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COMPUTING HOLES IN SEMI-GROUPS

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Abstract. In this paper we present an algorithm to compute an explicit description for the difference of a semi-group Q generated by vectors in $\mathbb{Z}^d$ and its saturation Q_{sat}. If $H = Q_{\text{sat}} \setminus Q$ is finite, we give an upper bound for the entries of $h \in H$. Finally, we present an algorithm to find all Q-minimal saturation points in Q.

1. Introduction

To specify the problem under consideration, let us start with a few definitions. For a matrix $A \in \mathbb{Z}^{d\times n}$, let C, L, and Q denote the cone, the lattice, and the semi-group (monoid) spanned by the columns $A_{.j}$, $j = 1, \ldots, n$, of A. Throughout this paper, we assume the cone C to be pointed. By $Q_{\text{sat}} = C \cap L$ we denote the *saturation* of Q and call Q *normal* if the set $H = Q_{\text{sat}} \setminus Q$ is empty. The elements of H are called *holes* and a hole $h \in H$ is *fundamental* if there is no other hole $h' \in H$ such that $h - h' \in Q$. While F is always finite [7], H could be infinite, see Example 1.1.

Finally, we call $s \in Q$ a *saturation point* of Q, if $s + Q_{\text{sat}} \subseteq Q$. The set of all saturation points of Q is denoted by S. By $\min(S;Q)$ we denote the set of all Q-minimal elements of S, that is, the set of all $s \in S$ for which there is no other $s' \in S$ with $s - s' \in Q$. Again, it can be shown that $\min(S;Q)$ is always finite [7, Prop. 4.4].

Example 1.1. Consider the 2×4 matrix

$$A = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 2 & 3 & 4 \end{pmatrix}.$$

The associated semi-group Q has infinitely many holes

$$H = \{(1,1)^\intercal + \alpha \cdot (1,0)^\intercal : \alpha \in \mathbb{Z}_+\},$$

out of which only $(1,1)^\intercal$ is fundamental, see Figure 1. Moreover, the semi-group Q has three Q-minimal saturation points: $(1,2)^\intercal$, $(1,3)^\intercal$, and $(1,4)^\intercal$. □

For given A, it is already an interesting combinatorial question to decide whether Q is normal or equivalently, whether $H = \emptyset$. Considering the enormous computational difficulties in deciding the existence or non-existence of holes in practice, it is probably not very surprising that there do not exist many studies on the *structure* and the *explicit computation* of the set H when $H \neq \emptyset$. In [7], Takemura and Yoshida established various conditions for *finiteness* of H. Moreover, they presented some results on the *location* of the holes inside of Q_{sat} [8]. In this paper, we present an algorithm that computes an *explicit* representation of H. If H is finite, we can use this approach to find bounds on the entries

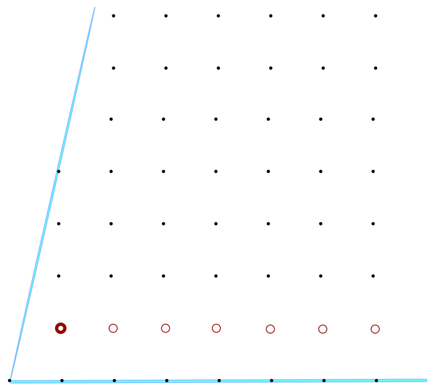

Figure 1: Non-holes, holes and fundamental hole for Example 1.1

of $h \in H$. Moreover, we can adapt this algorithmic idea to compute the set $\min(S;Q)$ of Q-minimal saturation points of Q.

The reader should note that for fixed matrix sizes d and n, there exists a *polynomial size* encoding of the generating function $f(H;z) = \sum_{h\in H} z^h$ (where $z^h := z_1^{h_1} \cdot \ldots \cdot z_d^{h_d}$) as a *short* rational generating function [7]:

$$f(H;z) = \sum_{i\in I} \gamma_i \frac{z^{\alpha_i}}{\prod_{j=1}^{d}(1-z^{\beta_{ij}})}.$$

Herein, I is a finite (polynomial size) index set and all appearing data $\gamma_i \in \mathbb{Q}$ and $\alpha_i, \beta_{ij} \in \mathbb{Z}^d$ is of size polynomial in the input size of A. In fact, this observation is based on a result by Barvinok and Woods [2], who showed that there are such short rational function encodings for Q and for Q_{sat}, and consequently, also for $f(H;z) = f(Q_{\text{sat}};z) - f(Q;z)$. However, although the proof by Barvinok and Woods is constructive, its practical usefulness still has to be proven by an efficient implementation. Finally, note that once $f(H;z)$ has been computed, one can also decide in polynomial time (when d and n are kept fix) whether the sum of rational functions $f(H;z)$ encodes a polynomial or an infinite series. Thus, one can decide finiteness of H [7]. If H is finite, one can then decide $H = \emptyset$ by checking whether $f(H;z) = 0$. Again, for fixed d and n, this can be done in polynomial time.

In the following, and in contrast to the *implicit* representation via rational generating functions, we present an algorithm to compute an *explicit* representation of H. Note that such an explicit representation needs not be of polynomial size in the input size of A, even when d and n are fixed. Moreover, an explicit representation of H cannot be recovered easily from an implicit short rational function encoding of $f(H;z)$.

Our algorithm follows three main steps:

(1) Compute the set F of fundamental holes.
(2) For each of the finitely many $f \in F$, compute the set $\min((f+Q)\cap Q;Q)$ of Q-minimal elements in $(f+Q)\cap Q$. Herein, $s \in (f+Q)\cap Q$ is called Q-minimal if there is no other $s' \in (f+Q)\cap Q$ with $s - s' \in Q$.
(3) From the Q-minimal elements in $(f+Q)\cap Q$, compute an explicit representation of the holes of Q lieing in $f+Q$.

Let us now demonstrate how to perform each task algorithmically. We accompany the theoretical constructions with a running example, Example 1.1.

2. Computing the fundamental holes F

The set F of fundamental holes is finite [7], since it is a subset of

$$P := \left\{ \sum_{j=1}^{n} \lambda_j A_{.j} : 0 \leq \lambda_1, \ldots, \lambda_n < 1 \right\}.$$

This can be seen as follows. Since each $f \in F$ lies also in C and thus can be written as $f = A\lambda = \sum_{j=1}^{n} \lambda_j A_{.j}$ for some $\lambda \geq 0$. If $\lambda_i \geq 1$ for some $i \in \{1, \ldots, n\}$ then $f' = f - A_{.i} \in C \cap L$ would contradict the Q-minimality of f, since $f - f' = A_{.i} \in Q$. Consequently, $\lambda_j < 1$ for all j.

This shows that F is finite. It also gives a finite procedure to enumerate F:

- Enumerate $P \cap L$.
- Check for each $z \in P \cap L$ whether z is a fundamental hole, that is, check infeasibility of $A\lambda = z, \lambda \in \mathbb{Z}_+^n$ and check whether $z - A_{.j} \in P \cap L \subseteq Q$ for some j.

This construction can be sped-up as follows. First compute the (unique) inclusion-minimal integral generating set B of $C \cap L$ [5]. Remember that B is called an *integral generating set* if every $z \in C \cap L$ can be written as a nonnegative integer linear combination of elements of B. Again, one can easily show that $B \subseteq P$. If $L = \mathbb{Z}^d$, an integral generating set is also known as a *Hilbert basis* of the cone C. If B contains no hole of Q, Q must be normal. Moreover, every hole of Q appearing in B must be fundamental, since B is minimal. Finally, if $f \in F$ is not in B, f can be written as a nonnegative integer linear combination of elements in B, since $f \in C \cap L$ and since B is an integral generating set of $C \cap L$. This representation cannot have summands that are not fundamental holes, since otherwise f is not fundamental. To see this, let

$$f = \sum_{b \in B \cap F} \lambda_b b + \sum_{b \notin B \cap F} \mu_b b, \quad \lambda_b, \mu_b \in \mathbb{Z}_+ \ \forall b.$$

Observe, that

$$f' = \sum_{b \in B \cap F} \lambda_b b$$

must be a hole of Q, as otherwise f is not a hole. But since

$$f - f' = \sum_{b \notin B \cap F} \mu_b b \in Q,$$

f cannot be a fundamental hole. Thus, we can enumerate F as follows:

- Compute the minimal integral generating set B of $C \cap L$.
- Check each $z \in B$ whether it is a fundamental hole or not, that is, compute $B \cap F$.
- Generate all nonnegative integer combinations of elements in $B \cap F$ that lie in P and check for each such z whether it is a fundamental hole or not.

Example 1.1 cont. In our example, the lattice L generated by the columns of A is simply $L = \mathbb{Z}^2$. With this, the minimal Hilbert basis B of $C \cap L$ consists of 5 elements:

$$B = \{(1,0)^\intercal, (1,1)^\intercal, (1,2)^\intercal, (1,3)^\intercal, (1,4)^\intercal\},$$

out of which only $(1,1)^\intercal$ is a hole. Being in B, $(1,1)^\intercal$ must be a fundamental hole. Thus, $B \cap F = \{(1,1)^\intercal\}$. Constructing nonnegative integer linear combinations of elements from $B \cap F$, we already see that the combination $2 \cdot (1,1)^\intercal = (2,2)^\intercal$ is an element of Q and consequently, there is no other fundamental hole in Q, i.e. $F = \{(1,1)^\intercal\}$. □

3. Computing the Q-minimal elements in $(f + Q) \cap Q$

Note that a point $z \in f + Q$ is either a hole, that is $z \in H$, or it satisfies $z \in Q$ and consequently $z + Q \subseteq Q$. Thus, to represent the non-holes in $f + Q$, it suffices to compute the Q-minimal elements in $(f + Q) \cap Q$. In order to compute these Q-minimal elements, we have to find an explicit representation for the solutions of

$$\{\lambda \in \mathbb{Z}_+^n : \exists \mu \in \mathbb{Z}_+^n \text{ such that } f + A\lambda = A\mu\}. \tag{1}$$

Every Q-minimal point $z \in (f + Q) \cap Q$ must correspond to a minimal inhomogeneous solution λ of this system. This can be seen by assuming that $0 \leq \lambda' \leq \lambda$ is a nonzero and smaller inhomogeneous solution to the above system. Then $z' = f + A\lambda' \in (f + Q) \cap Q$ and $z - z' = A(\lambda - \lambda') \in Q$, contradicting Q-minimality of z.

The (finitely many) minimal inhomogeneous solutions to the above linear system can be computed, for example, with `4ti2` [4]. However, `4ti2` currently only allows the computation of all minimal inhomogenous solutions (λ, μ) of the related system

$$\{(\lambda, \mu) \in \mathbb{Z}_+^{2n} : f + A\lambda = A\mu\}. \tag{2}$$

As every minimal solution λ to (1) must appear in a minimal solution (λ, μ) of (2), `4ti2` computes a set from which all desired minimal inhomogeneous solutions λ to (1) can be extracted. However, there may exist many more minimal inhomogeneous solutions to (2) than to (1). Here, an algorithmic improvement to compute the minimal inhomogenous solutions to (1) directly is desirable.

Example 1.1 cont. Let $f = (1,1)^\intercal$ and consider $(f + Q) \cap Q$. The linear system to solve is

$$\begin{array}{ccccccccccccccc} 1 & + & \lambda_1 & + & \lambda_2 & + & \lambda_3 & + & \lambda_4 & = & \mu_1 & + & \mu_2 & + & \mu_3 & + & \mu_4 \\ 1 & & & + & 2\lambda_2 & + & 3\lambda_3 & + & 4\lambda_4 & = & & & 2\mu_2 & + & 3\mu_3 & + & 4\mu_4 \end{array}$$

with $\lambda_i, \mu_j \in \mathbb{Z}_+, i, j \in \{1,2,3,4\}$.

`4ti2` gives the following 5 minimal inhomogeneous solutions (λ, μ) to system (2):

$$\begin{array}{rcl} (\lambda, \mu) & \rightarrow & z = f + A\lambda \\ (0,0,0,2,0,0,3,0)^\intercal & \rightarrow & (3,9)^\intercal \\ (0,1,0,0,1,0,1,0)^\intercal & \rightarrow & (2,3)^\intercal \\ (0,0,1,0,1,0,0,1)^\intercal & \rightarrow & (2,4)^\intercal \\ (0,0,1,0,0,2,0,0)^\intercal & \rightarrow & (2,4)^\intercal \\ (0,0,0,1,0,1,1,0)^\intercal & \rightarrow & (2,5)^\intercal \end{array}$$

As we can see, different minimal inhomogeneous solutions (λ, μ) may correspond to the same Q-minimal point in $f+Q$. Moreover, the point $(3,9)^\intercal$ is not Q-minimal, showing that there may exist minimal inhomogeneous solutions (λ, μ) that do not correspond to Q-minimal points in $f+Q$. While the first situation may also happen in general for different minimal inhomogeneous solutions λ, the second situation only occurs since we computed minimal inhomogeneous solutions (λ, μ) of system (2) instead of minimal inhomogeneous solutions λ of system (1). □

4. Computing the holes in $f+Q$

Having found the Q-minimal non-holes in $f+Q$, we can find an explicit representation for all holes in $f+Q$ as follows. First, let us construct a monomial ideal $I_{A,f} \in \mathbb{Q}[x_1, \ldots, x_n]$ generated by the monomials

$$I_{A,f} = \langle x^\lambda : \lambda \in \mathbb{Z}_+^n, f + A\lambda \in (f+Q) \cap Q \rangle.$$

Clearly, this monomial ideal is already determined by all λ such that $f + A\lambda$ is Q-minimal in $(f+Q) \cap Q$. Note that under our assumption that C is pointed, there are only finitely many $\lambda \in \mathbb{Z}_+^n$ such that $f + A\lambda = z$ for each $z \in f+Q$. Thus, by solving $f + A\lambda = z, \lambda \in \mathbb{Z}_+^n$ for all Q-minimal points in $(f+Q) \cap Q$, for example by using `4ti2`, we can find a finite generating set for $I_{A,f}$.

Note that the map $x^\lambda \mapsto z = A\lambda$ is not one-to-one. While the monomial x^λ corresponds to $z = f + A\lambda \in f + Q$, we have $z \in (f+Q) \cap Q$ if and only if $x^\lambda \in I_{A,f}$. Thus, the set of holes in $f+Q$ corresponds to the set of standard monomials of the monomial ideal $I_{A,f}$. It is not surprising that there exist algorithms to explicitly represent this set of standard monomials [6]. Mapping this explicit representation for the standard monomials x^λ back to $z \in f+Q$, we get a finite representation of the holes in $f+Q$.

Example 1.1 cont. Let us construct the generators of the monomial ideal $I_{A,f}$. For this, we have to find all representations of the form $z = f + A\lambda, \lambda \in \mathbb{Z}_+^4$ for each Q-minimal element z in $(f+Q) \cap Q$, i.e. for each $z \in \{(2,3)^\intercal, (2,4)^\intercal, (2,5)^\intercal\}$.

$$\begin{array}{rcl} z & = & f + A\lambda \\ (2,3)^\intercal & = & (1,1)^\intercal + A(0,1,0,0)^\intercal \\ (2,4)^\intercal & = & (1,1)^\intercal + A(0,0,1,0)^\intercal \\ (2,5)^\intercal & = & (1,1)^\intercal + A(0,0,0,1)^\intercal \end{array}$$

Thus, we get the monomial ideal

$$I_{A,f} = \langle x_2, x_3, x_4 \rangle,$$

whose set of standard monomials is $\{x_1^\alpha : \alpha \in \mathbb{Z}_+\}$. Thus, the set of holes in $f+Q$ is

$$\{f + \alpha A_{.1} : \alpha \in \mathbb{Z}_+\} = \{(1,1)^\intercal + \alpha(1,0)^\intercal : \alpha \in \mathbb{Z}_+\}$$

as already claimed above. □

5. Computing all Q-minimal saturation points

Let us now show how the above approach can be used in order to compute $\min(S;Q)$, the set of all Q-minimal saturation points of Q. Note that our construction recovers the known fact that $\min(S;Q)$ is always finite [7, Prop. 4.4].

We have the following equivalences:

$$\begin{aligned} s \in S \quad &\Leftrightarrow \quad s \in Q \text{ and } s + Q_{\text{sat}} \subseteq Q \quad \text{(by definition)} \\ &\Leftrightarrow \quad s \in Q \text{ and } s + H \subseteq Q \quad (\text{since } Q_{\text{sat}} = Q \cup H \text{ and } s + Q \subseteq Q,\ \forall s \in Q) \\ &\Leftrightarrow \quad s \in Q \text{ and } s + F \subseteq Q \quad (\text{since } H \subseteq F + Q) \\ &\Leftrightarrow \quad s + f \in f + Q \text{ and } s + f \subseteq Q \quad \forall f \in F \\ &\Leftrightarrow \quad s + f \in (f + Q) \cap Q \quad \forall f \in F. \end{aligned}$$

Consequently, we have

$$s \in S \Leftrightarrow s \in \bigcap_{f \in F} [((f + Q) \cap Q) - f]$$

and thus, with $s = A\lambda$ for some $\lambda \in \mathbb{Z}_+^n$ (as $s \in Q$), we get

$$s \in S \Leftrightarrow x^\lambda \in \bigcap_{f \in F} I_{A,f} =: I_A,$$

by definition of the monomial ideals $I_{A,f}$. The ideal I_A is in fact again a monomial ideal and can be found algorithmically, for example with the help of Gröbner bases [3]. The elements $s \in \min(S;Q)$ correspond exactly to the (finitely many!) ideal generators x^λ of I_A via the relation $s = A\lambda$. (Remember, however, that this relation need not be one-to-one.)

Example 1.1 cont. In our example, we have $I_A = I_{A,f} = \langle x_2, x_3, x_4 \rangle$, as there exists only one fundamental hole f. The three generators of I_A correspond to the three Q-minimal saturation points $(1,2)^\intercal$, $(1,3)^\intercal$, and $(1,4)^\intercal$. □

6. Computing bounds

For this section, let us assume that H is finite. Using the above approach, we establish a bound on the size of $\|h\|_\infty$ for all $h \in H$. Clearly, such a bound can then be used to show that H cannot be finite if a hole with sufficiently big entries has been found. Let upper indices denote components of vectors, e.g. $f^{(i)}$.

First, we can bound the elements $f \in F$ using again the relation

$$F \subseteq \left\{ \sum_{j=1}^n \lambda_j A_{\cdot j} : 0 \leq \lambda_1, \ldots, \lambda_n < 1 \right\}.$$

Thus, we get for all $f \in F$ the bound $\|f\|_\infty \leq M_F(A) := \max_{i=1,\ldots,d} \sum_{j=1}^n |A_{ij}| - 1$.

Next, as H is finite, all ideals $I_{A,f}$, $f \in F$, must have a finite set of standard pairs, which is equivalent to saying that there must be a monomial generator $x_j^{\alpha_j}$ for every $j = 1, \ldots, n$. In the language of [7, Thm. 3.3], this minimal value α_j is denoted by $\bar{\lambda}_{fj}$. Such a monomial generator corresponds to a minimal inhomogeneous solution $(\alpha_j, \mu) \in \mathbb{Z}_+^{n+1}$ to $f + \alpha_j A_{.j} = A\mu$. Let us now bound the values for such a minimal α_j.

First, the minimal inhomogeneous solutions $(\alpha_j, \mu) \in \mathbb{Z}_+^{n+1}$ to $f + \alpha_j A_{.j} = A\mu$ correspond exactly to the minimal homogeneous solutions $(u, \alpha_j, \mu) \in \mathbb{Z}_+^{n+2}$ to $fu + \alpha_j A_{.j} - A\mu = 0$ with $u = 1$. Each entry in a minimal homogeneous solution of this system, however, can be bounded by $(d+1)$ times the maximum absolute value $D(f\ A_{.j}\ -A)$ of the determinants of maximal submatrices of the coefficient matrix $(f\ A_{.j}\ -A)$.

Thus, in particular,

$$\alpha_j \leq (d+1)D(f\ A_{.j}\ -A) \leq (d+1)M_F(A) \cdot D(A_{.j}\ -A) = (d+1)M_F(A) \cdot D(A).$$

Conseqently, we can bound the entries $h^{(i)}$, $i = 1, \ldots, d$, of a hole $h \in (f + Q) \cap H$ by

$$f^{(i)} - \sum_{j=1}^{n} (\alpha_j - 1)|A_{ij}| \leq h^{(i)} \leq f^{(i)} + \sum_{j=1}^{n} (\alpha_j - 1)|A_{ij}|.$$

Therefore, we get

$$\begin{aligned} |h^{(i)}| &\leq |f^{(i)}| + \sum_{j=1}^{n} (\alpha_j - 1)|A_{ij}| \\ &\leq M_F(A) + \sum_{j=1}^{n} ((d+1)M_F(A)D(A) - 1)|A_{ij}| \\ &= M_F(A) + ((d+1)M_F(A)D(A) - 1) \sum_{j=1}^{n} |A_{ij}| \\ &\leq M_F(A) + ((d+1)M_F(A)D(A) - 1)M_F(A) \\ &= (d+1)M_F^2(A)D(A) \end{aligned}$$

As this bound is independent on $f \in F$, $h \in H$, and $i = 1, \ldots, d$, we have

$$\|h\|_\infty \leq (d+1)M_F^2(A)D(A) \quad \forall h \in H,$$

if H is finite.

Example 1.1 cont. In our example, we have

- $d + 1 = 3$,
- $M_F(A) = \max(1 + 1 + 1 + 1, 0 + 2 + 3 + 4) = 9$, and
- $D(A) = \max |2 \times 2 \text{ determinant of } A| = |\det \left(\begin{smallmatrix} 1 & 1 \\ 0 & 4 \end{smallmatrix}\right)| = 4$.

Thus, if H was finite, the bound $\|h\|_\infty \leq 3 \cdot 9^2 \cdot 4 = 972$ would hold for all $h \in H$. In this example, however, one can easily verify that $(1000, 1)^\intercal$ is a hole. As it violates the computed bound, H cannot be finite. □

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