Fundamental holes and saturation points of a commutative semigroup and their applications to contingency tables

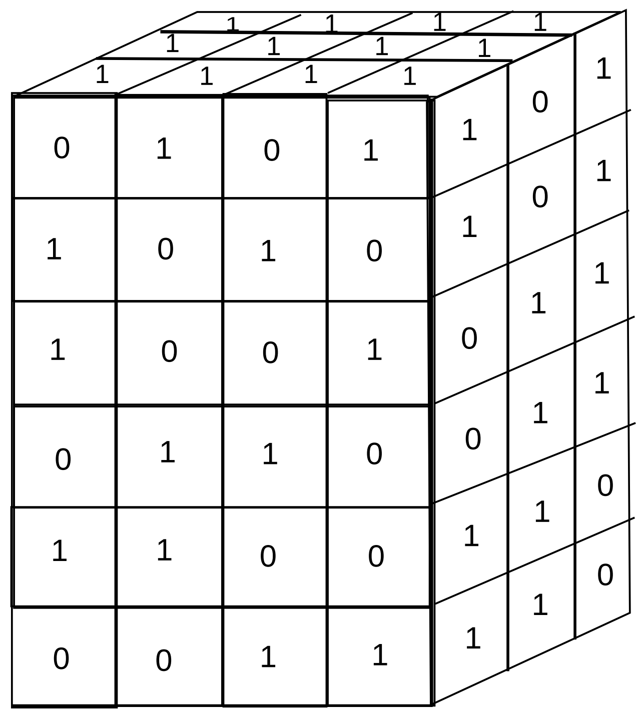
Ruriko Yoshida
Dept. of Mathematics Duke University

Joint work with A. Takemura

www.math.duke.edu/~ruriko

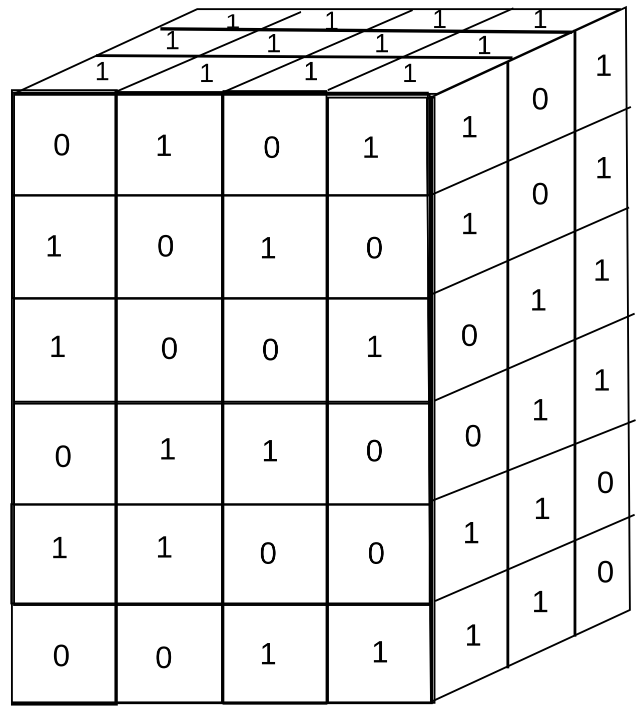
Puzzle

Is there a table satisfying these given margins?



Each cell has nonnegative integral value.

Answer



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

Problem

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**.

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 $\boldsymbol{a}_i$ of A, i.e. $Q = \{x \in \mathbb{R}^d : \sum_{i=1}^n \alpha_i \boldsymbol{a}_i,\ \alpha_i \in \mathbb{Z}_+\} \subset \text{cone}(A) \cap \mathbb{Z}^d$.

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

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

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 cone(A) is in Q.

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

Notation and definitions

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

$$
\begin{aligned}
Q &= A\mathbb{Z}_+^n = \{\lambda_1 \boldsymbol{a}_1 + \cdots + \lambda_n \boldsymbol{a}_n : \lambda_1, \cdots, \lambda_n \in \mathbb{Z}_+\} \\
K &= A\mathbb{R}_+^n = \{\lambda_1 \boldsymbol{a}_1 + \cdots + \lambda_n \boldsymbol{a}_n : \lambda_1, \cdots, \lambda_n \in \mathbb{R}_+\} \\
L &= A\mathbb{Z}^n = \{\lambda_1 \boldsymbol{a}_1 + \cdots + \lambda_n \boldsymbol{a}_n : \lambda_1, \cdots, \lambda_n \in \mathbb{Z}\} \\
Q_{\text{sat}} &= K \cap L = \text{saturation of } A \supset Q \\
H &= Q_{\text{sat}} \setminus Q = \text{holes in } Q_{\text{sat}} \\
S &= \{\boldsymbol{a} \in Q : \boldsymbol{a} + Q_{\text{sat}} \subset Q\} = \text{saturation points of } Q \\
\bar{S} &= Q \setminus S = \text{non-saturation points of } Q
\end{aligned}
$$

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

Minimal saturation points

We now consider minimal points of S with respect to S, Q and $Q_{\rm sat}$. We call $\boldsymbol{a} \in S$ an S-minimal (a Q-minimal, a $Q_{\rm sat}$-minimal, resp.) if there exists no other $\boldsymbol{b} \in S$, $\boldsymbol{b} \neq \boldsymbol{a}$, such that $\boldsymbol{a} - \boldsymbol{b} \in S$ (Q, $Q_{\rm sat}$, resp.). More formally $\boldsymbol{a} \in S$ is

a) an S-**minimal saturation point** if $(\boldsymbol{a} + (-(S \cup \{0\}))) \cap S = \{\boldsymbol{a}\}$,

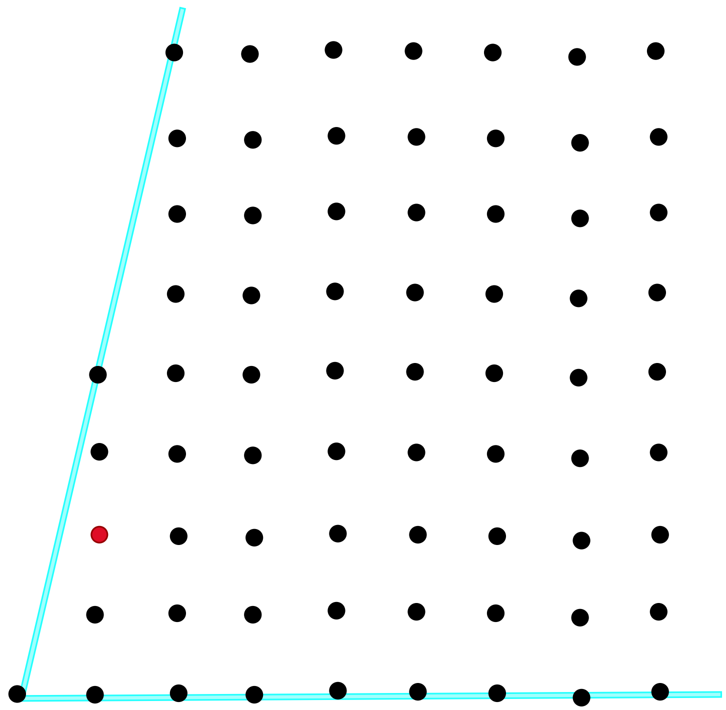
b) a Q-**minimal saturation point** if $(\boldsymbol{a} + (-Q)) \cap S = \{\boldsymbol{a}\}$,

c) a $Q_{\rm sat}$-**minimal saturation point** if $(\boldsymbol{a} + (-Q_{\rm sat})) \cap S = \{\boldsymbol{a}\}$.

Let $\min(S; S)$ denote the set of S-minimal saturation points, $\min(S; Q)$ the set of Q-minimal saturation points, and $\min(S; Q_{\rm sat})$ the set of $Q_{\rm sat}$-minimal saturation points.

Note. $\min(S; Q_{\rm sat}) \subset \min(S; Q) \subset \min(S; S)$.

Example



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

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 $\boldsymbol{a} \in H \subset Q_{\text{sat}}$, $\boldsymbol{a} \neq 0$, a **fundamental hole** if

$$Q_{\text{sat}} \cap (\boldsymbol{a} + (-Q)) = \{\boldsymbol{a}\}.$$

Let H_0 be the set of fundamental holes.

Ex. $A = (3\ \ 5\ \ 7)$. $Q_{\text{sat}} = \{0, 1, \ldots\}$, $Q = \{0, 3, 5, 6, 7, \ldots\}$, $-Q = \{0, -3, -5, -6, -7, \ldots\}$. $H = \{1, 2, 4\}$. 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

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

Fundamental holes

Lemma. [Takemura and Y., 2006]

H_0 is finite.

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

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

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

Thm. [Takemura and Y., 2006]

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

Thm. [Takemura and Y., 2006]

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

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

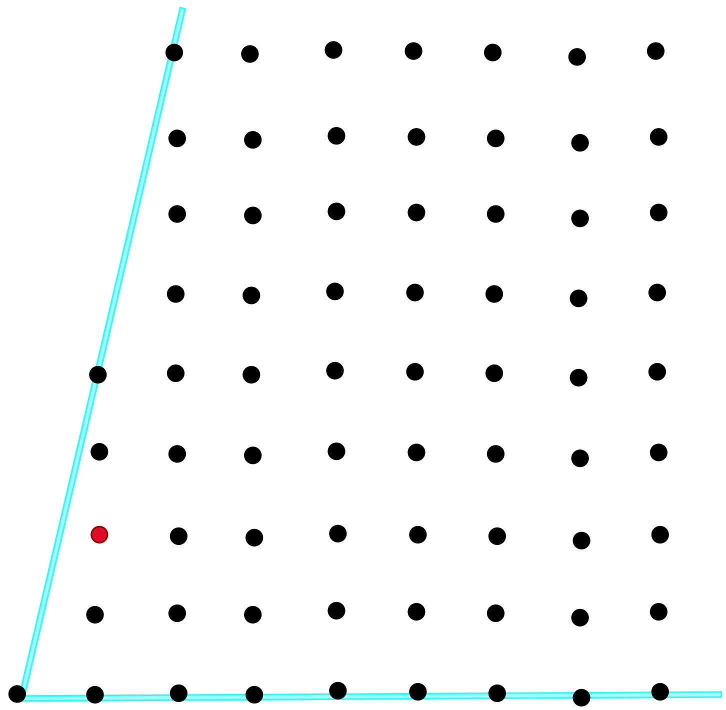
and $\bar{\mu}_{li} = \infty$ otherwise.

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

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

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

Example



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

Example

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

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

Thm. [Takemura and Y., 2006]

The following statements are equivalent.

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

2. cone(S) is a closed rational polyhedral cone.

3. There is some $s \in S$ on every extreme ray of K.

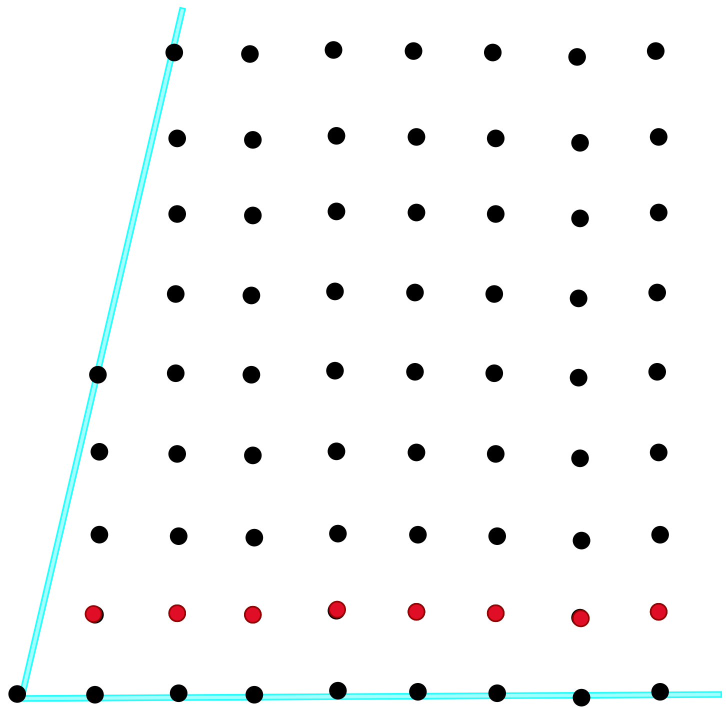
4. H is finite.

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-margins.

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

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

$$\boldsymbol{b}_{17} = (1\ 1\ \ldots\ 1)^t$$

consisting of all 1's.

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

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

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

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-margins and 3-margin 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

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

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

Then we set the system of linear equations such that:

$$\boldsymbol{b}_1 x_1 + \boldsymbol{b}_2 x_2 + \cdots + \boldsymbol{b}_{16} x_{16} = \boldsymbol{b}_{17}$$
$$x_1 \in \mathbb{Z}_-, \ x_i \in \mathbb{Z}_+, \ \text{for } i = 2, \cdots, 16.$$

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-margins 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:

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

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.ST/0603108

Thank you....