \ .$ 

- The A-grading of  $I_L$  forces every  $I_L$ -fiber to be finite.
- The fibers can be partially ordered by deg<sub>A</sub>.
- (the graded Nakayama Lemma "works") All minimal binomial generating sets of *I<sub>L</sub>* have the same cardinality and the same *A*-degrees.

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## Generating $I_L$ when $L \cap \mathbb{N}^n = 0$ (CKT 2007)

For every degree  $\mathbf{b} \in \mathcal{A}$  define a subideal of  $I_L$  generated by the binomials that have  $\mathcal{A}$ -degrees **less** than **b**.

Definition

$$\textit{I}_{\textit{L},<\textit{b}} = \textit{I}_{\textit{L},<\textit{F}} = (\textit{\textbf{x}}^{\textit{u}} - \textit{\textbf{x}}^{\textit{v}} \mid \textit{deg}_{\mathcal{A}}(\textit{\textbf{x}}^{\textit{u}}) = \textit{deg}_{\mathcal{A}}(\textit{\textbf{x}}^{\textit{v}}) \gneqq \textit{b}) \subset \textit{I}_{\textit{L}}$$

where *F* is the fiber at **b**.

Then we define two graphs.

#### Definition

First graph Let  $G(\mathbf{b})$  be the graph with vertices the elements of the fiber  $F = \deg_{\mathcal{A}}^{-1}(\mathbf{b})$  and edges all the sets  $\{\mathbf{x}^{\mathbf{u}}, \mathbf{x}^{\mathbf{v}}\}$  whenever  $\mathbf{x}^{\mathbf{u}} - \mathbf{x}^{\mathbf{v}} \in I_{L,<\mathbf{b}}$ .

## Generating $I_L$ when $L \cap \mathbb{N}^n = 0$ (CKT 2007)

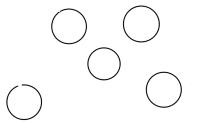
## Definition

The <u>Second graph</u> is the complete graph with vertex set the connected components of first graph  $G(\mathbf{b})$ . Let  $T_{\mathbf{b}}$  be a spanning tree of this graph.

For every edge of the tree  $T_{\mathbf{b}}$  joining two components of  $G(\mathbf{b})$  take one binomial by considering the difference of (two arbitrary) monomials, one from each component. For every **b**, choose a tree  $T_{\mathbf{b}}$  on the graph  $G(\mathbf{b})$  (whose vertices are the connected components of the fiber at **b**) and then choose the binomials. Denote this collection by  $\mathcal{F}_{T_{\mathbf{b}}}$ .

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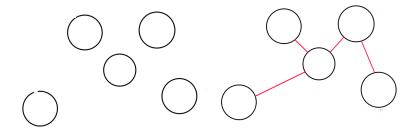
## Picture



Marius Vladoiu Markov bases of lattice ideals

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## Picture

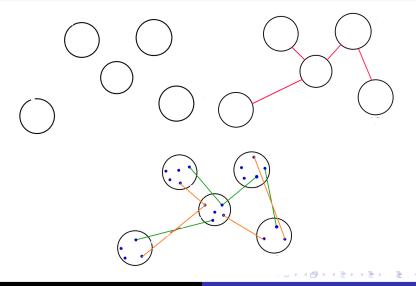


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## Picture



# Generating $I_L$ when $L \cap \mathbb{N}^n = 0$ (CKT 2007)

#### Theorem

The set  $\mathcal{F} = \cup_{\mathbf{b} \in \mathcal{A}} \mathcal{F}_{T_{\mathbf{b}}}$  is a Markov basis of  $I_L$ .

Let  $\mu(I_L)$  be the cardinality of a Markov basis,  $n_{\mathbf{b}}$  the number of connected components of  $G(\mathbf{b})$ , and  $t_i(\mathbf{b})$  the number of vertices of the *i*th component.

#### Theorem

$$\mu(I_L) = \sum_{\mathbf{b} \in \mathcal{A}} (n_{\mathbf{b}} - 1).$$

#### Theorem

The number of different Markov bases of IL is finite and equal to

$$\prod_{\mathbf{b}\in A} t_1(\mathbf{b})\cdots t_{n_{\mathbf{b}}}(\mathbf{b})(t_1(\mathbf{b})+\cdots+t_{n_{\mathbf{b}}}(\mathbf{b}))^{n_{\mathbf{b}}-2}$$

# $L \cap \mathbb{N}^n \neq \{\mathbf{0}\} \text{ (CTV1)}$

## Bad News!

• all fibers are infinite.

• there is no partial order between the fibers.

## But

We can consider equivalence classes of fibers under the following equivalence relation:

#### Definition

 $F \equiv_L G \Leftrightarrow (\exists) \mathbf{x}^{\mathbf{u}}, \mathbf{x}^{\mathbf{v}}$  monomials s.t.  $\mathbf{x}^{\mathbf{u}} F \subset G$  and  $\mathbf{x}^{\mathbf{v}} G \subset F$ .

and order the equivalence classes

#### Definition

Let  $\overline{F}$ ,  $\overline{G}$  be two equivalence classes of  $I_L$ -fibers. We say that  $\overline{F} \leq_{I_l} \overline{G}$  if there exists  $\mathbf{x}^{\mathbf{u}}$  such that  $\mathbf{x}^{\mathbf{u}} F \subset G$ .

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# $L \cap \mathbb{N}^n \neq \{\mathbf{0}\} \text{ (CTV1)}$

Note that:

1)  $L_{pure} = \{\mathbf{0}\}$  implies  $\overline{F} = \{F\}$ , and the order on the equivalence classes of fibers agrees with the degree-ordering of the fibers.

2) The cardinality of  $\overline{F}$  is fixed and is determined by  $L_{pure}$ .

3) The Noetherian property of the ring guarantees that all chains of equivalence classes of fibers have a minimal element.

#### Definition

$$\begin{split} I_{L,<\overline{F}} &= (\mathbf{x}^{\mathbf{u}} - \mathbf{x}^{\mathbf{v}} \mid \mathbf{x}^{\mathbf{u}}, \mathbf{x}^{\mathbf{v}} \in G, \overline{G} < \overline{F}) \subset I_L. \\ I_{L,<\overline{F}} &= (\mathbf{x}^{\mathbf{u}} - \mathbf{x}^{\mathbf{v}} \mid \mathbf{x}^{\mathbf{u}}, \mathbf{x}^{\mathbf{v}} \in G, \overline{G} \leq \overline{F}) \subset I_L. \end{split}$$

# $L \cap \mathbb{N}^n \neq \{\mathbf{0}\} \text{ (CTV1)}$

Recall 
$$L_{pure}$$
! Denote  $\sigma = \operatorname{supp}(L_{pure})$ , and  $\mathbf{u}^{\sigma} = (u_i)_{i \notin \sigma}$ .

## Definition

First graph Let  $G(\overline{F})$  be the graph with vertices the elements of  $G(M_F)^{\sigma}$ . The edges of  $G(\overline{F})$  correspond to binomials of  $I_{L < \overline{F}}$ .

Next consider the connected components of  $G(\overline{F})$ : these are the vertices of the second graph.

#### Definition

Second graph: The complete graph on the components of  $G(\overline{F})$ . We call this graph  $\Gamma(\overline{F})$ .

Consider, as before, spanning trees of  $\Gamma(\overline{F})$ .

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## **True Generalization**

- If  $L \cap \mathbb{N}^n = \{0\}$  then
  - $\sigma = \{\}$
  - $\overline{F} = \{F\}$
  - $G(M_F)$  is equal to F

•  $I_{L,<\overline{F}} = I_{L,<\mathbf{b}}$  where **b** is the  $\mathcal{A}$ -degree of any element in *F*. Thus we obtain the same graphs.

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## Markov bases of pure lattice ideals

#### Theorem

(CTV1)  $B = \mathbf{x}^{\mathbf{u}} - \mathbf{x}^{\mathbf{v}}$  belongs to a Markov basis of  $I_L$  if and only if B is not in  $I_{L,<\overline{F_{\mathbf{x}\mathbf{u}}}}$ .

#### Theorem

(ES95)  $I_{L_{pure}}$  is a complete intersection, generated minimally by rank( $L_{pure}$ ) elements.

We complete this theorem by giving a description of all generating sets of  $I_{L_{pure}}$  in terms of the exponents of the binomials.

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# Markov Bases of $I_L$ (CTV1)

#### Theorem

A set S of binomials of  $I_L$  is a Markov basis of  $I_L$  if and only if

- for every *F* the elements of S determine a spanning tree of Γ(*F*) and
- the binomials of S in the equivalence class of the fiber F<sub>x<sup>0</sup></sub> minimally generate the lattice generated by L ∩ N<sup>n</sup>.

What are the invariants of the Markov bases of  $I_L$ ?

#### Theorem

Let  $S = \{B_1, ..., B_s\}$  be a Markov basis of  $I_L$ . The equivalence classes of fibers that correspond to these binomials and their multiplicity in S are uniquely determined and are invariants of  $I_L$ .

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# Markov Bases of $I_L$ (CTV1)

## What can we compute?

We can compute the cardinality of a Markov basis, the Markov fibers, the indispensable fibers, the indispensable binomials, and the indispensable monomials.

#### Theorem

$$\mu(I_L) = r + \sum_{\overline{F} \neq \overline{F}_{\{1\}}} (t(\overline{F}) - 1),$$

where  $\mu(I_L)$  is the cardinality of a Markov basis, r is the rank of  $L_{pure}$ , and  $t(\overline{F})$  is the number of vertices of  $\Gamma_{\overline{F}}$ .

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# **Binomial Complete Intersection**

#### Definition

Let *L* be a lattice of rank *r*. The lattice ideal  $I_L$  is called a binomial complete intersection if there exist binomials  $B_1, \ldots, B_r$  such that  $I_L = \langle B_1, \ldots, B_r \rangle$ .

If  $L \cap \mathbb{N}^n = \{\mathbf{0}\}$  then complete intersection lattice ideals are automatically binomial complete intersections.

When is the lattice ideal a complete intersection ideal? The problem is completely solved when *L* is positively graded by a series of articles: Herzog (70), Delorne(76), Stanley (77), Ishida (78), Watanabe(80), Nakajima(85), Schafer (85), Rosales and Garcia-Sanchez (95), Fischer, Morris and Shapiro (95), Scheja, Scheja and Storch (99), Morales and Thoma (05).

# Mixed dominating matrices

The final conclusion of this series of articles is that  $I_L$  is a complete intersection if and only if the matrix M whose rows correspond to a basis of L is **mixed dominating**.

## Definition

A matrix M is mixed dominating if every row of M has a positive and negative entry and M contains no square submatrix with this property.

#### Example

$$\begin{bmatrix} 1 & -1 & 0 \\ 6 & 0 & -1 \end{bmatrix}$$

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# Complete intersections and mixed dominating matrices in the general case

We now consider arbitrary sublattices *L* of  $\mathbb{Z}^n$ . In (CTV1) we showed that the rank *L* is determined by the rank of  $L^{\sigma}$  (which is a positively graded lattice) and the rank of  $L_{pure}$ . Here  $L^{\sigma}$  is the sublattice of  $(\mathbb{Z}^n)^{\sigma}$  generated by the vectors  $\mathbf{u}^{\sigma}$ .

#### Theorem

$$\operatorname{rank}(L) = \operatorname{rank}(L^{\sigma}) + \operatorname{rank}(L_{pure}).$$

#### Theorem

(CTV1) Let  $L \subset \mathbb{Z}^n$  be a lattice. The ideal  $I_L$  is binomial complete intersection if and only if there exists a basis of  $L^{\sigma}$  so that its vectors give the rows of a mixed dominating matrix.

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## Universal Gröbner basis and Graver basis

Let *A* be a matrix in  $\mathbb{Z}^{m \times n}$ . The toric ideal  $I_A$  is the lattice ideal  $I_{L(A)}$ , where  $L(A) = \ker_{\mathbb{Z}}(A)$ . We assume that  $L(A) \cap \mathbb{N}^n = \{\mathbf{0}\}$ .

#### Theorem

(St 95) For any toric ideal  $I_A$  the following containments hold:

Universal Gröbner basis of A  $\subset$  Graver basis of A

What is the relation between the universal Gröbner basis of *A* and the universal Markov basis of *A*? What is the relation between the universal Markov basis of *A* and the Graver basis of *A*?

#### Example

Let  $I = (x_1x_2 - x_3x_4, x_5x_6 - x_7x_8, x_1^2x_2^2x_3x_4 - x_5x_6x_7x_8)$ . This generating set is not part of any reduced Gröbner basis of *I*.

## Example

Let

It can be shown that

$$I_{A} = (x_{1}x_{2} - x_{3}x_{4}, x_{5}x_{6} - x_{7}x_{8}, x_{1}^{2}x_{2}^{2}x_{3}x_{4} - x_{5}x_{6}x_{7}x_{8}).$$

The binomial  $x_1^2 x_2^2 x_3 x_4 - x_5 x_6 x_7 x_8$  does not belong to a reduced Gröbner basis of  $I_A$  since for any monomial order, the initial term of  $x_1 x_2 - x_3 x_4$  divides  $x_1^2 x_2^2 x_3 x_4$  while the initial term of  $x_5 x_6 - x_7 x_8$  divides  $x_5 x_6 x_7 x_8$ .

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## Markov Polytopes

#### Theorem

(CKT07, DSS09) **u** is in the universal Markov basis of A if and only if  $\mathbf{u}^+$  and  $\mathbf{u}^-$  belong to different connected components of  $G_{\mathbf{u}}$ .

We consider the convex hulls of the connected components of  $G_{u}$ .

## Definition

(CTV2) A Markov polytope is the convex hull of the elements in a connected component of this graph.

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## Universal Markov and universal Gröbner basis

#### Theorem

(StWeZi 95)  $\mathbf{u} \in L$  is in the universal Gröbner basis of A if  $\mathbf{u}$  is in the Graver basis of A and  $[\mathbf{u}^+, \mathbf{u}^-]$  is an edge of the convex hull of all points in  $\mathcal{F}_u$ .

We get the following characterization:

#### Theorem

(CTV2) An element **u** of the universal Markov basis of A belongs to the universal Gröbner basis of A if and only if  $\mathbf{u}^+$  and  $\mathbf{u}^-$  are vertices of two different (Markov) polytopes.

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# Example of Markov polytope

## Example

Let *A* be the matrix of the previous example. Recall that  $x_1^2 x_2^2 x_3 x_4 - x_5 x_6 x_7 x_8$  is in the universal Markov basis of  $I_A$  but not in the universal Gröbner basis of  $I_A$ . Let  $\mathbf{u} = (2, 2, 1, 1, -1, -1, -1, -1) \in L$ . Then  $|\mathcal{F}_{\mathbf{u}}| = 7$  and  $\mathcal{F}_{\mathbf{u}} =$  $\{(3, 3, 0, ..., 0), u^+, (1, 1, 2, 2, 0, 0, 0, 0), (0, 0, 3, 3, 0, 0, 0, 0)\}$ 

 $\cup \{(0,\ldots,0,2,2,0,0), u^-, (0,\ldots,0,2,2)\}$ 

The graph  $G_u$  has two connected components.

The Markov polytopes are line segments:  $\mathbf{u}^+$  and  $\mathbf{u}^-$  are not vertices of their Markov polytopes.

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## Universal Markov basis for positive toric ideals

Consider the toric ideal  $I_A$  such that  $L(A) \cap \mathbb{N}^n = \{\mathbf{0}\}$ . We have the following inclusions:

 $\mathcal{S}(I_A) \subseteq \mathcal{M}(I_A) \subseteq \mathcal{G}(I_A).$ 

- (St95): G(I<sub>A</sub>) is the subset of L(A) whose elements have no proper conformal decomposition.
- (HS2005+CTV3):  $S(I_A)$  is the subset of L(A) whose elements have no proper semiconformal decomposition.
- (CTV3): *M*(*I<sub>A</sub>*) is the subset of *L*(*A*) whose elements have no proper strongly semiconformal decomposition.

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Markov complexity m(A)

Let A be an arbitrary integer matrix.

- Santos, Sturmfels 2003: g(A) is equal to the maximum
   1-norm of an element in G(G(A)). Thus g(A) is finite.
- Santos, Sturmfels 2003:  $m(A) \leq g(A)$ .
- Hoşten, Sullivant 2005: m(A) ≥ the maximum 1-norm of any element in G(S(A)).

How to compute m(A) in general?

So far a mystery!!!

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# Markov complexity for monomial curves in $\mathbb{A}^3$

#### Theorem

(CTV3) Let  $A = \{n_1, n_2, n_3\}$  be a set of positive integers with  $gcd(n_1, n_2, n_3) = 1$ . Then m(A) = 2 if A is complete intersection, and m(A) = 3 if A is not complete intersection. Moreover, for any  $r \ge 2$  we have  $\mathcal{M}(A^{(r)}) = \mathcal{S}(A^{(r)})$ 

#### Theorem

(CTV3) Let  $A = \{n_1, n_2, n_3\}$  such that  $gcd(n_1, n_2, n_3) = 1$  and  $d_{ij} = gcd(n_i, n_j)$  for all  $i \neq j$ . Then

$$g(A) \geq rac{n_1}{d_{12}d_{13}} + rac{n_2}{d_{12}d_{23}} + rac{n_3}{d_{13}d_{23}}$$

In particular, if  $n_1, n_2, n_3$  are pairwise prime then  $g(A) \ge n_1 + n_2 + n_3$ .

## Examples

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(a) Let A = {3,4,5}. Computations with 4ti2 show that the maximum 1-norm of the elements of G(G(A)) is 12 = 3 + 4 + 5 and thus g(A) equals the the lower bound of the theorem.
(b) Let A = {2,3,17}. Computations with 4ti2 show that the maximum 1-norm of the elements of G(G(A)) is 30 and thus g(A) = 30, while the lower bound of the theorem is 22 = 2 + 3 + 17.

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