Markov Bases in Polymake

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Overview

Markov Basis

Definition

- Given a lattice $\mathcal{L} \subset \mathbb{Z}^n$ we define

$$\mathcal{F}_{\mathcal{L},b} := \{z : z = b \bmod \mathcal{L}, z \in \mathbb{Z}^n_+\}.$$

- For $S \subset \mathcal{L}$ we define $\mathcal{G}(\mathcal{F}_{\mathcal{L},b}, S)$ to be the undirected graph with vertices $\mathcal{F}_{\mathcal{L},b}$ and edges (u, v) for $u - v \in S$ or $v - u \in S$.
- We say S is a generating set of $\mathcal{F}_{\mathcal{L},b}$ if $\mathcal{G}(\mathcal{F}_{\mathcal{L},b}, S)$ is connected.
- We say S is a Markov basis if S is a generating set for $\mathcal{F}_{\mathcal{L},b}$ for any $b \in \mathbb{Z}^n$.

Remark

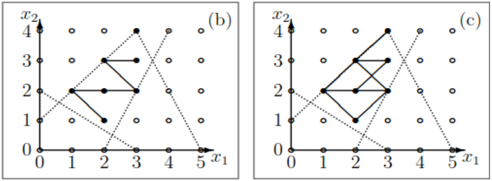
Note when $\mathcal{L} \cap \mathbb{Z}^n_+ = \{0\}$, $\mathcal{F}_{\mathcal{L},b}$ is finite for any $b \in \mathbb{Z}^n$.

Example

Let $S = \{(1,-1,-1,-3,-1,2),(1,0,2,-2,-2,1)\}$, and let $\mathcal{L}$ be the lattice spanned by S, then we have that $\mathcal{L}$ is the integer kernel of

$$A = \begin{bmatrix} -2 & -3 & 1 & 0 & 0 & 0 \\ 2 & -1 & 0 & 1 & 0 & 0 \\ 2 & 1 & 0 & 0 & 1 & 0 \\ -1 & 1 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Let $b = (2,2,4,2,4,1)$, and consider $\mathcal{F}_{\mathcal{L},b}$ projected onto the (x_1, x_2)-plane.



Lattice Ideals

Definition

Given a set $S \subset \mathbb{Z}^n$ define the $I(S)$ as

$$I(S) := \langle x^a - x^b : a - b \in \mathcal{L} \rangle = \langle x^{u_+} - x^{u_-} : u \in S \rangle$$

When $\mathcal{L} \subset \mathbb{Z}^n$ is a lattice, we call $I(\mathcal{L})$ a lattice ideal

Lemma

A set M is a Markov basis if and only if $I(M) = I(\mathcal{L})$

Term Order and Gröbner basis

Definition

- We call $\succ$ a term order for $\mathcal{L}$ if $\succ$ is a total well ordeing on $\mathcal{F}_{\mathcal{L},b}$ for all $b \in \mathbb{Z}^n$ and an additive order.
- We define $\mathcal{L}_{\succ} := \{u \in \mathcal{L} : u^+ \succ u^-\}$.
- We call $G \subset \mathcal{L}_{\succ}$ a Gröbner basis of $\mathcal{L}$ with respect to $\succ$ if for every $b \in \mathbb{Z}^n_+$ there exists a decreasing path in $\mathcal{G}(\mathcal{F}_{\mathcal{L},b})$ from b to the unique $\succ$-minimal element in $\mathcal{F}_{\mathcal{L},b}$.

Lemma

Given a term order $\succ$ a set $G \subset \mathcal{L}_{\succ}$ is a $\succ$-Gröbner basis of $\mathcal{L}$ if and only if for all $v \in \mathcal{L}_{\succ}$ there exists $u \in \mathcal{L}_{\succ}$ such that $u^+ \leq v^+$, that is, $v^+ - u \in \mathcal{F}_{\mathcal{L},v^+}$ and $v^+ \succ v^+ - u$.

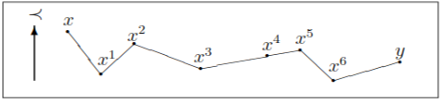
Reduction Paths

Definition

A path $(z_0, z_1, \dots, z_i)$ in $\mathcal{G}(\mathcal{F}_{\mathcal{L},b}, G$ is a reduction path with respect to $\succ$ if for no $i \in \{1, \dots, k-1\}$ both $z_i \succ z_0$ and $z_i \succ z_k$.

Lemma

Let $\succ$ be a term order of $\mathbb{Z}^n_+$. A set $G \subset \mathcal{L}_\succ$ is a $\succ$-Gröbner basis if and only if for any $b \in \mathbb{Z}^n$ and for each pair $u, v \in \mathcal{F}_{\mathcal{L},b}$ there exists a reduction in $\mathcal{G}(\mathcal{F}_{\mathcal{L},b})$ between u and v.



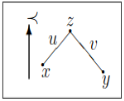
Critical Paths

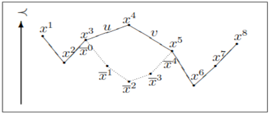
Definition

Given $G \subset \mathcal{L}_{\succ}$ and $b \in \mathbb{Z}^n$, a path (α, z, β) is a critical path if $z \succ \alpha$ and $z \succ \beta$.

Lemma

A set $G \subset \mathcal{L}_{\succ}$ is a Gröbner basis of $\mathcal{L}$ if and only if G is a generating set of $\mathcal{L}$ and if for all $b \in \mathbb{Z}^n$ and for every critical path (α, z, β) in $\mathcal{G}(\mathcal{F}_{\mathcal{L},b}, G)$ there exists a reduction path in $\mathcal{G}(\mathcal{F}_{\mathcal{L},b}, G)$.





Minimal Critical Paths

Definition

- A critical path (α, z, β) is minimal if there does not exist another critical path $(\alpha', z', \beta') = (\alpha + \gamma, z + \gamma, \beta + \gamma)$ for some $\gamma \in \mathbb{Z}_+^n$.
- The unique minimal critical path for a pair $(u, v) \in \mathcal{L}$ is denoted by $(\alpha^{(u,v)}, z^{(u,v)}, \beta^{(u,v)})$, where $z^{(u,v)} := max\{u^+, v^+\}$, $\alpha^{(u,v)} := z - u$, $\beta^{(u,v)} := z - v$.

Remark

Using minimal critical paths we reduce the amount of reduction paths to be checked to a finite number.

Projecting and Lifting

Lemma

- *If* $\mathcal{L} \cap \mathbb{Z}_+^n \neq 0$, *then let* $a \in \mathcal{L} \cap \mathbb{Z}_+^n$, *and we know there is an* i *such that* $a_i > 0$. *Let* $M \subset \mathcal{L}$ *be such that* M^i *is a Markov basis of* $\mathcal{L}^i$, *then* $M \cup \{a\}$ *is a Markov basis for* $\mathcal{L}$
- *If* $\mathcal{L} \cap \mathbb{Z}_+^n = 0$, *then we can find a term order* $\succ_c$ *on* $\mathcal{L}$.
- *A set* $G \subset \mathcal{L}_{\succ_c}$ *is a* $\succ_c$ *Gröbner basis for* $\succ_\rfloor$ *if and only if* G^i *is a* $\succ_c^i$*-Gröbner basis for* $\mathcal{L}^i$.

Geometric Buchberger

Input: a term ordering $\succ$ and a set $S \subset \mathcal{L}$
Output: a set $G \subset \mathcal{L}$ such that if α, β are connected in $\mathcal{G}(\mathcal{F}_{\mathcal{L},\alpha}, G)$ then there exists a reduction path between α and β in $\mathcal{G}(\mathcal{F}_{\mathcal{L},\alpha}, G)$.

$G \leftarrow \{u : u^+ \succ u^-, u \in S\} \cup \{u : u^- \succ u^+, u \in S\}$
$C \leftarrow \{(u, v) : u, v \in G\}$
while $C \neq \emptyset$ **do**
  select $(u, v) \in C$
  $C \leftarrow C \setminus (u, v)$
  $r \leftarrow MDPA(\alpha^{(u,v)}, G) - MDPA(\beta^{(u,v)}, G)$
  if $r \neq 0$ **then**
    if $r^- \succ r^+$ **then**
      $r \leftarrow -r$
    end if
    $C \leftarrow C \cup \{(r, s) : s \in G\}$
    $G \leftarrow G \cup r$
  end if
end while
return G

Maximal Decreasing Path Algorithm

Input: a vector $\alpha \in \mathbb{Z}_+^n$ and a set $G \subset \mathcal{L}_\succ$.
Output: a vector α' where there is a maximal decreasing path in $\mathcal{G}(\mathcal{F}_{\mathcal{L},\alpha}, G)$ from α to α'.

1: $\alpha' \leftarrow \alpha$
2: **while** there is some $u \in G$ such that $u^+ \leq \alpha^+$ **do**
3: $\quad \alpha' \leftarrow \alpha' - u$
4: **end while**
5: **return** α'

Project and Lift

Input: A lattice $\mathcal{L}$.
Output: A Markov basis M of $\mathcal{L}$.

Find a set $\sigma \subset \{1, 2, \ldots, n\}$ such that $\ker^\sigma(\mathcal{L}) = 0$
Find a set $M \subset \mathcal{L}$ such that M^σ is a Markov basis $\mathcal{L}^i$
while $\sigma \neq \emptyset$ **do**
    Select $i \in \sigma$
    if There exists $a \in \mathcal{L}$ such that $a^\sigma \geq 0$ and $a_i > 0$ **then**
        $M \leftarrow M \cup \{a\}$
    else
        Find $c \in \mathbb{R}^n_+$ such that $c_\sigma = 0$ and $c^T u = -u_i$ for all $u \in \mathcal{L}$
        Using M, compute $G \subset \mathcal{L}$ such that G^σ is a $\succ^\sigma_c$ - Gröbner basis of $\mathcal{L}^\sigma$
        $M \leftarrow G$
    end if
    $\sigma \leftarrow \sigma \setminus \{i\}$
end while
return M

References

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