4ti2

A software package for algebraic, geometric and combinatorial problems on linear spaces

Raymond Hemmecke

University of Magdeburg, Germany

Version 1.3 now available from www.4ti2.de!

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What is 4ti2?

Algorithmic mathematics

- Extreme rays and Hilbert bases of polyhedral cones
- Circuits and Graver bases
- Gröbner bases and generating sets of lattice ideals
- (Atomic fibers)

Software

- Demonstration of practical usefulness of algorithms

Tool for proving/disproving mathematical conjectures

- Full Markov basis for $4 \times 4 \times 4$ tables (Sullivant's Challenge)
- Counter-example to normality of a certain semi-graphoid (Studený's conjecture)

Who is 4ti2?

4ti2 team/contributors of version 1.3

- University of Magdeburg, Germany
  - Raymond Hemmecke
  - Matthias Köppe
  - Matthias Walter
- CORE, Université catholique de Louvain, Belgium
  - Peter Malkin
- RISC, University of Linz, Austria
  - Ralf Hemmecke

In preparation: Computation of atomic fibers

- University of Magdeburg, Germany
  - Elke Eisenschmidt

Let us start with linear systems

Solving linear systems

Problem

$$\begin{array}{rcl} Ax & = & a \\ Bx & \leq & b \\ x & \in & \mathbf{R}^n \end{array}$$

Weyl's theorem

For every rational polyhedron P there exist finite sets $V, E \subseteq \mathbf{Q}^n$ such that

$$P = \text{conv}(V) + \text{cone}(E).$$

Description of all real solutions

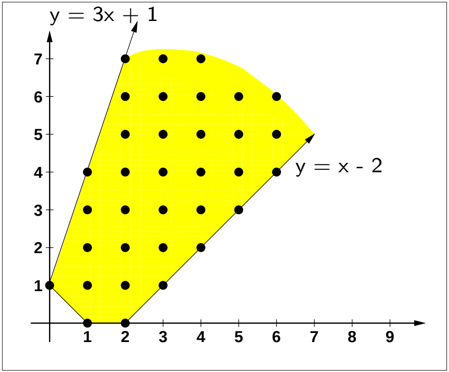
$$x = \sum \alpha_i \, x_{\text{inhom},i} + \sum \beta_j \, x_{\text{hom},j}, \quad \alpha_i, \beta_j \geq 0, \sum \alpha_i = 1$$

Goal

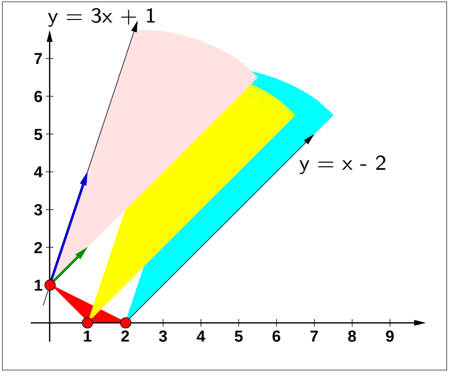
Find the finite sets V and E of *minimal* inhomogeneous and homogeneous solutions.

Example

$$
\begin{aligned}
x - y &\leq 2 \\
-3x + y &\leq 1 \\
x + y &\geq 1 \\
x, y &\geq 0 \\
x, y &\in \mathbf{R}
\end{aligned}
$$



$$\text{conv}\left(\begin{pmatrix}1\\0\end{pmatrix},\begin{pmatrix}2\\0\end{pmatrix},\begin{pmatrix}0\\1\end{pmatrix}\right)+\text{cone}\left(\begin{pmatrix}1\\1\end{pmatrix},\begin{pmatrix}1\\3\end{pmatrix}\right)$$



The homogeneous case

Extreme rays

The *extreme rays* E of a pointed rational polyhedral cone

$$C = \{x \in \mathbf{R}^n : Ax \leq 0\}$$

minimally generate the cone C, that is

$$C = \text{cone}(E).$$

Thus, every point $z \in C$ can be written as $z = \sum \alpha_i h_i$ with $h_i \in E$ and $\alpha_i \in \mathbf{R}_+$.

The inhomogeneous case

Given system

$$P = \{x \in \mathbf{R}^n : Ax \leq b\}$$

Homogenized system

$$C = \{(x, u) \in \mathbf{R}^n \times \mathbf{R}_+ : Ax - bu \leq 0\}$$

Fact

Minimal *homogeneous* solutions correspond to extreme rays with $u = 0$. $\longrightarrow E$

Minimal *inhomogeneous* solutions correspond to extreme rays with $u = 1$. $\longrightarrow V$

The double description method (Motzkin, Raiffa et al., 1953)

Problem

Compute the extreme rays of the cone $C = \{x : Ax \leq 0\}$.

Idea of double description method

$$C_j = \{x : a_i^\intercal x \leq 0 : 1 \leq i \leq j\} = \{x : A^{(j)}x \leq 0\}.$$

Use extreme rays of C_j to compute extreme rays of C_{j+1} recursively.

Facts

- Every extreme ray of C_{j+1} is a conic combination of two adjacent extreme rays of C_j.
- Two extreme rays r_1, r_2 are adjacent if there is no extreme ray r of C_j with

$$\overline{\text{supp}}(A^{(j)}r) \subseteq \overline{\text{supp}}(A^{(j)}r_1) \cap \overline{\text{supp}}(A^{(j)}r_2).$$

- This results in a simple completion algorithm for $\text{rays}(C_j) \to \text{rays}(C_{j+1})$.

A special case

Problem

Compute the extreme rays of the cone $C = \{x : Ax = 0, x \geq 0\}$.

Solution

- Compute generating set for linear space $\{x : Ax = 0\}$.
- Apply idea of double description method iteratively to $x_1 \geq 0, \ldots, x_n \geq 0$.

Project-and-lift idea

Lifting of support minimal elements

$$\text{Proj}_I(\{x : Ax = 0\}) \cap \mathbf{R}^I_+ \rightarrow \text{Proj}_{I\cup\{i\}}(\{x : Ax = 0\}) \cap \mathbf{R}^{I\cup\{i\}}_+.$$

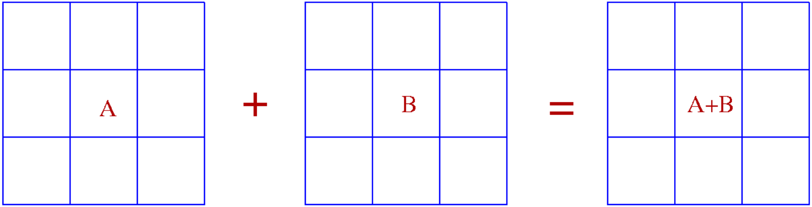
Fact

Same idea works for support minimal elements in $\{x : Ax = 0\}$, the *circuits* of A.

$\rightarrow$ output-polynomial time algorithm

Computational experiments I

Magic squares



The set of magic squares forms a pointed rational polyhedral cone.

Computational experiments on Sun Fire V890 Ultra Sparc IV, 1200 MHz

Extreme rays for magic 6×6 squares

- 97,548 extreme rays
- 43 seconds (with `4ti2`)
- 572 seconds (with `lrs`)
- 1,800 seconds (with `cdd`)

Extreme rays for magic 7×7 squares

- 5,920,184 extreme rays
- 31.74 hours (with `lrs`)
- 49.40 hours (with `4ti2`)

Circuits for example posed by Beerenwinkel

- 772,731 circuits
- 519 seconds (with `4ti2`)

Let us continue with the integer situation

Solving integer linear systems

Problem

$$\begin{array}{rcl} Ax & = & a \\ Bx & \leq & b \\ x & \in & \mathbf{Z}^n \end{array}$$

Integer analogue to Weyl's theorem

For every rational polyhedron P there exist finite sets $V, E \subseteq \mathbf{Q}^n$ such that

$$P \cap \mathbf{Z}^n = (\mathrm{conv}(V) \cap \mathbf{Z}^n) + (\mathrm{cone}(E) \cap \mathbf{Z}^n)\,.$$

Description of all integer solutions

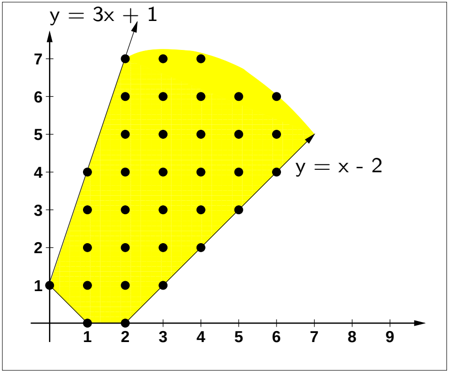
$$x = x_{\mathrm{inhom},i} + \sum \beta_j\, x_{\mathrm{hom},j}, \quad \beta_j \geq 0$$

Goal

Find the finite sets V and E of *minimal* inhomogeneous and homogeneous *integer* solutions.

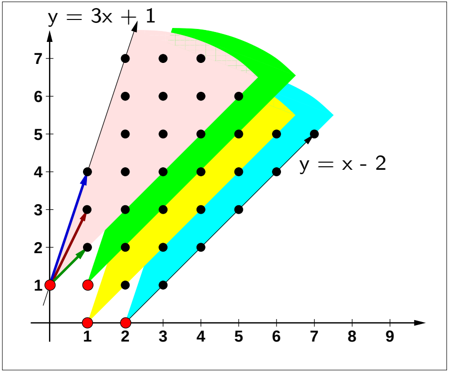
Example

$$\begin{array}{rcl} x - y & \leq & 2 \\ -3x + y & \leq & 1 \\ x + y & \geq & 1 \\ x, y & \geq & 0 \\ x, y & \in & \mathbf{Z} \end{array}$$



Solution over $\mathbb{Z}$

$$\left\{\binom{1}{0},\binom{2}{0},\binom{0}{1},\binom{1}{1}\right\} + \text{monoid}\left(\binom{1}{1},\binom{1}{2},\binom{1}{3}\right)$$



Hilbert basis

A finite set $H \subseteq C \cap \mathbf{Z}^n$ is a *Hilbert basis* of C if

$$C \cap \mathbf{Z}^n = \text{monoid}(H).$$

Thus, every point $z \in C \cap \mathbf{Z}^n$ can be written as $z = \sum \alpha_i h_i$ with $h_i \in H$ and $\alpha_i \in \mathbf{Z}_+$.

The inhomogeneous case

Given system

$$P = \{x \in \mathbf{R}^n : Ax \leq b\}$$

Homogenized system

$$C = \{(x, u) \in \mathbf{R}^n \times \mathbf{R}_+ : Ax - bu \leq 0\}$$

Fact

Minimal *homogeneous* integer solutions correspond to Hilbert basis elements with $u = 0$. $\rightarrow E$

Minimal *inhomogeneous* integer solutions correspond to Hilbert basis elements with $u = 1$. $\rightarrow V$

Normality problem

Let $A \subseteq \mathbf{Z}^{d\times n}$ such that lattice$(A) = \mathbf{Z}^d$. Decide whether monoid$(A) =$ cone$(A) \cap \mathbf{Z}^d$.

Solution

If monoid(A) has *holes*, there must be one in hilbert(cone(A)).

Harder problem: find *all* holes

If monoid$(A) \subsetneq$ cone$(A) \cap \mathbf{Z}^d$, find a finite description for cone$(A) \cap \mathbf{Z}^d \setminus$ monoid(A).

$\rightarrow$ H.+Takemura+Yoshida: "Computing holes in semi-groups"

"Integer double description method" (Contejean, Devie, ...)

Problem

Compute the Hilbert basis of the cone $C = \{x : Ax \leq 0\}$.

Idea

$$C_j = \{x : a_i^\intercal x \leq 0 : 1 \leq i \leq j\} = \{x : A^{(j)} x \leq 0\}.$$

- Use Hilbert basis of C_j to compute Hilbert basis of C_{j+1} recursively.
- This leads again to a simple completion algorithm for hilbert$(C_j) \rightarrow$ hilbert(C_{j+1}).

Special case (H., 2002)

Idea gives again a project-and-lift algorithm for hilbert$(\{x : Ax = 0, x \geq 0\})$.

Graver basis of A (H., 2002)

Algorithm can be adapted to compute graver$(A) := \bigcup_j$ hilbert$\{x \in \mathcal{O}_j : Ax = 0\})$.

$\rightarrow$ output-polynomial time algorithm

Computational experiments II

Computational experiments on Sun Fire V890 Ultra Sparc IV, 1200 MHz

Hilbert basis for magic 6×6 squares

- 522,347 elements
- ca. 10 days (with `4ti2`)

Homogeneous primitive partition identities

- Example:

$$1 + 1 + 4 = 2 + 2 + 2$$

- $$\text{graver} \begin{pmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & 2 & 3 & \dots & 20 \end{pmatrix}$$

- 1,254,767 elements
- 5.25 days (with `4ti2`)

Let us conclude with lattice ideals

Problem

- In statistics, we wish to test using a sample of data whether a population has a specific distribution.
- For example, we may want to know if eye colour is independent of hair colour.

	Black	Brown	Red	Blonde	Total
Brown	68	119	26	7	220
Blue	20	84	17	94	215
Hazel	15	54	14	10	93
Total	103	257	57	111	528

- We want to know if the sample data is statistically significantly different from its expected values.
- Significantly different is defined in comparison to all other possible contingency tables with the same column and row sums.

However

- There may be too many other tables to enumerate them all.
- Thus, we sample them using basic moves to set up a *Markov chain*.
- The set of basic moves is called a *Markov basis*.

Markov bases

- We sample in the fiber $\{z : Az = b, z \in \mathbf{Z}^n_+\}$ for fixed b.
- Moves are integer solutions to $Ax = 0$.
- $M \subseteq \ker_{\mathbf{Z}}(A)$ is called a Markov basis of A if it connects $\{z : Az = b, z \in \mathbf{Z}^n_+\}$ for every b.

Fact (Diaconis+Sturmfels)

M is a Markov basis of A if and only if $\{x^{m^+} - x^{m^-} : m \in M\}$ is a generating set of

$$I_A := \langle x^u - x^v : Au = Av, u, v \in \mathbf{Z}^n_+\rangle.$$

Test sets in integer programming

Problem

$$\min\{c^\intercal z : Az = b, z \in \mathbf{Z}^n_+\} \quad (*)$$

Augmentation algorithm

- Find a feasible solution $z_0 \in \mathbf{Z}^n$ to $Az = b, z \geq 0$.
- While there is an improving direction $t \in \mathbf{Z}^n$, set $z_0 := z_0 - t$.

Test sets

A set $T \subseteq \mathbf{Z}^n$ is called a *test set* for (*) if

- for every right-hand side b and
- for every non-optimal feasible solution z_0 to (*)
- there exists some improving direction $t \in T$.

Toric Gröbner bases constitute test sets for c fixed, b variable (Conti+Traverso)

$$I_A := \langle x^u - x^v : Au = Av, u, v \in \mathbf{Z}^n_+ \rangle$$

$$x^u \succ x^v \Leftrightarrow (c^\intercal u > c^\intercal v) \text{ or } (c^\intercal u = c^\intercal v \text{ and } u \succ v)$$

Universal test sets

Universal test sets

A set $T \subseteq \mathbf{Z}^n$ is called a *universal test set* if T is a test set for (*) for every b and c.

Graver bases are finite universal test sets (Graver)

Using Graver basis directions, only *polynomially many* augmentation steps are necessary. (Schulz+Weismantel)

Finite test sets for certain convex objectives (Murota+Saito+Weismantel, H.)

There are finite test sets also for problems

$$\min \left\{ \sum_{i=1}^{s} f_i(c_i^\intercal z + c_{i,0}) + c^\intercal z : Az = b, z \in \mathbf{Z}_+^n \right\}$$

for any collection of convex functions $f_i : \mathbf{R} \to \mathbf{R}$.

Toric Gröbner bases and Markov bases

Main problem

Find a generating set for I_A. $\rightarrow$ *Markov basis*

A little history

- 1991: Conti+Traverso: Eliminate y from

$$\{y_1 - x^{A_{.1}}, \ldots, y_n - x^{A_{.n}}\}.$$

- 1995: Hoşten+Sturmfels: Saturation algorithm, F is a lattice basis of $\ker(A)$

$$I_A \quad = \quad \langle x^{u^+} - x^{u^-} : u \in F\rangle : (x_1 x_2 \ldots x_n)^\infty$$

- 1999: Bigatti+LaScala+Robbiano: implementation of saturation in `CoCoA`
- 2005: Malkin: Project-and-lift algorithm and implementation in `4ti2`

Project-and-lift algorithm (Malkin)

Idea

1. Choose $J \subseteq \{1,\ldots,n\}$ and compute generating set for

$$I_{A,J} := \langle x^u - x^v : Au = Av, u, v \in \mathbf{Z}_+^n \rangle \subseteq k(x_{\overline{J}})[x_J]$$

   for example via the saturation algorithm.
2. For $i \in \overline{J}$, compute a certain degrevlex Gröbner basis for $I_{A,J}$, where the term ordering depends on i-th component.
3. Translate Gröbner basis into polynomial ring $k\left(x_{\overline{J}\setminus\{i\}}\right)\left[x_{J\cup\{i\}}\right]$ and repeat.

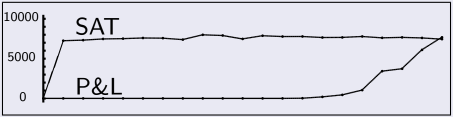
Nice fact implied by special term ordering

The Gröbner basis of $I_{A,J}$ in $k(x_{\overline{J}})[x_J]$ lifts to a Gröbner basis in $k\left(x_{\overline{J}\setminus\{i\}}\right)\left[x_{J\cup\{i\}}\right]$.

Advantages

Size of Gröbner bases

Intermediate Gröbner bases increase only slowly in size.



Critical-pair criteria

more efficient $\rightarrow$ cancelation criterion

Truncated generating sets of lattices (Malkin, 2006)

Truncation (Thomas+Weismantel) can be combined with project-and-lift idea.

Computational experiments III

Computational experiments on Sun Fire V890 Ultra Sparc IV, 1200 MHz

Markov basis for $4 \times 4 \times 4$ table (Sullivant's challenge)

- 148,654 elements
- ca. 2.5 days (with `4ti2`)

Markov bases of phylogenetic trees (Eriksson)

- Successful computations with $2,048$ variables.
- ca. 15 minutes (with `4ti2`)

Normality of semi-group (Studený's question)

- 32×80 matrix
- `4ti2` was used to find a non-squarefree *indispensible* Markov basis element.
- This move was translated into a hole of the semi-group.
- `4ti2` was used to give a computational proof of hole-property.

www.4ti2.de

Thank you for your attention!