Gröbner bases of toric ideals and their application

Hidefumi Ohsugi

Kwansei Gakuin University

ISSAC 2014 tutorial, Kobe, July 22, 2014

Contents

Part I. Introduction to Gröbner bases

Gröbner bases

Part II. Gröbner bases of toric ideals

- 2 Toric ideals
- Application to integer programming
- Application to triangulations of convex polytopes
- Application to contingency tables (statistics)
- Quadratic Gröbner bases (if possible)

Gröbner bases and toric ideals

Gröbner bases

- A "very good" set of polynomials
- keyword: division of a polynomial (by several polynomials in n variables.)
- invented by B. Buchberger in 1965.
 ("standard bases" H. Hironaka in 1964.)
- Elimination Theorem for systems of polynomial equations
- implemented in a lot of mathematical software

 Mathematica, Maple,

 Macauley2, Singular, CoCoA, Risa/Asir,

Gröbner bases and toric ideals

Toric ideals

- Prime ideals generated by binomials
- Gröbner bases of toric ideals have a lot of application
 - commutative algebra, algebraic geometry
 - triangulations of convex polytopes
 - integer programming
 - contingency tables (statistics)
 - <u>. . . .</u>

System of linear equations

Example

$$\begin{cases}
f_1 = x_1 + x_3 + 3x_4 = 0 \\
f_2 = x_2 - x_3 - 2x_4 = 0 \\
f_3 = 2x_1 + 3x_2 - x_3 = 0
\end{cases}$$

$$\left(\begin{array}{cccc} 1 & 0 & 1 & 3 \\ 0 & 1 & -1 & 2 \\ 2 & 3 & -1 & 0 \end{array}\right) \rightarrow \left(\begin{array}{cccc} 1 & 0 & 1 & 3 \\ 0 & 1 & -1 & 2 \\ 0 & 3 & -3 & -6 \end{array}\right) \rightarrow \left(\begin{array}{cccc} 1 & 0 & 1 & 3 \\ 0 & 1 & -1 & 2 \\ 0 & 0 & 0 & 0 \end{array}\right)$$

$$f_3 = 2f_1 + 3f_2$$
.

Division?

Gröbner bases

$$\begin{array}{c|c} x & +1 \\ \hline) & x^2 \\ \hline & x^2 & -x \\ \hline & & x \\ \hline & & x & -1 \\ \hline & & 1 \end{array}$$

For example, which monomial in

$$f = x_1^2 + 2x_1x_2x_3 - 3x_1 + x_3^5 + 5$$

shoud be the largest?

Definition

Gröbner bases

 \mathcal{M}_n : set of all monomials in the variables x_1, \ldots, x_n A total order < on \mathcal{M}_n is called a monomial order

if < satisfies the following:

Lexicographic order

Example (Lexicographic order $(x_1 > \cdots > x_n)$)

$$x_1^{a_1} x_2^{a_2} \cdots x_n^{a_n} >_{\text{lex}} x_1^{b_1} x_2^{b_2} \cdots x_n^{b_n} \overset{\text{def}}{\Longrightarrow}$$
 $a_1 > b_1$
or
 $a_1 = b_1 \text{ and } a_2 > b_2$
or
 $a_1 = b_1, a_2 = b_2, \text{ and } a_3 > b_3$
or
 \vdots

For example,

$$X_1 >_{\text{lex}} X_2^{100} X_3$$

 $X_1^2 X_2^2 X_5 >_{\text{lex}} X_1^2 X_2 X_3 X_4$

(Degree) Reverse lexicographic order

Example (Reverse lexicographic order $(x_1 > \cdots > x_n)$)

$$x_1^{a_1} x_2^{a_2} \cdots x_n^{a_n} >_{\text{revlex}} x_1^{b_1} x_2^{b_2} \cdots x_n^{b_n} \stackrel{\text{def}}{\Longleftrightarrow}$$

$$\sum_{i=1}^n a_i > \sum_{i=1}^n b_i \quad \text{or}$$

$$\sum_{i=1}^n a_i = \sum_{i=1}^n b_i \quad \text{and} \quad a_n < b_n \quad \text{or}$$

$$\sum_{i=1}^n a_i = \sum_{i=1}^n b_i, \quad a_n = b_n \quad \text{and} \quad a_{n-1} < b_{n-1}$$

$$\vdots$$

For example,

$$X_1 <_{\text{revlex}} X_2^{100} X_3$$

 $X_1^2 X_2^2 X_5 <_{\text{revlex}} X_1^2 X_2 X_3 X_4$

Weight order

Gröbner bases

Example (Weight order $>_{\mathbf{w}}$)

$$\mathbf{w} = (w_1, w_2, \dots, w_n) \in \mathbb{R}^n_{>0}$$

<: a monomial order (for "tie break")

$$X_1^{a_1}X_2^{a_2}\cdots X_n^{a_n}>_{\mathbf{W}} X_1^{b_1}X_2^{b_2}\cdots X_n^{b_n} \stackrel{\mathrm{def}}{\Longleftrightarrow}$$

$$\sum_{i=1}^n a_i w_i > \sum_{i=1}^n b_i w_i$$

$$\sum_{i=1}^n a_i w_i = \sum_{i=1}^n b_i w_i \text{ and } x_1^{a_1} x_2^{a_2} \cdots x_n^{a_n} > x_1^{b_1} x_2^{b_2} \cdots x_n^{b_n}$$

Remark

Gröbner bases

If n=1, then a monomial order is unique.

In fact, if < is a monomial order on monomials in x_1 , then

$$x_1 > 1 \Longrightarrow x_1^2 > x_1 \Longrightarrow x_1^3 > x_1^2 \Longrightarrow x_1^4 > x_1^3 \Longrightarrow \cdots$$

Hence, we have

$$1 < x_1 < x_1^2 < x_1^3 < \cdots$$

If n > 2, then there exist infinitely many monomial orders.

 $K[x_1,\ldots,x_n]$: polynomial ring over a field K (e.g., $K=\mathbb{C}$)

• The set of all polynomials in variables x_1, \ldots, x_n with coefficients in K.

Fix a monomial order < on $K[x_1, \ldots, x_n]$.

$$0 \neq f \in K[x_1, \ldots, x_n]$$

 $in_{<}(f)$: the largest monomial among the monomials in f the initial monomial of f

Example

 $>_{lex}$: lexicographic order $(x_1 > \cdots > x_5)$

 $>_{\text{revlex}}$: reverse lexicographic order ($x_1 > \cdots > x_5$)

$$f = x_1^2 + 2x_1x_2x_3 - 3x_1 + x_3^5 + 5$$

Then, $\operatorname{in}_{\geq_{\operatorname{lex}}}(f) = x_1^2$ and $\operatorname{in}_{\geq_{\operatorname{revlex}}}(f) = x_3^5$

Division algorithm

Gröbner bases

Theorem (Division algorithm)

<: monomial order

$$0 \neq f, g_1, g_2, \ldots, g_s \in K[x_1, \ldots, x_n]$$

Then, there exist $f_1, \ldots, f_s, r \in K[x_1, \ldots, x_n]$ such that

- $f = f_1g_1 + f_2g_2 + \cdots + f_sg_s + r$.
- If $r \neq 0$, then any monomial in r is divided by none of $\operatorname{in}_{<}(g_1), \ldots, \operatorname{in}_{<}(g_s)$.
- If $f_i \neq 0$, then $\operatorname{in}_{<}(f) \geq \operatorname{in}_{<}(f_i g_i)$.

r is called a remainder of f w.r.t. $\{g_1, \ldots, g_s\}$.

Example

Gröbner bases

$$x^2y + xy^2 + y^2 = (x + y)(xy - 1) + 1 \cdot (y^2 - 1) + x + y + 1$$

Example

Gröbner bases

$$n = 2$$
, lexicographic order $(x > y)$
 x
 $xy - 1$
 $y^2 - 1$
 $x^2y + xy^2 + y^2$
 $x^2y - x$
 $xy^2 + x + y^2$
 $xy^2 - x$
 $xy^2 - x$

$$x^2y + xy^2 + y^2 = x \cdot (xy - 1) + (x + 1) \cdot (y^2 - 1) + 2x + 1$$

Ideals of polynomial rings

Definition

Let $f_1, \ldots, f_s \in K[x_1, \ldots, x_n]$. Then, we define

$$\langle f_1,\ldots,f_s\rangle:=\{h_1f_1+\cdots+h_sf_s\mid h_i\in K[x_1,\ldots,x_n]\}$$

ideal generated by $f_1, \ldots, f_s \in K[x_1, \ldots, x_n]$.

Proposition

$$f_1, \ldots, f_s, g_1, \ldots, g_t \in K[x_1, \ldots, x_n]$$
 $If \langle f_1, \ldots, f_s \rangle = \langle g_1, \ldots, g_t \rangle$, then
$$\begin{cases} f_1 = 0 \\ \vdots & \text{and} \end{cases} \begin{cases} g_1 = 0 \\ \vdots & \text{have the same solutions.} \\ g_t = 0 \end{cases}$$

Gröbner bases

Fix a monomial order <.

$$f_1, \ldots, f_s \in K[x_1, \ldots, x_n]$$

 $I = \langle f_1, \ldots, f_s \rangle \subset K[x_1, \ldots, x_n]$: ideal

Definition

$$in_{<}(I) := \langle in_{<}(f) \mid 0 \neq f \in I \rangle$$
 the initial ideal of I

Integer programming

Definition

$$\{g_1, \ldots, g_t\} \subset I$$
 is a Gröbner basis of I w.r.t. $\iff in_<(I) = \langle in_<(g_1), \ldots, in_<(g_t) \rangle$
 \iff For any nonzero element $f \in I$, $in_<(f)$ is divided by $in_<(g_i)$ for some i .

Example

Gröbner bases

Example

$$f_1 = x^2 + y^2$$
, $f_2 = xy$
 $I = \langle f_1, f_2 \rangle$, lexicographic order $(x > y)$

Then, $\{f_1, f_2\}$ is not a Gröbner basis of I since

• $f = yf_1 - xf_2 = y(x^2 + y^2) - x \cdot xy = y^3$ belongs to *I*.

Integer programming

- So, $\operatorname{in}_{<}(I) = y^3$ belongs to $\operatorname{in}_{<}(I)$.
- $\operatorname{in}_{\sim}(f) = y^3$ is divided by neither in_< $(f_1) = x^2$ nor in_< $(f_2) = xy$.

 \longrightarrow In this case, $\{f_1, f_2, f\}$ is a Gröbner basis of I.

Gröbner bases

Basic properties of a Gröbner basis \mathcal{G} of an ideal I:

- Always exists.
- Not unique.
- G generates I.
- For any nonzero polynomial $f \in K[x_1, \dots, x_n]$, the remainder of f with respect to \mathcal{G} is unique.
- For any nonzero polynomial $f \in K[x_1, \dots, x_n]$, $f \in I \iff$ the remainder of f with respect to \mathcal{G} is 0.

 $\mathcal{G} = \{g_1, \dots, g_t\}$: a Gröbner basis of an ideal I

Definition

Gröbner bases

 \mathcal{G} is called minimal if each g_i is monic and

• $\operatorname{in}_{<}(g_i)$ is not divided by $\operatorname{in}_{<}(g_i)$ if $i \neq j$.

 \mathcal{G} is minimal $\iff \mathcal{G} \setminus \{g_i\}$ is not a Gröbner basis for $\forall i$.

Definition

 \mathcal{G} is called reduced if each g_i is monic and

• Any monomial in g_i is not divided by $\operatorname{in}_{<}(g_i)$ if $i \neq j$.

If we fix an ideal and a monomial order, then the reduced Gröbner basis exists (and unique).

Example

Gröbner bases

Example

$$I = \langle x_1 - x_2, x_1 - x_3 \rangle$$

 $<_{lex}$: lexicographic order
 $in_{<_{lex}}(I) = \langle x_1, x_2 \rangle$
 $\{x_1 - x_2, x_1 - x_3, x_2 - x_3\}$: Gröbner basis , not minimal
 $\{x_1 - x_2, x_2 - x_3\}$: minimal Gröbner basis , not reduced
 $\{x_1 - x_3, x_2 - x_3\}$: reduced Gröbner basis

Triangulations

S-polynomial

$$(0 \neq) f, g \in K[x_1, \dots, x_n]$$

$$m := LCM(\operatorname{in}_{<}(f), \operatorname{in}_{<}(g))$$

$$f = c_f \cdot \operatorname{in}_{<}(f) + \cdots$$

$$g = c_g \cdot \operatorname{in}_{<}(g) + \cdots$$

Then, we define S-polynomial of f and g by

$$S(f,g) := rac{m}{c_f \cdot \operatorname{in}_{<}(f)} f - rac{m}{c_g \cdot \operatorname{in}_{<}(g)} g.$$

Example

$$f = x_1x_4 - x_2x_3$$
, $g = 2x_4x_7 - x_5x_6$, $<_{lex}$: lexicographic order

$$S(f,g) = \frac{x_1 x_4 x_7}{x_1 x_4} (x_1 x_4 - x_2 x_3) - \frac{x_1 x_4 x_7}{2 x_4 x_7} (2 x_4 x_7 - x_5 x_6)$$

$$= -x_2 x_3 x_7 + \frac{1}{2} x_1 x_5 x_6$$

Theorem

 $I = \langle g_1, \ldots, g_t \rangle \subset K[x_1, \ldots, x_n]$

Then, $\{g_1, \ldots, g_t\}$ is a Gröbner basis of I

 \iff

The remainder of $S(g_i, g_j)$ with respect to $\{g_1, \ldots, g_t\}$ is 0 for all $i \neq j$.

Integer programming

Triangulations

```
Input: g_1, \ldots, g_t \in K[x_1, \ldots, x_n], monomial order <
```

- Output: A Gröbner basis \mathcal{G} of $I = \langle g_1, \dots, g_t \rangle \subset K[x_1, \dots, x_n]$ w.r.t. <
- Step 1. $G = \{g_1, ..., g_t\}$

Gröbner bases

- Step 2. Apply Buchberger criterion to \mathcal{G} .
- Step 3. If it satisfies the condition of the criterion. then G is a Gröbner basis. If not, then there exists a nonzero remainder. Add it to \mathcal{G} and back to step 2.

Gröbner bases

Example

$$f=x_1x_4-x_2x_3,\ g=x_4x_7-x_5x_6$$
 $I=\langle f,g\rangle$
lexicographic order $(x_1>\cdots>x_n)$
 $\mathcal{G}=\{f,g\}$
 $S(f,g)=x_7f-x_1g=x_1x_5x_6-x_2x_3x_7$
A remainder of $S(f,g)$ w.r.t. $\{f,g\}$ is $x_1x_5x_6-x_2x_3x_7=:h$
 $\mathcal{G}=\{f,g,h\}$
 $S(f,h)=x_5x_6f-x_4h=x_2x_3x_4x_7-x_2x_3x_5x_6=x_2x_3g$
 $S(g,h)\longrightarrow$ remainder w.r.t. \mathcal{G} is zero.
Thus, $\{f,g,h\}$ is a Gröbner basis of I .

Improving the efficiency of Buchberger algorithm

Proposition

```
(0 \neq) f, g \in K[x_1, \dots, x_n]

GCD(in_{<}(f), in_{<}(g)) = 1

\implies the remainder of S(f, g) with respect to \{f, g\} is 0.
```

- Strategies for selecting S-polynomials
 Sugar Selection Strategy (in Proc. ISSAC 1991)
 → first implemented in CoCoA
- Homogenization (to avoid unnecessary intermediate coefficient swells)
- <u>a</u> . . .

Theorem

Gröbner bases

0 < m < n: integers

<: monomial order on $K[x_1, \ldots, x_n]$

 $\{0\} \neq I \subset K[x_1, \dots, x_n]$: ideal

G: Gröbner basis of I w.r.t. <

If < satisfies the condition

$$g \in \mathcal{G}, \text{in}_{<}(g) \in K[x_1, \dots, x_m] \Longrightarrow g \in K[x_1, \dots, x_m],$$

then $G \cap K[x_1, ..., x_m]$ is a Gröbner basis of $I \cap K[x_1, ..., x_m]$.

Example

In order to solve the system of equations

$$\begin{cases} f_1 = x^2 + y + z - 1 = 0, \\ f_2 = x + y^2 + z - 1 = 0, \\ f_3 = x + y + z^2 - 1 = 0, \end{cases}$$

we compute a Gröbner basis of the ideal $\langle f_1, f_2, f_3 \rangle$ with respect to the lexicographic order $<_{\text{lex}} (x > y > z)$:

$$\begin{cases} g_1 &= x + y + z^2 - 1, \\ g_2 &= y^2 - y - z^2 + z, \\ g_3 &= 2yz^2 + z^4 - z^2, \\ g_4 &= z^6 - 4z^4 + 4z^3 - z^2. \end{cases}$$

 $<_{\mathrm{lex}}$ satisfies the condition in Elimination Theorem. Since $\langle f_1, f_2, f_3 \rangle = \langle g_1, g_2, g_3, g_4 \rangle$ holds, $f_1 = f_2 = f_3 = 0$ and $g_1 = g_2 = g_3 = g_4 = 0$ have the same solutions.

Triangulations

Toric ideals

 $\mathbb{Z}^{d\times n}$: the set of all $d\times n$ integer matrices

$$A = (\mathbf{a}_1, \dots, \mathbf{a}_n) \in \mathbb{Z}^{d \times n}$$

- A is called a configuration if $\exists \mathbf{w} \in \mathbb{R}^d$ s.t. $\mathbf{w} \cdot \mathbf{a}_1 = \cdots = \mathbf{w} \cdot \mathbf{a}_n = 1$.
- We usually assume that A is a configuration.

$$K$$
: field (e.g., $K = \mathbb{C}$)

$$K[X] = K[x_1, \dots, x_n]$$
: poly. ring in *n* variables over *K*

•
$$\mathbf{u} = (u_1, \dots, u_n) \in \mathbb{Z}_{>0}^n \Longrightarrow X^{\mathbf{u}} = X_1^{u_1} \cdots X_n^{u_n}$$

$$I_{A} = \left\langle X^{\mathbf{u}} - X^{\mathbf{v}} \in K[X] \mid \mathbf{u}, \mathbf{v} \in \mathbb{Z}_{\geq 0}^{n}, A\mathbf{u} = A\mathbf{v} \right\rangle$$
$$= \left\langle X^{\mathbf{u}^{+}} - X^{\mathbf{u}^{-}} \in K[X] \mid \mathbf{u} \in \mathbb{Z}^{n}, A\mathbf{u} = \mathbf{0} \right\rangle$$

Toric ideal of A

Example

Gröbner bases

Example

$$A = \left(\begin{array}{ccccccc} 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \end{array}\right)$$

$$I_A = \langle x_1 x_5 - x_2 x_4, x_1 x_6 - x_3 x_4, x_2 x_6 - x_3 x_5 \rangle$$

(For example,
$$x_1x_5 - x_2x_4 \in I_A$$
 since $A\begin{pmatrix} 1 \\ -1 \\ 0 \\ -1 \\ 1 \\ 0 \end{pmatrix} = \mathbf{0}.$)

$$K[A] = K[t_1t_3, t_1t_4, t_1t_5, t_2t_3, t_2t_4, t_2t_5] \cong K[X]/I_A$$

Gröbner bases

Properties of toric ideals:

- prime ideal
- The reduced Gröbner basis of I_A consists of binomials.
- A is a configuration $\iff I_A$ is homogeneous w.r.t. a usual grading
- $A \in \mathbb{Z}_{>0}^n$ \implies I_A is homogeneous w.r.t. some positive grading
- If each **a**_i is a nonnegative integer vector, then

$$I_A = \langle x_1 - T^{\mathbf{a}_1}, \dots, x_n - T^{\mathbf{a}_n} \rangle \cap K[X].$$

So, we can compute a Gröbner basis of I_A by Elimination theorem.

However, this method is not effective in practice.

Algorithm computing generators of I_A

Lemma

Gröbner bases

 $J \subset K[X]$: homogeneous ideal

<: reverse lexicographic order

G: the reduced Gröbner basis of J w.r.t. <

 $(J: X_n^{\infty}) := \{ f \in K[X] \mid \exists r \in \mathbb{N} \text{ s.t. } X_n^r f \in J \}$

Then, a GB of $(J : x_n^{\infty})$ w.r.t. < is obtained by dividing each $g \in \mathcal{G}$ by the highest power of x_n that divides g.

Proposition

 $A \in \mathbb{Z}^{d \times n}$: configuration

B: lattice basis of $\{\mathbf{u} \in \mathbb{Z}^n \mid A\mathbf{u} = \mathbf{0}\}$

$$J:=\left\langle X^{\mathbf{u}^{+}}-X^{\mathbf{u}^{-}}\mid \mathbf{u}\in B
ight
angle$$

Then $I_A = (J : (x_1 \cdots x_n)^{\circ}) = ((\cdots (J : x_1^{\circ}) : x_2^{\circ}) \cdots) : x_n^{\circ})$

Gröbner bases Toric ideals Integer programming Triangulations Contingency tables

Three breakthroughs

Toric ideals

- 0. Commutative algebra
 - Toric ideals have been studied by commutative algebraists for a long time.
 - For example,
 - J. Herzog
 Generators and relations of abelian semigroups and semigroup rings

 Manuscripta Math., 3 (1970), 175 193.

is an early reference in commutative algebra.

Three breakthroughs

- 1. Integer programming
 - P. Conti and C. Traverso
 Buchberger algorithm and integer programming
 in Proceedings of AAECC-9 (New Orleans)
 Springer LNCS **539** (1991), 130 139.

Three breakthroughs

Gröbner bases

- 2. Triangulations of convex polytopes.
- I. M. Gel'fand, A. V. Zelevinskii and M. M. Kapranov Hypergeometric functions and toral manifolds *Functional Analysis and Its Applications*, **23** (1989), 94 106.
- B. Sturmfels
 Gröbner bases of toric varieties *Tôhoku Math. J.* **43** (1991), 249 261.

Three breakthroughs

Gröbner bases

- 3. Conditional test of contingency tables (Markov chain Monte Carlo method)
 - P. Diaconis and B. Sturmfels Algebraic algorithms for sampling from conditional distributions

Annals of Statistics, **26** (1998), 363 – 397. (Received June 1993; revised April 1997.)

Three breakthroughs

One can study three breakthroughs in

B. Sturmfels Gröbner bases and convex polytopes Amer. Math. Soc., Providence, RI, 1995.

See also

- D. Cox, J. Little and D. O'Shea Using algebraic geometry GTM 185, Springer, Berlin, 1998.
- T. Hibi (Ed.) Gröbner bases –Statistics and Software Systems– Springer, 2013.

B.1. Integer programming

Example (CLO, "Using algebraic geometry")

Each pallet from a customer A: 400 kg, 2 m³ Each pallet from a customer B: 500 kg, 3 m³

The customer A will pay \$ 11 for each pallet, and the customer B will pay \$ 15 for each pallet.

We use trucks that can carry any load

up to 3700 kg, and up to 20 m^3 .

How to maximize the revenues generated?

Subject to
$$\left\{ \begin{array}{lcl} 4a & + & 5b & \leq & 37 \\ 2a & + & 3b & \leq & 20 \\ & & a,b & \geq & 0 \end{array} \right. ,$$

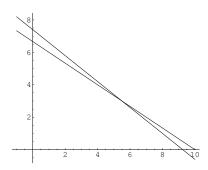
find integers a, b which maximize 11a + 15b.

Example

Gröbner bases

Subject to
$$\left\{ \begin{array}{lcl} 4a & + & 5b & \leq & 37 \\ 2a & + & 3b & \leq & 20 \\ & & a,b & \geq & 0 \end{array} \right. ,$$

find integers a, b which maximize 11a + 15b.



Standard form

Gröbner bases

Subject to
$$\begin{cases} 4a + 5b \leq 37 \\ 2a + 3b \leq 20 \\ a, b \geq 0 \end{cases}$$

find integers a, b which maximize 11a + 15b.

↓ the standard form

Subject to
$$\begin{cases} 4a + 5b + c & = 37 \\ 2a + 3b & + d = 20 \\ a, b, c, d \ge 0 \end{cases}$$

find integers a, b, c, and d which minimize -11a - 15b.

Triangulations

Gröbner bases

Subject to
$$A \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \begin{pmatrix} 37 \\ 20 \end{pmatrix}$$
 where $A = \begin{pmatrix} 4 & 5 & 1 & 0 \\ 2 & 3 & 0 & 1 \end{pmatrix} \cdots$

$$\mathbf{w} := (-11, -15, 0, 0) + 2 \cdot (6, 8, 1, 1) = (1, 1, 2, 2).$$

$$\mathcal{G} = \{x_3^4 x_4^2 - x_1, x_2 x_3^3 x_4 - x_1^2, x_1 x_3 x_4 - x_2, x_1^4 x_4 - x_2^3 x_3, x_2^2 x_3^2 - x_1^3\}$$

is a Gröbner basis of I_A with respect to $<_{\mathbf{w}}$

(a, b, c, d) = (0, 0, 37, 20) satisfies the constraints.

Therefore, we compute the remainder of $x_3^{37}x_4^{20}$ w.r.t. \mathcal{G} .

The remainder is $x_1^4 x_2^4 x_3$.

Hence, (a, b, c, d) = (4, 4, 1, 0) is a solution.

Answer: Four pallets from A and four pallets from B.

B.2. Triangulations of convex polytopes

In this section, we always assume that $A = (\mathbf{a}_1, \dots, \mathbf{a}_n) \in \mathbb{Z}^{d \times n}$ is a configuration, and often identify A with the set $\{\mathbf{a}_1, \dots, \mathbf{a}_n\} \subset \mathbb{Z}^d$.

Definition

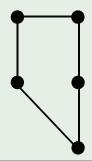
Gröbner bases

$$\operatorname{Conv}(A) := \left\{ \sum_{i=1}^n r_i \ \mathbf{a}_i \in \mathbb{Q}^d \ \middle| \ 0 \leq r_i \in \mathbb{Q}, \ \sum_{i=1}^n r_i = 1 \right\}$$

the convex hull of A.

Example

$$A = \begin{pmatrix} 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 \end{pmatrix}$$
. Then, Conv(A) is



Gröbner bases Toric ideals Integer programming Triangulations Contingency tables

Triangulation

Definition

An integral convex polytope P is called simplex if the number of vertex of P is $1 + \dim P$. (ex. line, triangle, tetrahedron.)

Definition

A covering Δ of A is a set of simplices whose vertices belong to A such that $Conv(A) = \bigcup_{F \in \Delta} F$.

Definition

A covering \triangle of A is called a triangulation if

- **1** F' is a face of $F \in \Delta \Longrightarrow F' \in \Delta$
- 2 $F, F' \in \Delta \Longrightarrow F \cap F'$ is a face of F and a face of F'.

Initial complex

Definition (initial complex)

$$A = \{\mathbf{a}_1, \dots, \mathbf{a}_n\} \subset \mathbb{Z}^d$$

< : monomial order

$$\Delta(in_{<}(I_{A})) := \left\{ \operatorname{Conv}(B) \mid \begin{array}{c} B \subset A \\ \prod_{\mathbf{a}_{i} \in B} x_{i} \notin \sqrt{in_{<}(I_{A})} \end{array} \right\}$$

Theorem

 $\Delta(in_{<}(I_A))$ is a triangulation of A.

- (Gel'fand et al.) For $\mathbf{w} \in \mathbb{R}^n$, a triangulation $\Delta_{\mathbf{w}}$ is defined geometricaly. (regular triangulation)
- (Sturmfels) We have $\Delta(in_{\mathbf{w}}(I_A)) = \Delta_{\mathbf{w}}$.

Example

$$A = \left(\begin{array}{ccccc} 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 \end{array}\right)$$

$$I_A = \langle x_1 x_2 - x_3 x_5, x_1 x_4 - x_2 x_3, x_2^2 - x_4 x_5 \rangle$$

 $<_1$: lexicographic order $(x_2 > x_1 > x_3 > x_4 > x_5)$

Gröbner bases of I_A with respect to $<_1$ is

$$\{X_1X_2 - X_3X_5, X_2X_3 - X_1X_4, X_2^2 - X_4X_5, X_1^2X_4 - X_3^2X_5\}$$

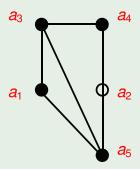
$$in_{<_1}(I_A) = \langle x_1 x_2, x_2 x_3, x_2^2, x_1^2 x_4 \rangle, \quad \sqrt{in_{<_1}(I_A)} = \langle x_1 x_4, x_2 \rangle$$

Examples

Gröbner bases

Example

$$A = \begin{pmatrix} 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 \end{pmatrix}, \sqrt{in_{<_1}(I_A)} = \langle x_1 x_4, x_2 \rangle$$



Examples

Gröbner bases

Example

$$A = \left(\begin{array}{ccccc} 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 \end{array}\right)$$

Integer programming

$$I_A = \langle x_1 x_2 - x_3 x_5, x_1 x_4 - x_2 x_3, x_2^2 - x_4 x_5 \rangle$$

 $<_2$: lexicographic order($x_5 > x_3 > x_4 > x_2 > x_1$)

Gröbner bases of I_A with respect to $<_2$ is

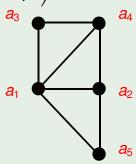
$$\{X_3X_5 - X_1X_2, X_2X_3 - X_1X_4, X_4X_5 - X_2^2\}$$

$$in_{<_2}(I_A) = \sqrt{in_{<_2}(I_A)} = \langle x_2x_3, x_3x_5, x_4x_5 \rangle$$

Example

Example

$$A = \begin{pmatrix} 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 \end{pmatrix}, \sqrt{in_{<_2}(I_A)} = \langle x_2 x_3, x_3 x_5, x_4 x_5 \rangle$$



Unimodular triangulations

Definition

Gröbner bases

A covering (triangulation) \triangle of A is called unimodular, if for the vertex set B of any maximal simplex in Δ , we have $\mathbb{Z}A=\mathbb{Z}B$,

Integer programming

(Here,
$$\mathbb{Z}A = \left\{ \sum_{i=1}^n z_i \mathbf{a}_i \mid z_i \in \mathbb{Z} \right\}$$
.)

Theorem

$$\Delta(in_{<}(I_A))$$
 is unimodular $\iff \sqrt{in_{<}(I_A)} = in_{<}(I_A)$

Important properties

- (i) A is unimodular (any triangulation of A is unimodular) $(\Leftrightarrow \sqrt{in_{<}(I_A)} = in_{<}(I_A) \text{ for any } <)$
- (ii) A is compressed $(\Leftrightarrow \sqrt{in_{<}(I_A)} = in_{<}(I_A)$ for any reverse lex. order <)
- (iii) A has a regular unimodular triangulation $(\Leftrightarrow \sqrt{in} \langle (I_A) = in \langle (I_A) \text{ for some } <)$
- (iv) A has a unimodular triangulation
- (v) A has a unimodular covering
- (vi) K[A] is normal $(\Leftrightarrow \mathbb{Z}_{>0}A = \mathbb{Z}A \cap \mathbb{Q}_{>0}A)$
- Then, (i) \Rightarrow (ii) \Rightarrow (iii) \Rightarrow (iv) \Rightarrow (v) \Rightarrow (vi) hold. However, the converse of them are false in general.

G: finite connected graph on the vertex set $\{1, 2, \dots, d\}$ $E(G) = \{e_1, \dots, e_n\}$: the edge set of G(no loop, no multiple edges)



For each edge $e = \{i, j\} \in E(G)$, let $\rho(e) := \mathbf{e}_i + \mathbf{e}_i \in \mathbb{Z}^d$.

$$A_G := (\rho(e_1), \dots, \rho(e_n)) \in \mathbb{Z}^{d \times n}$$

 $Conv(A_G)$ is called an edge polytope of G.

Edge polytopes

Theorem (O-Hibi (1998), Simis et al. (1998))

For a finite connected graph G, TFAE:

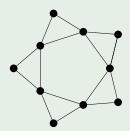
- \bullet $K[A_G]$ is normal;
- A_G has a unimodular covering;
- For any two odd cycles C and C' of G without common vertices, there exists an edge of G which joins a vertex of C with a vertex of C'.

An interesting edge polytope

Example (O-Hibi (1999))

Let *G* be the following graph. Then,

- For any monomial order <, $\sqrt{in_<(I_{A_G})} \neq in_<(I_{A_G})$
- A_G has a unimodular triangulation.
 (Checked by the software PUNTOS by De Loera.)



B.3. Contingency tables

5×5 contingency table:

algebra \ statistics	5	4	3	2	1	total
5	2	1	1	0	0	4
4	8	3	3	0	0	14
3	0	2	1	1	1	5
2	0	0	0	1	1	2
1	0	0	0	0	1	1
total	10	6	5	2	3	26

Is there a correlation between the two scores?

Markov chain Monte Carlo method

Integer programming

By a random walk on F, we sample elements of F and compare certain features (χ^2 -statistics). (In this example, $\sharp |F| = 229, 174$.)

Markov chain Monte Carlo method

For example, fix α_i , β_j such that $\sum_i \alpha_i = \sum_i \beta_j$ and let

$$F = \left\{ T = (t_{ij}) \, \left| \, \begin{array}{c|cc} t_{11} & t_{12} & t_{13} & \alpha_1 \\ t_{21} & t_{22} & t_{23} & \alpha_2 \\ \hline \beta_1 & \beta_2 & \beta_3 \end{array} \right|, \quad 0 \leq t_{ij} \in \mathbb{Z} \, \right\}.$$

Then by adding or subtracting one of the elements of

$$\textit{M} = \left\{ \left(\begin{array}{ccc} 1 & -1 & 0 \\ -1 & 1 & 0 \end{array} \right), \left(\begin{array}{ccc} 1 & 0 & -1 \\ -1 & 0 & 1 \end{array} \right), \left(\begin{array}{ccc} 0 & 1 & -1 \\ 0 & -1 & 1 \end{array} \right) \right\},$$

any of two elements T, T' of F are connected:

$$T = T_0 \longrightarrow T_1 \in F \longrightarrow T_2 \in F \longrightarrow \cdots \longrightarrow T_s = T'.$$
 for any alpha_i & beta_j. Such an M is called a Markov basis.

Markov bases and toric ideals

Example (continued)

Gröbner bases

$$A = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \end{pmatrix}, A \begin{pmatrix} t_{11} \\ t_{12} \\ t_{13} \\ t_{21} \\ t_{22} \\ t_{23} \end{pmatrix} = \begin{pmatrix} t_{11} + t_{12} + t_{13} \\ t_{21} + t_{22} + t_{23} \\ t_{11} + t_{21} \\ t_{12} + t_{22} \\ t_{13} + t_{23} \end{pmatrix}$$

$$I_A = \langle x_1 x_5 - x_2 x_4, \quad x_1 x_6 - x_3 x_4, \quad x_2 x_6 - x_3 x_5 \rangle$$

$$\left\{ \left(\begin{array}{ccc} 1 & -1 & 0 \\ -1 & 1 & 0 \end{array} \right), \left(\begin{array}{ccc} 1 & 0 & -1 \\ -1 & 0 & 1 \end{array} \right), \left(\begin{array}{ccc} 0 & 1 & -1 \\ 0 & -1 & 1 \end{array} \right) \right\}$$

Diaconis-Sturmfels

Theorem (Diaconis-Sturmfels)

Let M be a finite set of integer matrices. Then, M is a Markov basis if and only if I_A is generated by the corresponding binomials.

- 2 way contingency tables: It is known that I_A has a quadratic Gröbner basis.
- ≥ 3 way contingency tables:
 Except for some classes, the set of generators of I_A is unknown and it is not easy to compute in general.
 (You should try to use powerful software 4ti2.)

No *n* way interaction models

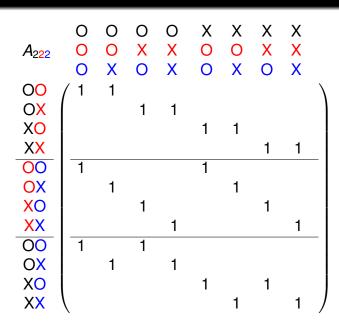
For $r_1 \times r_2 \times \cdots \times r_\ell$ contingency table $(r_1 \ge r_2 \ge \cdots \ge r_\ell \ge 2)$

$$T=(t_{i_1i_2\cdots i_\ell})_{i_\ell=1,2,\ldots,r_\ell},\quad 0\leq t_{i_1i_2\cdots i_\ell}\in\mathbb{Z},$$

we associates a configuration $A_{r_1r_2\cdots r_\ell}$ consisting of the following vectors:

$$\boldsymbol{e}_{i_2i_3\cdots i_\ell}^{(1)}\oplus\boldsymbol{e}_{i_1i_3\cdots i_\ell}^{(2)}\oplus\cdots\oplus\boldsymbol{e}_{i_1i_2\cdots i_{\ell-1}}^{(\ell)}$$

where each i_k belongs to $\{1, 2, \ldots, r_k\}$ and $\mathbf{e}_{i_1 \cdots i_{k-1} i_{k+1} \cdots i_{\ell}}^{(k)}$ is a unit vector in $\mathbb{R}^{r_1 \cdots r_{k-1} r_{k+1} \cdots r_{\ell}}$.



Classification

Gröbner bases

Classification

$r_1 \times r_2$	unimodular				
$r_1 \times r_2 \times 2 \times \cdots \times 2$					
$r_1 \times 3 \times 3$	compressed,				
	not unimodular				
$5 \times 5 \times 3$	normal				
$5 \times 4 \times 3$	(4ti2 & Normaliz)				
$4 \times 4 \times 3$	not compressed				
otherwise, i.e.,					
$\ell \geq$ 4 and $r_3 \geq 3$	not normal				
$\ell=3$ and $r_3\geq 4$					
$\ell = 3, r_3 = 3, r_1 \ge 6 \text{ and } r_2 \ge 4$					

Decompositions/constructions

- Algebras of Veronese type
- Segre–Veronese configurations (O–Hibi 2000)
- Extended Segre-Veronese configurations (Aoki-Hibi-O-Takemura 2010)
- Nested configurations (Aoki–Hibi–O–Takemura 2008, O–Hibi 2010)
- Higher Lawrence configurations (Santos–Sturmfels 2003) → N-fold configurations
- Toric fiber product (Sullivant 2007)

Segre-Veronese configurations

 $\tau >$ 2, *n*: integers

$$\mathbf{b} = (b_1, \dots, b_n), \mathbf{c} = (c_1, \dots, c_n), \mathbf{p} = (p_1, \dots, p_n),$$

 $\mathbf{q} = (q_1, \dots, q_n)$: integer vectors satisfying

$$0 \le c_i \le b_i$$
 for all $1 \le i \le n$

Let A be the matrix whose columns are all vectors $(f_1,\ldots,f_d)\in\mathbb{Z}^d_{\geq 0}$ s.t.

$$\sum_{j=1}^{d} f_j = \tau$$

$$c_i \leq \sum_{i=p_i}^{q_i} f_j \leq b_i \text{ for all } 1 \leq i \leq n$$

A is called Segre–Veronese configuration.

Segre-Veronese configurations

Example

$$\tau = 2, n = 2, d = 5$$

$$\mathbf{b} = (1, 1), \mathbf{c} = (0, 0), \mathbf{p} = (1, 3), \mathbf{q} = (2, 5)$$

Let A be the matrix whose columns are all vectors $(f_1, \ldots, f_5) \in \mathbb{Z}_{>0}^5$ s.t.

$$0 < f_1 + f_2 < 1$$

$$0 \le f_3 + f_4 + f_5 \le 1$$

Then
$$A = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ \hline 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \end{pmatrix}$$
.

Gröbner bases Toric ideals Integer programming Triangulations Contingency tables

Segre-Veronese configurations

Theorem

Suppose that A is a Segre–Veronese configuration. Then the toric ideal I_A has a quadratic Gröbner basis.

- S. Aoki, T. Hibi, H. Ohsugi and A. Takemura Markov basis and Gröbner basis of Segre-Veronese configuration for testing independence in group-wise selections
 - Annals of the Institute of Statistical Math. **62** (2010), 299–321.
- S. Aoki, T. Otsu, A. Takemura and Y. Numata Statistical Analysis of Subject Selection Data in NCUEE Examination Oyo Tokeigaku, **39**, (2)–(3), 2010, 71–100. (Japanese)

Nested configurations

Gröbner bases

$$A = (\mathbf{a}_1, \dots, \mathbf{a}_n) \in \mathbb{Z}_{>0}^{d \times n}$$
: configuration

For each i = 1, 2, ..., d:

$$B_i \in \mathbb{Z}_{>0}^{\mu_i \times \lambda_i}$$
: configuration

$$K\left[u_1^{(i)},\ldots,u_{\mu_i}^{(i)}
ight]$$
 : polynomial ring in μ_i variables

$$K[B_i] = K\left[m_1^{(i)}, \dots, m_{\lambda_i}^{(i)}\right] \subset K\left[u_1^{(i)}, \dots, u_{\mu_i}^{(i)}\right]$$

$$K[A(B_1,\ldots,B_d)] := K \left[\begin{array}{c|c} m_{j_1}^{(i_1)} \cdots m_{j_r}^{(i_r)} & r \in \mathbb{N} \\ \mathbf{e}_{i_1} + \cdots + \mathbf{e}_{i_r} \in A \\ 1 \leq j_k \leq \lambda_{i_k} \text{ for } \forall k \end{array} \right]$$

The configuration $A(B_1, \ldots, B_d)$ is called the nested configuration of $A, B_1, ..., B_d$.

Example

Gröbner bases

$$A = \begin{pmatrix} 2 & 1 \\ 0 & 1 \end{pmatrix}, B_1 = \begin{pmatrix} 2 & 1 & 0 \\ 0 & 1 & 2 \end{pmatrix}, B_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

- You have 2 coupons.
- Shop α accepts at most 2 coupons.
- Shop β accepts at most 1 coupon.
- Each shop has 2 different items.
- A coupon allows you to buy 2 items at a discount at α .
- A coupon allows you to buy 1 item at a discount at β .

Nested configurations

Theorem

Let n > 2.

- $I_A, I_{B_1}, \dots, I_{B_d}$ have Gröbner bases of degree $\leq n$ $\implies I_{A(B_1,\dots,B_d)}$ has a Gröbner basis of degree $\leq n$.
- I_A , I_{B_1} , ..., I_{B_d} have squarefree initial ideals $\implies I_{A(B_1,...,B_d)}$ has a squarefree initial ideal.

Theorem

K[A], $K[B_1]$,..., $K[B_d]$ are normal $\implies K[A(B_1,...,B_d)]$ is normal. (The converse is not true in general.)

References

- S. Aoki, T. Hibi, H. Ohsugi and A. Takemura Gröbner bases of nested configurations J. Algebra, 320 (2008) no. 6, 2583 – 2593.
- H. Ohsugi and T. Hibi
 Toric rings and ideals of nested configurations

 J. commutative algebra, 2 (2010), 187 208.
- T. Shibuta
 Gröbner bases of contraction ideals
 Journal of Algebraic Combinatorics, **36** (2012), 1 19.

0. Quadratic Gröbner bases

The following properties of Gröbner bases of toric ideals are studied by many researchers:

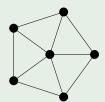
- (i) There exists a monomial order such that a Gröbner basis of I_A consists of quadratic binomials.
- (ii) K[A] is "Koszul algebra."
- (iii) I_A is generated by quadratic binomials.
 - (i) \Rightarrow (ii) \Rightarrow (iii) hold.
 - But neither (ii) \Rightarrow (i) nor (iii) \Rightarrow (ii) holds in general.

Quadratic Gröbner bases

Example (O-Hibi (1999))

Let G be the following graph. Then,

- I_{A_G} is generated by quadratic binomials.
- $K[A_G]$ is not Koszul.
- Hence, for any monomial order <,
 the reduced Gröbner basis of I_{AG} is not quadratic.



Infinite family of counterexamples

Hibi-Nishiyama-Ohsugi-Shikama (2008 2014)

Using software <code>Risa/Asir</code>, <code>Macauley2</code>, <code>CaTS</code>, ..., we chacked that there are a lot of graphs of \leq 8 vertices whose edge polytope is a counterexample.

Moreover, we proved that

Theorem

 $n \geq 5$

 C_n : cycle of length n

 K_{n+1} : the complete graph with n+1 vertices

 $G:=K_{n+1}-E(C_n)$

Then,

- *I*_{AG} is generated by quadratic binomials
- I_{Ac} has no quadratic Gröbner basis .

Configurations arising from root systems

Gel'fand-Graev-Postnikov (1997)

$$\overline{A_{d-1}} = \{\mathbf{e}_i - \mathbf{e}_j \mid 1 \le i < j \le d\}$$
 $(\mathbf{e}_i \in \mathbb{Z}^d \text{ is a unit vector})$

$$\widetilde{A_{d-1}} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \hline 1 \mid 1 & \cdots & 1 \end{pmatrix}$$

There exists a monomial order such that a Gröbner basis of I_{A-1} consists of quadratic binomials. (They constructed a "regular unimodular triangulation.")

O-Hibi (2002)

$$egin{aligned} \overline{D_d} &= \{ \mathbf{e}_i + \mathbf{e}_j \mid 1 \leq i < j \leq d \} \cup A_{d-1} \ B_d &= \{ \mathbf{e}_1, \dots, \mathbf{e}_d \} \cup D_d \ C_d &= \{ 2\mathbf{e}_1, \dots, 2\mathbf{e}_d \} \cup D_d \end{aligned}$$

Let
$$\mathcal{B} = \{B_1, \dots, B_n\}$$
 where

- Each B_i is an r-subset of {1, 2, ..., d};
- (Basis Exchange Axiom)

For each
$$1 \le i, j \le n$$
, for $\forall x \in B_i \setminus B_i$,

$$\exists y \in B_j \setminus B_i \text{ s. t. } (B_i \setminus \{x\}) \cup \{y\} \in \mathcal{B}.$$

Let
$$A_{\mathcal{B}} = (\mathbf{a}_1, \dots, \mathbf{a}_n) \in \mathbb{Z}^{d \times n}$$
 where $\mathbf{a}_i = \sum_{i \in B_i} \mathbf{e}_i \in \mathbb{R}^d$.

Conjecture (White (1980))

 I_{A_R} is generated by quadratic binomials.

Conjecture

 I_{A_R} has a quadratic Gröbner basis.