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Computing holes of a commutative semigroup

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Puzzle

Is there a table satisfying these given marginals?

The diagram shows a 3D cube representing a 4x4x4 table. The front face is a 4x4 grid with the following values:

0	1	0	1
1	0	1	0
1	0	0	1
0	1	1	0

The top face shows marginal values: 1, 1, 1, 1, 1, 1, 1, 1.

The right face shows marginal values: 1, 0, 1, 1, 1, 0, 1, 0.

The bottom face shows marginal values: 1, 1, 0, 0, 1, 1, 1, 1.

Each cell has nonnegative integral value.

Answer

0	1	0	1	1	0	1
1	0	1	0	1	0	1
1	0	0	1	0	1	1
0	1	1	0	0	1	1
1	1	0	0	1	1	0
0	0	1	1	1	1	0

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

Problem

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

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

This is called the **multi-dimensional integer planar transportation 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

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

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

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

Let Q be the semigroup generated by the columns \mathbf{a}_i of A , i.e. $Q = \{x \in \mathbb{R}^d : \sum_{i=1}^n \alpha_i \mathbf{a}_i, \alpha_i \in \mathbb{Z}_+\} \subset \text{cone}(A) \cap \mathbb{Z}^d$.

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

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

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

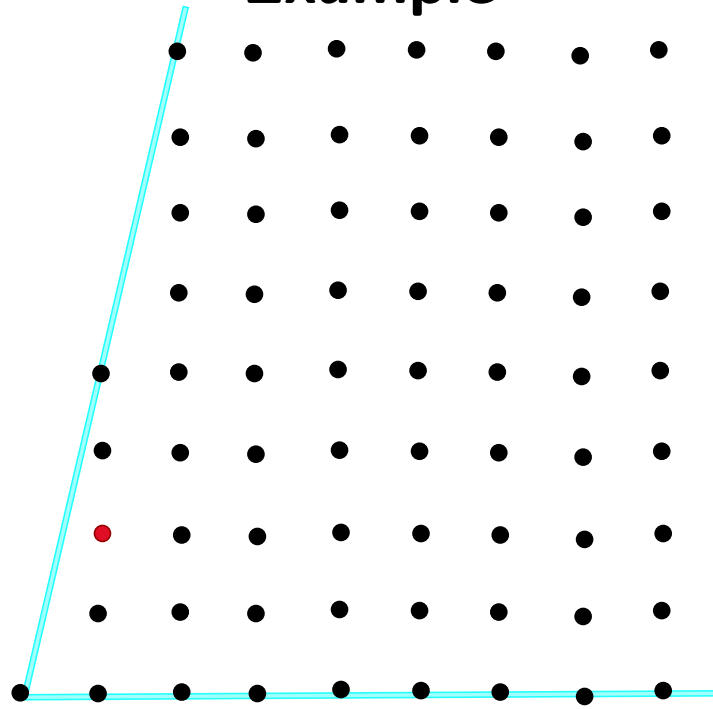
Motivation:

- (Algebra): Almost all focus in the algebraic literature on this topic is on the normal case (i.e. there are no holes).
- (Statistics): This is significant for statistics because many affine semigroups with statistical connections are not normal.

Note: Q is normal iff the Hilbert basis of $\text{cone}(A)$ is in Q .

Problem: Find **the necessary and sufficient conditions for H 's finiteness.**

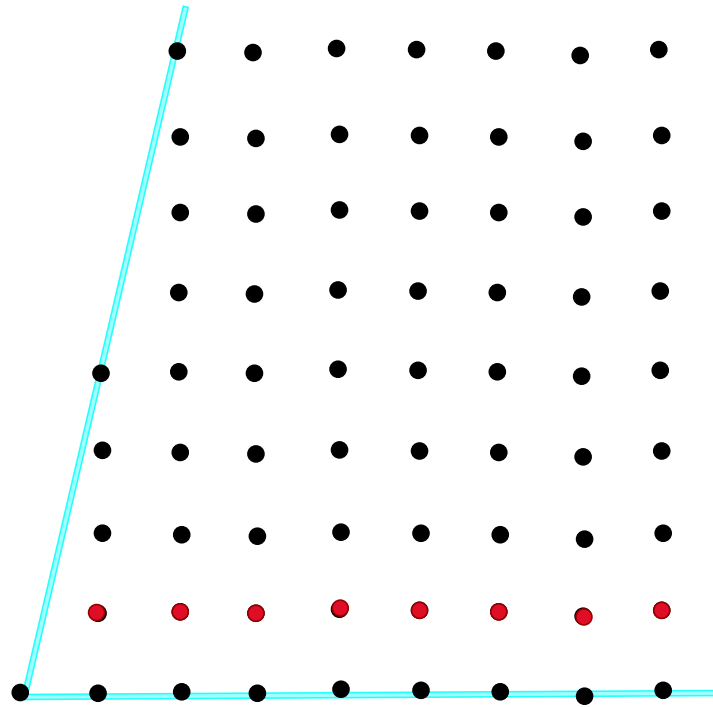
Example



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

The red dot represents a hole and there is only one hole for A .

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

There are infinitely many holes for A . How can we determine whether there are finite or infinite?

Notation and definitions

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 $H = Q_{\text{sat}} - Q$).

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 . Let $\bar{S} = Q - S$.

Note. If $\text{cone}(A)$ is pointed then $S \neq \emptyset$.

$s \in S$ is called a **Q -minimal** of S there is no other $s' \in S$ with $s - s' \in Q$.

$s \in S$ is called a **S -minimal** of S there is no other $s' \in S$ with $s - s' \in S$.

Under the assumption above K and Q are **pointed** and S is non-empty by Problem 7.15 of [Miller and Sturmfels, 2004].

Let $\min(S; S)$ denote the set of S -minimal saturation points, $\min(S; Q)$ the set of Q -minimal saturation points.

Example

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

$$H = \{(1, 2)^t\}.$$

$$\bar{S} = \{(0, 0)^t, (1, 0)^t, (1, 1)^t\}.$$

$$\min(S; S) = \{(1, 3)^t, (1, 4)^t, (2, 0)^t, (2, 1)^t, (2, 2)^t, (2, 3)^t, (2, 4)^t, (2, 5)^t, (3, 0)^t, (3, 1)^t, (3, 2)^t\}.$$

Thus, H , \bar{S} , and $\min(S; S)$ are all finite.

Fundamental holes

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

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

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

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

Fundamental holes

Lemma. [Takemura and Y., 2006]

H_0 is finite.

Let $H_0 = \{\mathbf{y}_1, \dots, \mathbf{y}_M\}$. For each $\mathbf{y}_h \in H_0$ and each \mathbf{a}_i , if there exists some $\lambda \in \mathbb{Z}$ such that $\mathbf{y}_h + \lambda\mathbf{a}_i \in Q$, let

$$\bar{\lambda}_{hi} = \min\{\lambda \in \mathbb{Z} \mid \mathbf{y}_h + \lambda\mathbf{a}_i \in Q\}.$$

Otherwise define $\bar{\lambda}_{hi} = \infty$.

Thm. [Takemura and Y., 2006]

H is finite if and only if $\bar{\lambda}_{hi} < \infty$ for all $h = 1, \dots, M$ and all $i = 1, \dots, n$.

Thm. [Takemura and Y., 2006]

Let $B = \{\mathbf{b}_1, \dots, \mathbf{b}_L\}$ denote the Hilbert basis of Q_{sat} . If $\mathbf{b}_l + \lambda \mathbf{a}_i \in Q$ for some $\lambda \in \mathbb{Z}$, let

$$\bar{\mu}_{li} = \min\{\lambda \in \mathbb{Z} \mid \mathbf{b}_l + \lambda \mathbf{a}_i \in Q\}$$

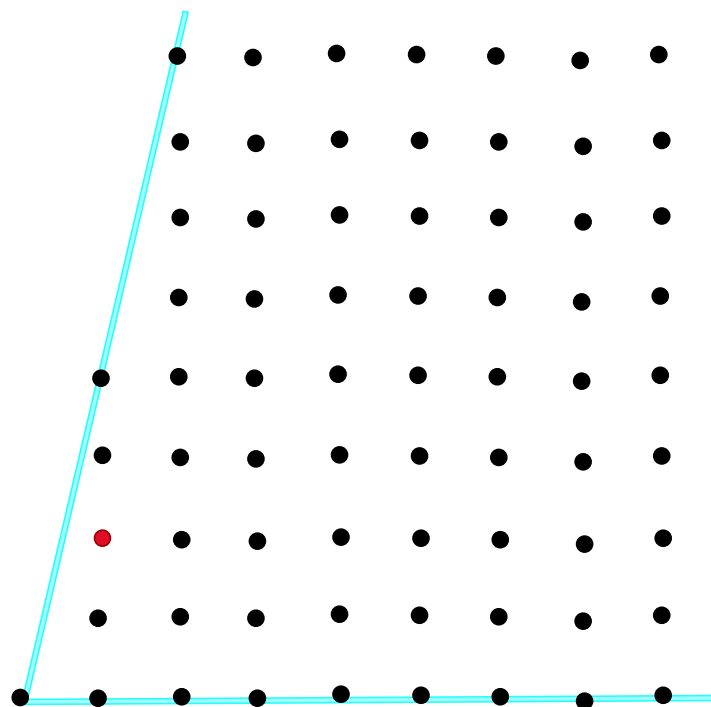
and $\bar{\mu}_{li} = \infty$ otherwise.

Then H is finite if and only if $\bar{\mu}_{li} < \infty$ for all $l = 1, \dots, L$ and all $i = 1, \dots, n$.

Remark. For each $1 \leq i \leq n$, let $\tilde{Q}_{(i)} = \{\sum_{j \neq i} \lambda_j \mathbf{a}_j \mid \lambda_j \in \mathbb{Z}_+, j \neq i\}$ be the semigroup spanned by $\mathbf{a}_j, j \neq i$. For each extreme \mathbf{a}_i and for each $\mathbf{b}_l \notin Q$, we only have to check

$$\mathbf{b}_l \in (-\mathbb{Z}_+ \mathbf{a}_i) + \tilde{Q}_{(i)}, \text{ for } l = 1, \dots, L.$$

Example



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

Example

$$B = \{\mathbf{b}_1 = (1, 0)^t, \mathbf{b}_2 = (1, 1)^t, \mathbf{b}_3 = (1, 2)^t, \mathbf{b}_4 = (1, 3)^t, \mathbf{b}_5 = (1, 4)^t\}.$$

Then we can write \mathbf{b}_3 as the following:

$$\begin{aligned} (1, 2)^t &= -(1, 0)^t + 2 \cdot (1, 1)^t \\ &= (1, 0)^t - (1, 1)^t + (1, 3)^t \\ &= (1, 1)^t - (1, 3)^t + (1, 4)^t \\ &= 2 \cdot (1, 3)^t - (1, 4)^t. \end{aligned}$$

We have $\bar{\mu}_{3i} = 1$ for each $i = 1, \dots, 4$ and $\bar{\mu}_{li} = 0$, where $l \neq 3$ for each $i = 1, \dots, 4$. Thus by Theorem above, the number of elements in H is finite. Note that H consists of only one elements $\{\mathbf{b}_3 = (1, 2)^t\}$.

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Thm. [Takemura and Y., 2006]

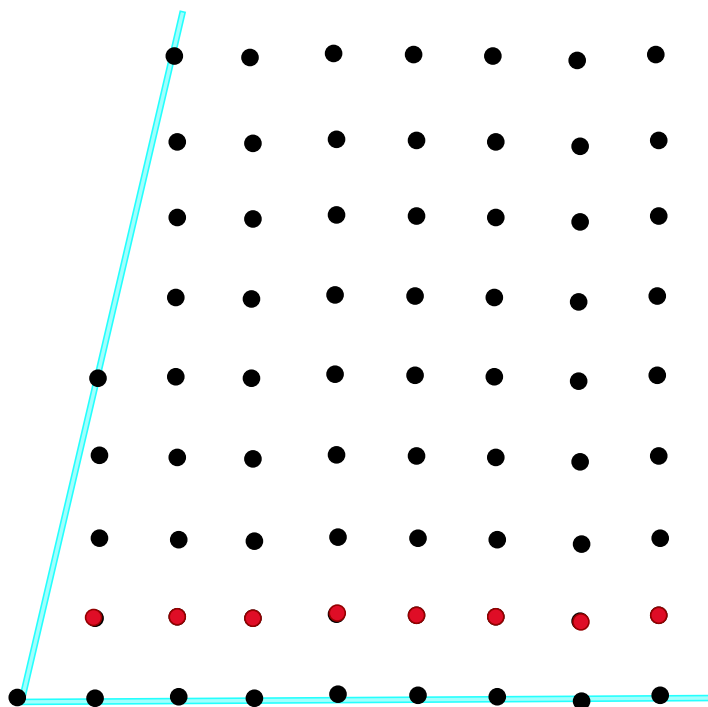
The following statements are equivalent.

1. $\min(S; S)$ is finite.
2. $\text{cone}(S)$ is a rational polyhedral cone.
3. There is some $s \in S$ on every extreme ray of K .
4. H is finite.
5. \bar{S} is finite.

Prop. [Takemura and Y., 2006]

$\min(S; Q)$ is finite.

Example



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

Example

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

H consists of elements $\{(k, 1) : k \in \mathbb{Z}, k \geq 1\}$.

$$\bar{S} = \{(i, 0)^t : i \in \mathbb{Z}, i \geq 0\},$$

$$\min(S; S) = \{(k, j)^t : k \in \mathbb{Z}, k \geq 1, 2 \leq j \leq 3\} \cup \{(1, 4)\}.$$

Thus, H , \bar{S} , and $\min(S; S)$ are all infinite. However, $\min(S; Q) = \{(1, 2)^t, (1, 3)^t, (1, 4)^t\}$ is finite.

Applications to contingency tables

$2 \times 2 \times 2 \times 2$ tables with 2-marginals.

The semigroup has 16 generators $\mathbf{a}_1, \dots, \mathbf{a}_{16}$ in \mathbb{Z}^{24} .

The Hilbert basis of the cone generated by these 16 vectors contains 17 vectors $\mathbf{b}_1, \dots, \mathbf{b}_{17}$. The first 16 vectors are the same as \mathbf{a}_i , i.e. $\mathbf{b}_i = \mathbf{a}_i$, $i = 1, \dots, 16$. The 17-th vector \mathbf{b}_{17} is

$$\mathbf{b}_{17} = (1 \ 1 \ \dots \ 1)^t$$

consisting of all 1's.

Thus, $\mathbf{b}_{17} \notin Q$. Then we set the 16 systems of linear equations such that:

$$P_j : \quad \mathbf{b}_1 x_1 + \mathbf{b}_2 x_2 + \cdots + \mathbf{b}_{16} x_{16} = \mathbf{b}_{17}$$
$$x_j \in \mathbb{Z}_-, \quad x_i \in \mathbb{Z}_+, \quad \text{for } i \neq j,$$

for $j = 1, 2, \dots, 16$.

Using LattE, we showed that the 16 systems of linear equations have integral solutions.

Thus by theorems above, H , \bar{S} , and $\min(S; S)$ are finite.

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

The semigroup is generated by 16 vectors in \mathbb{Z}^{12} .

The Hilbert basis consists of these 16 vectors and two additional vectors

$$\mathbf{b}_{17} = (1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 0 \ 0 \ 0)^t, \quad \mathbf{b}_{18} = (1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 0 \ 1 \ 1 \ 1)^t.$$

Thus, $\mathbf{b}_{17}, \mathbf{b}_{18} \notin Q$.

Then we set the system of linear equations such that:

$$\mathbf{b}_1x_1 + \mathbf{b}_2x_2 + \cdots + \mathbf{b}_{16}x_{16} = \mathbf{b}_{17}$$
$$x_1 \in \mathbb{Z}_-, x_i \in \mathbb{Z}_+, \text{ for } i = 2, \dots, 16.$$

We solved the system via lrs, CDD and LattE.

We noticed that this system has no real solution (infeasible).

Thus by theorems above, H , \bar{S} , and $\min(S; S)$ are infinite.

Prop. [Takemura and Y., 2006]

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

Sketch of pf.

					sum
	c	0	0	0	c
	0	0	0	0	0
	0	0	0	0	0
sum	c	0	0	0	c

Table 1: the 7-th 3×4 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:

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

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.

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Questions?

A preprint is available at arxiv:

<http://arxiv.org/abs/math.ST/0603108>

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Thank you....