

The Project-And-Lift Algorithm for the Computation of Toric Gröbner Bases

An Implementation in Mathematica

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Outline

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 - Saturation Algorithm
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Integer Linear Programming

Standard Form

$$\min\{cy : Ay = b, y \in \mathbb{N}^n\}$$

Selected Applications

- Travelling Salesman
- Knapsack, Bin Packing
- Schedule Optimization
- Frequency Planning for Mobile Phone Networks
- Capacity Planning for Telecommunication Networks

Applying Gröbner-Bases

Definition (Test Set)

T is a **test set** for $\min\{cy : Ay = b, y \in \mathbb{N}^n\}$ if

- 1 all $y \in T$ have negative cost ($cy < 0$),
- 2 all $y \in T$ solve $Ay = 0$ and
- 3 for each non-optimal solution $y_s \in \mathbb{N}^n$ of $Ay_s = b$ there is a $y \in T$ s.t. $y_s + y \in \mathbb{N}^n$.

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Optimization Algorithm

- 1 Find *any* solution $y_s \in \mathbb{N}^n$ of $Ay_s = b$.
- 2 While $\exists y \in T : y_s + y \in \mathbb{N}^n$, let $y_s \leftarrow y_s + y$.
- 3 Return y_s .

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How can we find a *finite* (small) test set???

Polynomial Ideals

Notation

- $\mathbb{K}[X]$ = ring of polynomials over \mathbb{K} in variables $X = \{x_1, \dots, x_n\}$
- $I \subset \mathbb{K}[X]$ is an ideal iff for all $a, b \in I, r \in \mathbb{K}[X]$
 - 1 $a + b \in I$ and
 - 2 $ar \in I$.
- $\langle f_1, \dots, f_s \rangle$ = ideal generated by $f_1, \dots, f_s \in \mathbb{K}[X]$

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Example

- $\mathbb{Q}[x_1, x_2, x_3] \ni x_1^2 - x_2x_3, x_1x_2^2x_3 - 1, x_2^5x_3^3 - 1$
- $\langle x_1^2 - x_2x_3, x_1x_2^2x_3 - 1, x_2^5x_3^3 - 1 \rangle \ni x_1 - x_2^3x_3^2 = x_2^2x_3(x_1^2 - x_2x_3) - x_1(x_1x_2^2x_3 - 1)$

Monomial Orderings

Definition

A total ordering \prec of the monomials $x^\alpha = x_1^{\alpha_1} \cdots x_n^{\alpha_n}$ is **admissible** iff for all $\alpha, \beta, \gamma \in \mathbb{N}^n$ ($0 \in \mathbb{N}$)

- ① $x^\alpha \prec x^\beta \Rightarrow x^\alpha x^\gamma \prec x^\beta x^\gamma$ and
- ② $1 \prec x^\alpha$ for $x^\alpha \neq 1$.

LM(f) = largest monomial of $f \in \mathbb{K}[X]$ wrt. \prec

Monomial Orderings (2)

Example

- **Lexicographic Ordering:**

$x^\alpha \prec x^\beta$ iff first nonzero entry of $\alpha - \beta$ is negative.

$$x_1 \succ x_2^3 x_3^2 \succ x_2^2 x_3^3$$

- **Graded Reverse Lexicographic Ordering:**

$x^\alpha \prec x^\beta$ iff $\deg(x^\alpha) < \deg(x^\beta)$ or $\deg(x^\alpha) = \deg(x^\beta)$ and last nonzero entry of $\alpha - \beta$ is positive.

$$x_2^3 x_3^2 \succ x_2^2 x_3^3 \succ x_1$$

Monomial Orderings (3)

Definition (Matrix Orderings)

Given a matrix $C \in \mathbb{K}^{s,n}$, let $x^\alpha \prec x^\beta$ iff the first nonzero entry of $C\alpha - C\beta$ is positive.

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Notes

Any admissible monomial ordering can be

- represented by a matrix $C \in \mathbb{R}^{n,n}$.
- approximated up to an arbitrary, fixed degree by a matrix $C \in \mathbb{Z}^{n,n}$.

Common monomial orderings can be represented by a matrix $C \in \mathbb{Z}^{n,n}$

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Example ($n = 3$)

Lexicographic
Ordering: $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

Graded Reverse-
lexicographic
Ordering: $\begin{pmatrix} 1 & 1 & 1 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}$

Gröbner Bases

Definition

G is a **Gröbner basis** of I wrt. a monomial ordering \prec iff

- 1 $I = \langle G \rangle$ and
- 2 $\langle \text{LM}(I) \rangle = \langle \text{LM}(G) \rangle$.

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Example

Consider $I = \langle x_1^2 - x_2x_3, x_1x_2^2x_3 - 1, x_2^5x_3^3 - 1 \rangle$ and the lexicographic monomial ordering.

- $G_1 = \{x_1^2 - x_2x_3, x_1x_2^2x_3 - 1, x_2^5x_3^3 - 1\}$ is no Gröbner basis of I since $x_1 \in \langle \text{LM}(I) \rangle$ but $x_1 \notin \langle \text{LM}(G_1) \rangle$
- $G_2 = \{x_1^2 - x_2x_3, x_1x_2^2x_3 - 1, x_2^5x_3^3 - 1, x_1 - x_2^3x_3^2\}$ is a Gröbner basis of I .

Problem Statement

Definition (Toric Ideals)

Given a matrix $A \in \mathbb{Z}^{k,n}$, the associated **toric ideal** is defined as

$$I(A) = \langle x^\alpha - x^\beta : \alpha, \beta \in \mathbb{N}^n : \alpha - \beta \in \ker(A) \rangle$$

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Example

$$A = \begin{pmatrix} 1 & -3 & 5 \end{pmatrix}$$

$$\Rightarrow I(A) = \langle x_2^5 x_3^3 - 1, x_1 - x_2^3 x_3^2 \rangle$$

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Task

Given

- matrix $A \in \mathbb{Z}^{k,n}$ and
- monomial ordering \prec (as matrix)

compute a Gröbner basis of $I(A)$ wrt. \prec .

"Blue Print" of an Toric Ideal Algorithm

Input: Matrix A , monomial ordering \prec defined by matrix C

Output: Gröbner basis of $I(A)$

Calculate lattice basis B of $\ker_{\mathbb{Z}}(A)$

Compute Markov basis M of $\ker_{\mathbb{Z}}(A)$ resp. ideal basis F of $I(A)$

Compute Gröbner basis of $I(A)$

Lattice Basis

Definition

A **lattice** L is a set of the form

$$L = \mathbb{Z}v_1 + \mathbb{Z}v_2 + \dots + \mathbb{Z}v_s \subset \mathbb{Z}^n.$$

The set $\{v_1, \dots, v_s\}$ is a **lattice basis** of L .

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Example

$$A = \begin{pmatrix} 1 & -3 & 5 \end{pmatrix}$$

$$\Rightarrow \ker_{\mathbb{Z}}(A) = \mathbb{Z} \begin{pmatrix} 2 & -1 & -1 \end{pmatrix}^T + \mathbb{Z} \begin{pmatrix} 1 & 2 & 1 \end{pmatrix}^T$$

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Computation

- Since $A \in \mathbb{Z}^{k,n}$, $L = \ker_{\mathbb{Z}}(A)$ is a lattice.
1. Triangulate A with unimodular operations (Hermite decomposition).
 2. Lattice basis B of $L = \ker_{\mathbb{Z}}(A)$ can be read off the triangular form.

Markov Basis

Let α^+ be defined by $\alpha_i^+ = \max\{\alpha_i, 0\}$ and $\alpha^- = (-\alpha)^+$.

Definition

Given a lattice $L = \ker_{\mathbb{Z}}(A)$, B is a **Markov basis** of L iff $J(B) = \{x^{\alpha^+} - x^{\alpha^-} : \alpha \in B\}$ is an ideal basis of $I(A)$.

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Computation

- 1 Saturation algorithm (Sturmfels, Bigatti et. al)
- 2 Shadow algorithm (Kesh, Metha)
- 3 Project-and-Lift algorithm (Hemmecke, Malkin)

Saturation Algorithm

Definition

$I : f^\infty = \{h \in \mathbb{K}[X] : f^k h \in I \text{ for some } k \in \mathbb{N}\}$ **saturation** of I wrt. f .

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Fact

Given a basis B of the lattice $L = \ker_{\mathbb{Z}}(A)$, $\langle J(B) \rangle : (x_1 \cdots x_n)^\infty = I(A)$.

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Computation

- $\langle g_1, \dots, g_s \rangle : f^\infty = \langle g_1, \dots, g_s, tf - 1 \rangle \cap \mathbb{K}[X]$
- \Rightarrow Compute Gröbner basis of $\langle g_1, \dots, g_s, tx_1 \cdots x_n - 1 \rangle$ wrt. elimination ordering (e.g. lexicographic).
- ⚡ Extra variable necessary.

Saturation Algorithm (2)

Optimization

I ω -graded iff for all $x^\alpha - x^\beta \in I : \omega \cdot \alpha = \omega \cdot \beta, \omega_i > 0$

- If I is ω -graded, then $I : x_k^\infty = \langle \text{GB}(I, \prec_{\omega,k}) : x_k^\infty \rangle$.
- $I : (x_1 \cdots x_n)^\infty = (\cdots ((I : x_1^\infty) : x_2^\infty) \cdots) : x_n^\infty$

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Input: $F = J(B)$ for basis B of lattice L

Output: $G =$ ideal basis of $I(L)$

$G \leftarrow F$

for $k \leftarrow 1$ **to** n **do**

$G \leftarrow \text{GB}(G, \prec_{\omega,k}) : x_k^\infty$

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end

- Can be optimized to maximal $\frac{n}{2}$ saturation steps.
- ⚡ $\frac{n}{2}$ Gröbner basis computations in n variables.
- ⚡ Only for graded ideals, otherwise extra variable.

Shadow Algorithm

Projections

Let π_k be the projection on the first k variables ($x_{k+1}, \dots, x_n \leftarrow 1$).

- Further optimizes Saturation Algorithm
- $G = \text{GB}_k(I, \prec_{\omega,k}) \subset I$ such that $\pi_k(G) = \text{GB}(\pi_k(I), \prec_{\omega,k})$

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⚡ Only for graded ideals, otherwise extra variable.

Project-and-Lift Algorithm

Markov Bases

- Also uses projections: π_σ projects onto $\mathbb{K}[x_i : i \in \sigma]$.
- Instead of computing Gröbner bases, compute Markov bases.
- Sometimes we can simply add a polynomial to lift to larger projection.
- In remaining cases ideal is graded, so no extra variable.

Project-and-Lift Algorithm (2)

Input: Basis B of lattice L

Output: $M =$ Markov basis of L

Find (maximal) $\sigma \subset \{1, \dots, n\}$ s.t. $\ker(\pi_\sigma(L)) = \{0\}$.

Find $M \subset L$ s.t. $\pi_\sigma(M)$ is Markov basis of $\pi_\sigma(L)$.

while $\exists k \in \bar{\sigma} = \{1, \dots, n\} \setminus \sigma$ **do**

if $\exists u \in L : \pi_\sigma(u) \geq 0, u_k > 0$ **then**

$M \leftarrow M \cup \{u\}$

else

 Find $c \in \mathbb{Q}_+^n$ s.t. $\pi_{\bar{\sigma}}(c) = 0$ and $\forall u \in L : c \cdot u = -u_k$.

$M \leftarrow \text{GB}_\sigma(M, \prec_c)$

end

$\sigma \leftarrow \sigma \cup \{k\}$

end

Project-and-Lift Algorithm (3)

Optimizations

- Preprocess lattice L with `LatticeReduce` \Rightarrow short vectors.
- Use `Minimize` or extreme ray algorithm in order to find $u \in L : \pi_\sigma(u) \geq 0, u_k > 0 \Rightarrow$ short vectors.
- Lift variables x_k last for which no Gröbner basis computation is necessary.

S-Polynomial

Definition

$$S(f, g, \prec) = \frac{\text{LM}(g)}{\text{gcd}(\text{LM}(f), \text{LM}(g))} \cdot f - \frac{\text{LM}(f)}{\text{gcd}(\text{LM}(f), \text{LM}(g))} \cdot g$$

Example

$$S(x_1^2 - x_2x_3, x_1x_2^2x_3 - 1) = x_2^2x_3(x_1^2 - x_2x_3) - x_1(x_1x_2^2x_3 - 1) = x_1 - x_2^3x_3^2$$

Reduction

Reduce(f, F, \prec)

Input: Polynomial f , $F = \{f_1, \dots, f_s\}$, monomial ordering \prec

Output: $h \equiv f \pmod{\langle f_1, \dots, f_s \rangle}$ s.t. no monomial of h is in $\langle \text{LM}(F) \rangle$

$h \rightarrow 0$

while $f \neq 0$ **do**

if $\exists f_i : \text{LM}(f_i) \mid \text{LM}(f)$ **then**

$$f \rightarrow f - \frac{\text{LM}(f)}{\text{LM}(f_i)} f_i$$

else

$$h \rightarrow h + \text{LM}(f)$$

$$f \rightarrow f - \text{LM}(f)$$

end

end

Example

$$\text{Reduce}(x_1 x_2^2 x_3, \{x_1 - x_2^3 x_3^2, x_2^5 x_3^3 - 1\}, \prec_{\text{lex}}): x_1 x_2^2 x_3 \xrightarrow{x_1 - x_2^3 x_3^2} x_2^5 x_3^3 \xrightarrow{x_2^5 x_3^3 - 1} 1$$

Buchberger Algorithm

Input: Basis F of ideal I , monomial ordering \prec

Output: $G =$ Gröbner basis of I

$G \leftarrow F$

$Pairs \leftarrow \{(i, j) : 1 \leq i < j \leq \#G\}$

while $\exists(i, j) \in Pairs$ **do**

$Pairs \leftarrow Pairs \setminus \{(i, j)\}$

$h \leftarrow S(g_i, g_j, \prec)$

$h \leftarrow \text{Reduce}(h, G, \prec)$

if $h \neq 0$ **then**

$G \leftarrow G \cup \{h\}$

$Pairs \leftarrow Pairs \cup \{(i, \#G) : 1 \leq i < \#G\}$

end

end

Geometric Buchberger Algorithm

Criteria

- Buchberger: Discard (i, j) if $\text{LM}(g_i), \text{LM}(g_j)$ relatively prime.
- Gebauer-Möller: Basis of syzygies is sufficient. \Rightarrow Discard superfluous pairs (only approximation, still expensive).
- Bigatti, Hemmecke-Malkin: Criterion-Tail (only for toric ideals)
Discard (i, j) if $S(g_i, g_j)$ reduces to polynomial with smaller grading.

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Vector Arithmetic

- Use vectors $\alpha - \beta$ instead of binomials $x^\alpha - x^\beta$.
- Automatically cancels common factors (i.e. partly saturates).
- Only works for toric ideals.

Example

$$x_1^3 x_2^2 x_3 - x_1 x_2^5 x_3^3 \longrightarrow (2 \quad -3 \quad -2)^T \longrightarrow x_1^2 - x_2^3 x_3^2$$

Geometric Buchberger Algorithm (2)

Data Structures

- Originally, G is a vector.
 - Many searches in G for $\text{LM}(g_i) \mid m$ for given monomial m .
 - Vector notation: search $g_i^+ \leq m$.
- ⇒ Use multidimensional search data structure.

Geometric Buchberger Algorithm (2)

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Suggestions

- kd-Lists
- kd-Trees

Geometric Buchberger Algorithm (3)

kd-Lists

- First level: sorted array of first coordinates
- Each entry points to substructure representing all elements with this value.
- i -th level: sorted arrays of i -th coordinates of resp. substructure

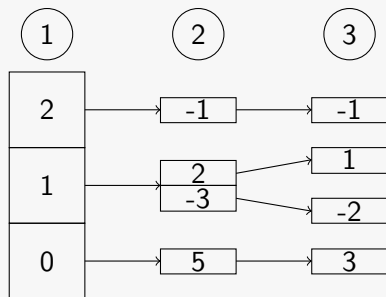


Figure: kd-List for $(2 \ -1 \ -1)$,
 $(1 \ 2 \ 1)$, $(0 \ 5 \ 3)$, $(1 \ -3 \ -2)$

Geometric Buchberger Algorithm (4)

kd-Trees

- Each level: two subtrees
- Vectors stored at leaves
- Equally balances if possible

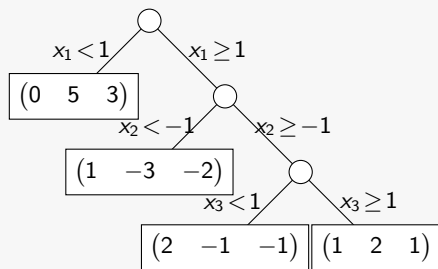


Figure: kd-Tree for $(2 \ -1 \ -1)$,
 $(1 \ 2 \ 1)$, $(0 \ 5 \ 3)$, $(1 \ -3 \ -2)$

Experimental Results

Input	P&L (uses LR)			ToricGB	ToricGB + LR
	List	KDL	KDT		
Random 1x5	0.06	0.12	0.11	0.00	0.00
Random 2x5	0.25	0.48	0.42	0.01	0.01
Random 3x5	2.45	3.42	3.54	0.35	0.31
Random 4x5	0.74	1.00	1.00	2.90	0.01
Random 5x5	0.11	0.22	0.22	0.00	0.00
Frobenius 6x 10 dig.	7.56	26.86	14.33	429.76	0.49
Frobenius 7x 10 dig.	168.33	714.25	293.49	383.29	56.80
Frobenius 8x 5 dig.	22.87	64.75	44.31	5.55	1.25
Frobenius 10x 4 dig.	24.98	50.32	43.51	3.38	1.56

Attention:

- ToricGB is implemented natively, P&L not.
- Statistic biased by memory leaks.

Conclusion

Data Structures

- Performance gain possible if implemented natively.
- kd-Lists can degenerate, thus kd-trees more promising

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Data Structures

- Performance gain possible if implemented natively.
- kd-Lists can degenerate, thus kd-trees more promising

Mathematica Implementation

- Add Criterion Tail to GroebnerBasis 'ToricGroebnerBasis.
- Add capability of projections to GroebnerBasis 'ToricGroebnerBasis.
- Use Project-and-Lift algorithm for saturation.

Thank you!