# An algorithm to compute holes of semi-groups

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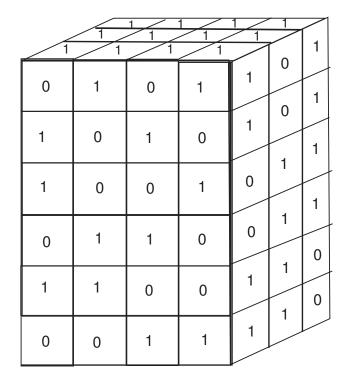
Joint work with A. Takemura and R. Hemmecke

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### Puzzle

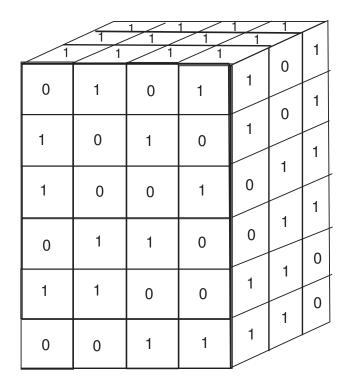
Is there a nonnegative integral valued table satisfying these given margins?



Each cell has nonnegative integral value.

Hint: There exists a nonnegative real valued table satisfying the constraints.

### Answer



There does not exist such a nonnegative integral valued table, although the marginals are consistent.

Suppose we have a given set of margins for contingency tables.

Want: decide whether there exists a table satisfying the given margins.

This is called the **multi-dimensional integer planar transportation problem** and it can be applied to **data sequrity problem**.

In terms of Optimization, we can rewrite this problem as an **integral feasibility problem**, that is:

Decide whether there exists an integral solution in the system

$$Ax = b, x \ge 0,$$

where  $A \in \mathbb{Z}^{d \times n}$  and  $b \in \mathbb{Z}^d$ .

### Observation

Assume the lattice L generated by the columns of A is  $\mathbb{Z}^d$ .

Let cone(A) be the cone generated by the columns of A and  $P_b = \{x \in \mathbb{R}^n : Ax = b, x \ge 0\}.$ 

We assume that cone(A) is pointed.

$$P_b \neq \emptyset \Leftrightarrow b \in \operatorname{cone}(A).$$

### **Observation**

Let Q be the semigroup generated by the columns  $a_i$  of A, that is,  $Q = \{\sum_{i=1}^n \alpha_i a_i : \alpha_i \in \mathbb{Z}_+\} \subset \operatorname{cone}(A) \cap \mathbb{Z}^d.$ 

 $P_b \cap \mathbb{Z}^n \neq \emptyset \Leftrightarrow b \in Q.$ 

 $(P_b \neq \emptyset) \bigwedge (P_b \cap \mathbb{Z}^n = \emptyset) \Leftrightarrow b \in (\operatorname{cone}(A) \cap \mathbb{Z}^d - Q).$ 

We study on the set of holes of Q,  $H := (\operatorname{cone}(A) \cap \mathbb{Z}^d) - Q$ .

**Motivation**: One of motivations is that once we solve this problem, then we can solve an integer linear feasibility problem efficiently if we vary the right-hand-side b.

**Note**: Q is normal (i.e.  $H = \emptyset$ ) iff the Hilbert basis of cone(A) is in Q.

**Note**: Barvinok and Woods showed that: suppose we fix d and n. We can compute all holes of Q in polynomial time using **short rational functions**.

**However**: It is an **implicit representation** of H, and also their method cannot be implemented at this moment.

**Problem**: Find an explicit representation of *H*.

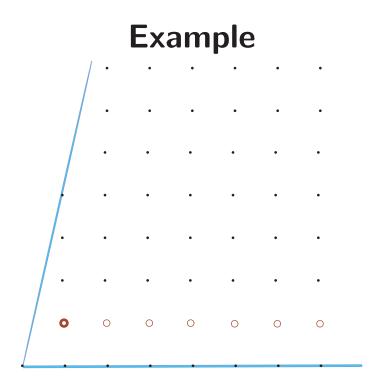


Figure 1: Red dots represent holes.

$$A = \left( \begin{array}{rrrr} 1 & 1 & 1 & 1 \\ 0 & 2 & 3 & 4 \end{array} \right).$$

### **Fundamental holes**

**Def.** The semigroup  $Q_{\text{sat}} = \text{cone}(A) \cap L$  is called the saturation of Q (i. e.  $Q_{\text{sat}} = Q + H$  or  $H = Q_{\text{sat}} - Q$ ).

**Def.** We call  $a \in H \subset Q_{\text{sat}}$ ,  $a \neq 0$ , a **fundamental hole** if there is no other hole  $h' \in H$  such that  $h - h' \in Q$ . Let F be the set of fundamental holes.

**Ex.**  $A = (3 \ 5 \ 7)$ .  $Q_{sat} = \{0, 1, ...\}$ ,  $Q = \{0, 3, 5, 6, 7, ...\}$ ,  $H = \{1, 2, 4\}$ . Among the 3 holes, 1 and 2 are fundamental. For example,  $2 \in H$  is fundamental because

$$\{0, 1, \ldots\} \cap \{2, -1, -3, -4, -5, \ldots\} = \{2\}.$$

On the other hand  $4 \in H$  is not fundamental because

$$4-1=3\in Q.$$

RIMS

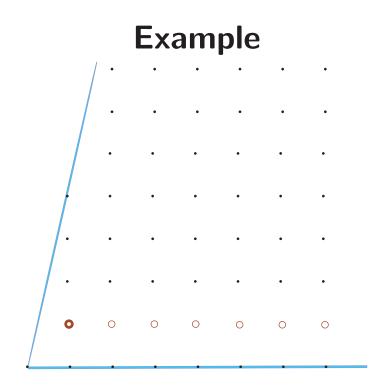


Figure 2: Non-holes, holes and fundamental hole for Example.

$$A = \left( \begin{array}{rrrr} 1 & 1 & 1 & 1 \\ 0 & 2 & 3 & 4 \end{array} \right).$$

### Example cont.

 $\boldsymbol{Q}$  has infinitely many holes

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

out of which only  $(1,1)^{\intercal}$  is fundamental,

The **output** from our algorithm looks like:

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

# Computing the holes in f + Q

Let  $f \in F$  and  $I_{A,f} \in \mathbb{Q}[x_1, \ldots, x_n]$  be the monomial ideal generated by

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

**Note.** If  $\operatorname{cone}(A)$  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 minimal inhomogenuous solutions in  $(f + Q) \cap Q$ , we can find a finite generating set for  $I_{A,f}$ .

**Theorem.** (Hemmecke, Takemura, Y, 2006) While the monomial  $x^{\lambda}$  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  $I_{A,f}$ .

### Algorithm

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

**Output**: An explicit representation of *H*.

- 1. Compute the set F of fundamental holes.
- 2. For each of the finitely many  $f \in F$ , compute all minimal inhomogenous solutions  $(\lambda, \mu)$  of

$$\{(\lambda,\mu)\in\mathbb{Z}_{+}^{2n}:f+A\lambda=A\mu\}.$$
(1)

3. From the minimal inhomogenous solutions  $(\lambda, \mu)$  of (1), compute an explicit representation of the holes of Q in f + Q.

## **Computing fundamental holes**

The set F of fundamental holes is finite, since it is a subset of the lattice points in

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

Algorithm. (Computing fundamental holes)

- Compute the minimal integral generating set B of  $cone(A) \cap L$ .
- 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 ∩ F that lie in P and check for each such z whether it is a fundamental hole or not.

### **Example cont**

In our example, the lattice  $L = \mathbb{Z}^2$ . With this, the minimal Hilbert basis B of  $cone(A) \cap L$  consists of 5 elements:

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

out of which only  $(1,1)^{\mathsf{T}}$  is a hole.

Being in B,  $(1,1)^{\intercal}$  must be a fundamental hole. Thus,  $B \cap F = \{(1,1)^{\intercal}\}$ .

Note that  $2 \cdot (1,1)^{\intercal} = (2,2)^{\intercal} \in Q$  and consequently, there is no other fundamental hole in  $Q_{\text{sat}}$ , i.e.  $F = \{(1,1)^{\intercal}\}$ .

# **Computing minimal inhomogenous solutions**

The (finitely many) minimal inhomogeneous solutions to the above linear system can be computed, for example, with 4ti2.

**Example cont.** Let  $f = (1,1)^{\mathsf{T}}$  and consider  $(f+Q) \cap Q$ . The linear system to solve is

### **Example cont**

4ti2 gives the following 5 minimal inhomogeneous solutions  $(\lambda, \mu)$  to system (1):

Thus, we have  $\{(2,3)^{\intercal}, (2,4)^{\intercal}, (2,5)^{\intercal}, (3,9)^{\intercal}\}$ .

#### **Example cont**

Construct the generators of the monomial ideal  $I_{A,f}$  by finding all representations of the form  $z = f + A\lambda, \lambda \in \mathbb{Z}_+^4$  for each z in  $(f + Q) \cap Q$  for each  $z \in \{(2,3)^\intercal, (2,4)^\intercal, (2,5)^\intercal, (3,9)^\intercal\}$ .

$$z = f + A\lambda$$

$$(2,3)^{\mathsf{T}} = (1,1)^{\mathsf{T}} + A(0,1,0,0)^{\mathsf{T}}$$

$$(2,4)^{\mathsf{T}} = (1,1)^{\mathsf{T}} + A(0,0,1,0)^{\mathsf{T}}$$

$$(2,5)^{\mathsf{T}} = (1,1)^{\mathsf{T}} + A(0,0,0,1)^{\mathsf{T}}$$

$$(3,9)^{\mathsf{T}} = (1,1)^{\mathsf{T}} + A(0,0,0,4)^{\mathsf{T}}$$

### **Example**

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  $f+Q\ {\rm is}$ 

$$\{f + \alpha A_1 : \alpha \in \mathbb{Z}_+\} = \{(1, 1)^{\mathsf{T}} + \alpha(1, 0)^{\mathsf{T}} : \alpha \in \mathbb{Z}_+\}$$

# Applications to contingency tables

# Sequencial Importance Sampling (SIS)

For a formal definition of SIS, see (Chen, 2001), (Chen, Diaconis, Holmes, Liu 2005), (Chen, Dinwoodie, Sullivant, 2006), etc., etc.

#### How does SIS work?

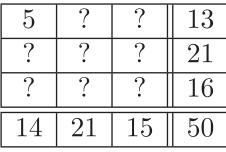
For example, suppose we have the following table.

7	5	1	13
5	10	6	21
2	6	8	16
14	21	15	50

Now we consider  $\tau$ , all integral valued tables with the same column sums  $c_i$  and row sums  $r_i$  for i = 1, 2, 3.

### Example cont...

We want to sample a table from  $\tau$ . We pick an integer from  $[0, \min\{8, 9\}]$  with some distribution (say a uniform distribution). For example, we picked 5.



Then update  $r_1$  and  $c_1$  as follows:

5	?	?	8
?	?	?	21
?	?	?	16
9	21	15	50

### Example cont...

We do this process untill we fill up all cells. Then we get a table:

5	7	1	13
7	8	6	21
2	6	8	16
14	21	15	50

**Questions**: How can we choose a sample which does not end up a non-consistant table? Relations between holes and samples.

### SIS and holes

Suppose  $(T_{i_1,\dots,i_m}) \in \tau$  be a  $d_1 \times \dots \times d_m$  table and we set:

$$b = Ax,$$

where 
$$x = (T_{1,1,\dots,1}, T_{1,1,\dots,2}, \dots, T_{d_1,d_2,\dots,d_m})$$
 and  $b = (\sum_{i_1} T_{i_1,\dots,i_m}, \dots, \sum_{i_m} T_{i_1,\dots,i_m}).$ 

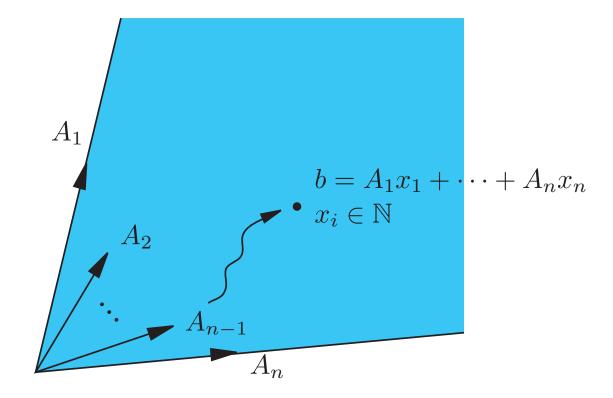
Thus we can rewrite:

$$b = A_1 x_1 + A_2 x_2 + \dots + A_n x_n, \ x_i \in \mathbb{Z}_+.$$

To get a table satisfying the given marginals, we take a path

$$A_1x_1 \to A_1x_1 + A_2x_2 \to \cdots \to A_1x_1 + A_2x_2 + \cdots + A_nx_n.$$

### From the view of Q



Taking a sample via SIS can be viewed as a path from the origin to  $b \in Q$ .

## SIS and holes

Suppose Q is not normal (such as three-way tables).

To sample via SIS, we need to check if it is possible to reach b from the current point  $s = A_1y_1 + A_2y_2 + \cdots + A_ny_n$ .

To check there is a path from s to b by adding  $z_i \in \mathbb{Z}_+$  to  $y_i$  for some i:

- If  $b s \in Q$ , then there is a path.
- If  $b s \in H$ , then we reject.

Thus knowing H, one might be speed up some computation of SIS. (we need to investigate how practical our algorithm is).

# Finiteness of holes of Q

**Theorem**: (Takemura and Y, 2006): Suppose we fix d and n. Then, there is a polynomial time algorithmm to decide whether the set of holes H of Q for a matrix A is finite or not.

**Examples**: The matrix for defining  $2 \times 2 \times 2 \times 2$  tables with 2-marginals has finitely many holes.

 $2 \times 2 \times 2 \times 2$  tables with 2-marginals and 3-marginal i.e. [12][13][14][123] and with levels of 2 on each node has infinitely many holes.

#### Prop. [Takemura and Y., 2006]

 $3 \times 4 \times 7$  table with 2-marginals has infinite number of holes.

Sketch of pf.

					sum
	С	0	0	0	C
	0	0	0	0	0
	0	0	0	0	0
sum	С	0	0	0	С

Table 1: the 7-th  $3 \times 4$  slice is uniquely determined by its row and its column sums. c is an arbitrary positive integer. Thus for each choice of positive integer the beginning  $3 \times 4 \times 6$  part remains to be a hole. Since the positive integer is arbitrary,  $3 \times 4 \times 7$  table has infinite number of holes.

### **Future work**

**Known.** Results on the saturation of 3-DIPTP are summarized in Theorem 6.4 of a paper by Ohsugi and Hibi, (2006). They show that a normality (i.e. Q is saturated) or non-normality (i.e. Q is not saturated) of Q is not known only for the following three cases:

$$5 \times 5 \times 3$$
,  $5 \times 4 \times 3$ ,  $4 \times 4 \times 3$ .

**Note.**  $4 \times 4 \times 3$  is solved! We want to decide whether semigroups of these tables above are normal or not.

Also we want to decide whether  $3 \times 4 \times 6$  table with 2-margins have a finite number of holes.

# Questions?

# A preprint is available at arxiv:

http://arxiv.org/abs/math.CO/0607599

# Thank you....