Holes in semigroups and their applications to the two-way common diagonal effect model

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Abstract—A *two-way subtable sum model* is a statistical model for two-way contingency tables such that sufficient statistics for the model are row sums, column sums and an additional constraint that the sum of a subtable is also fixed. From a statistical viewpoint this model is related to a block interaction model, a two-way change-point model proposed by Hirotsu, and the quasi-independence model for incomplete two-way contingency tables which contain some structural zeros. When the set of square-free moves of degree two does not form a Markov basis, we know that the semigroup generated by columns of the design matrix for the sufficient statistics of the model is not normal. One such model is the *common diagonal effect model*. In this paper, we first summarize the results in [Takemura and Yoshida, 2007] and then we study how the difference between the semigroup generated by columns of the design matrix for a common diagonal effect model and its saturation are distributed.

keyword: contingency tables, Hilbert bases, integer linear feasibility problem, semigroup.

1 Introduction

Let $A = \{\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n\}$, $\boldsymbol{a}_i \in \mathbb{Z}^d$, $i = 1, \ldots, n$, be a finite set of integral points and let $Q = Q(A)$ denote the commutative semigroup generated by $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n$. In our previous paper [Takemura and Yoshida, 2007, 2008] we studied properties of *holes*, which are the difference between the semigroup and its *saturation*. We gave some necessary and sufficient conditions for the finiteness of the set of holes and also we gave detailed descriptions of how holes are located and when there are infinitely many holes.

Recently Hara et al. [2007] considered Markov bases for two-way contingency tables with fixed row sums, column sums and an additional constraint that the sum of a subtable is also fixed. We call this problem a *two-way subtable sum problem*. From a statistical viewpoint this problem is motivated by a block interaction model or a two-way change-point model proposed by [Hirotsu, 1997], which has been studied from both theoretical and practical viewpoints [Ninomiya, 2004] and has important applications to dose-response clinical trials with ordered categorical responses. It has been well-known that for two-way contingency tables with fixed row sums and column sums, the set of square-free moves of degree two forms a Markov basis. However when we impose an additional constraint that the sum of a subtable is also fixed, then these moves do not necessarily form a Markov basis. Hara et al. [2007] showed a necessary and sufficient condition on a subtable so that a corresponding Markov basis consists of square-free moves of degree two. Shortly after that Ohsugi and Hibi showed that the semigroup generated by the columns of the design matrix for a subtable sum problem is *normal* (i.e., there is no hole) if and only if a set of square-free moves of degree two forms a Markov basis [Ohsugi and Hibi, 2007].

The *common diagonal effect model* (CDEM) models diagonal effects which arise mainly in analyzing contingency tables with common categories for the rows and the columns [Hara et al., 2008]. Under the CDEM, we consider contingency tables with fixed row sums, column sums, and an additional constraint that the sum of diagonal cells is also fixed. Note that a set of square-free moves of degree two does not form a Markov basis for the design matrix under the CDEM. Therefore, the semigroup generated by the columns of the design matrix for the CDEM is not normal by the results from [Ohsugi and Hibi, 2007].

In this paper we focus on the semigroup generated by the columns of the design matrix for the CDEM and we will study details of the distribution of the holes using the methods in [Takemura and Yoshida, 2007, 2008]. This paper is organized as follows: in section 2 we will summarize the previous results from [Takemura and Yoshida, 2007, 2008]. In Section 3 we will show our main theorem on holes of the semigroups for the CDEM and some computational results.

2 Basic notation and definitions

In this section we summarize some relevant definitions and results from [Takemura and Yoshida, 2007, 2008]. For more details, see [Takemura and Yoshida, 2007, 2008].

Let $K = \mathrm{cone}(\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n)$ be the rational polyhedral cone generated by $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n$ and let $L \subset \mathbb{Z}^d$ denote the lattice generated by them. The saturation Q_{sat} of Q is defined by $Q_{\mathrm{sat}} = K \cap L$. The elements of $H = Q_{\mathrm{sat}} \setminus Q$ are called *holes* of Q. We assume that K is a *pointed* cone with non-empty interior. In many examples L coincides with $\mathbb{Z}^d$ and in this case let B denote the unique minimal *Hilbert basis* of K (i.e., the unique minimal generator of $K \cap \mathbb{Z}^d$). In the following we simply say the Hilbert basis instead of the unique minimal Hilbert basis.

We call $\boldsymbol{a} \in Q_{\mathrm{sat}}$, $\boldsymbol{a} \neq 0$, a *fundamental hole* if $Q_{\mathrm{sat}} \cap (\boldsymbol{a} + (-Q)) = \{\boldsymbol{a}\}$. Let H_0 be the set of all fundamental holes in Q. H_0 is always finite for any given semigroup by Proposition 3.1 in Takemura and Yoshida [2008]. $\boldsymbol{a} \in Q$ is called a *saturation point* if $\boldsymbol{a} + Q_{\mathrm{sat}} \subset Q$. Let S be the set of all saturation points of the semigroup Q. Let $\bar{S} = Q \setminus S =$ *non-saturation points* of Q. Under the assumption that K is pointed, S is nonempty by Problem 7.15 of [Miller and Sturmfels, 2005].

First we state one of the results from [Takemura and Yoshida, 2008]. In the following theorem we assume that $L = \mathbb{Z}^d$ without essential loss of generality.

Theorem 2.1. *Let $B = \{\boldsymbol{b}_1, \dots, \boldsymbol{b}_L\}$ denote the Hilbert basis of K. 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. H is finite if and only if $\bar{\mu}_{li} < \infty$ for all $l = 1, \dots, L$ and all $i = 1, \dots, n$.

Remark 2.2. *Let $\boldsymbol{b}_h \in B$ but $\boldsymbol{b}_h \notin Q$. For each $1 \le i \le n$, let*

$$\tilde{Q}_{(i)} = \{\sum_{j \neq i} \lambda_j \boldsymbol{a}_j \mid \lambda_j \in \mathbb{N},\ j \neq i\}$$

be the semigroup spanned by $\boldsymbol{a}_j, j \neq i$. Furthermore write

$$\bar{Q}_{(i)} = \mathbb{Z}\boldsymbol{a}_i + \tilde{Q}_{(i)}.$$

For each h and i, $\bar{\mu}_{hi}$ is finite if and only if $\boldsymbol{b}_h \in \bar{Q}_{(i)}$. Since $\boldsymbol{b}_h$ is a hole, we actually only need to check

$$\boldsymbol{b}_h \in (-\mathbb{N}\boldsymbol{a}_i) + \tilde{Q}_{(i)}.$$

But $(-\mathbb{N}\boldsymbol{a}_i) + \tilde{Q}_{(i)}$ is another semigroup, where $\boldsymbol{a}_i$ in A is replaced by $-\boldsymbol{a}_i$. Therefore this problem is a standard membership problem in a semigroup.

We call a face F of K *almost saturated* if there exists a saturation point of $Q = Q(A)$ on F. Otherwise (i.e., if no point of F is a saturation point) we call F *nowhere saturated*. We now state the following result from Takemura and Yoshida [2007]. Again we assume $L = \mathbb{Z}^d$.

Theorem 2.3. *A face F is nowhere saturated if and only if for some element $\boldsymbol{b}$ of the Hilbert basis B*

$$\boldsymbol{b} \;=\; x_1\boldsymbol{a}_1 + \cdots + x_n\boldsymbol{a}_n, \qquad (1)$$

$$x_j \in \mathbb{Z}, \forall j, \text{ and } x_j \geq 0 \text{ for } \boldsymbol{a}_j \notin F.$$

does not have a feasible solution.

In the next section, we are going to apply Theorem 2.1 and Theorem 2.3 to design matrices for contingency tables under the CDEM.

3 Applications to contingency tables under the CDEM

Now we consider $R \times C$ tables with fixed row sums, column sums, and the diagonal sum and we investigate (1) whether the set of holes in Q of each design matrix of a table is finite or infinite by Theorem 2.1 and (2) which faces of the polyhedral cone defined by this matrix are almost saturated or nowhere saturated by Theorem 2.3.

To compute minimal Hilbert bases of cones, we used `normaliz` [Bruns and Koch, 2001] and to compute each hyperplane representation and vertex representation we used `lrs` [Avis, 2005]. Also we used `4ti2` [4ti2 team, 2006] to compute defining matrices. To count the number of integral solutions in each system, we used `LattE` [DeLoera et al., 2003].

First we want to see whether a 3×3 table under the CDEM has infinitely many holes or not. After removing redundant rows (using `cddlib`) [Fukuda, 2005], a 3×3 table with fixed row, column sums and the diagonal sum has a 6×9 design matrix. Thus the semigroup is generated by 9 (column) vectors in $\mathbb{Z}^6$:

```
1 1 1 0 0 0 0 0 0
0 0 0 1 1 1 0 0 0
0 0 0 0 0 0 1 1 1
1 0 0 1 0 0 1 0 0
0 1 0 0 1 0 0 1 0
1 0 0 0 1 0 0 0 1
```

By calculating the Smith normal form, it can be checked that the lattice L generated by the columns coincides with $\mathbb{Z}^6$. All of these vectors are extreme rays of the cone (verified via `cddlib`). The Hilbert basis of the cone generated by these 9 vectors consists of these 9 vectors and three additional vectors

$$\begin{aligned} \boldsymbol{b}_{10} &= (1\ 1\ 0\ 1\ 1\ 1)^t, \\ \boldsymbol{b}_{11} &= (1\ 0\ 1\ 1\ 0\ 1)^t, \\ \boldsymbol{b}_{12} &= (0\ 1\ 1\ 0\ 1\ 1)^t. \end{aligned} \tag{2}$$

These vectors are the fundamental holes of the semigroup. We set a system of linear equations such that:

$$\boldsymbol{b}_1 x_1 + \boldsymbol{b}_2 x_2 + \cdots + \boldsymbol{b}_9 x_9 = \boldsymbol{b}_{10}$$
$$x_1 \in \mathbb{Z}_-,\ x_i \in \mathbb{Z}_+,\ \text{for } i = 2, \cdots, 9$$

where $\mathbb{N} = \mathbb{Z}_+ := \{0, 1, \ldots\}$ and $\mathbb{Z}_- := \{0, -1, \ldots\}$. We solved the system via `lrs`. We noticed that this system has no real solution (infeasible). This means that

$$\boldsymbol{b}_{10} \notin (-\mathbb{N}\boldsymbol{a}_1) + \tilde{Q}_{(1)}.$$

Thus by Theorem 2.1, the number of elements in H is infinite.

If we write the marginal sums of the fundamental holes in (2), we see that these correspond to three 2×3 diagonal subtables of the 3×3 table. This suggests that we investigate the case of a 2×3 table. Let $y_{11}, y_{12}, y_{13}, y_{21}, y_{22}, y_{23}$ denote the variables corresponding to six cells of a 2×3 table. Fix the marginals as follows

$$\begin{aligned} c &= y_{11} + y_{12} + y_{13} = y_{21} + y_{22} + y_{23} \\ &= y_{11} + y_{21} = y_{12} + y_{22} = y_{11} + y_{22}, \\ 0 &= y_{13} + y_{23}. \end{aligned} \tag{3}$$

The unique solution of these equations is given as

$$\frac{c}{2} = y_{11} = y_{12} = y_{21} = y_{22}, \quad 0 = y_{13} = y_{23}$$

Therefore if $c = 2k + 1$ is an odd positive integer, then the unique solution is not integral. Moreover, as suggested in Section 6 of Ohsugi and Hibi [2008] the following element of the lattice L

$$\begin{pmatrix} c & c & 0 \\ 0 & 0 & 2c \end{pmatrix} - \begin{pmatrix} 0 & 0 & c \\ 0 & 0 & c \end{pmatrix}$$

has the marginals in (3). It follows that (3) is a hole for all positive odd integer c.

Remark 3.1. *The above argument suggests that we take a look at 2×2 tables with*

$$2k + 1 = y_{11} + y_{12} = y_{21} + y_{22} =$$
$$y_{11} + y_{21} = y_{12} + y_{22} = y_{11} + y_{22}$$

which has the unique solution $k + 1/2 = y_{11} = y_{12} = y_{21} = y_{22}$. However, this is not a hole. In the 2×2 case the design matrix (after removing a redundant row) can be written as

```
1 1 0 0
0 0 1 1
1 0 1 0
1 0 0 1
```

By calculating the Smith normal form, we find 2 is an elementary divisor of this matrix and the columns do not generate $\mathbb{Z}^4$. In fact the semigroup generated by the columns is normal. This follows from the fact that the columns are linearly independent and $\boldsymbol{b} = A\boldsymbol{x}$ has a unique solution for a 2×2 case.

Now based on the fact that 2×3 tables have infinitely many holes, we can prove the following theorem.

Theorem 3.2. *Let $R, C \in \mathbb{Z}$ be positive integers such that $\min\{R, C\} \geq 2$ and $\max\{R, C\} \geq 3$. The semigroup generated by columns of the design matrix of a $R \times C$ table with fixed row, column sums and the diagonal sum has infinitely many holes.*

Proof: Suppose we consider a 2×3 table x with fixed row sums, column sums, and the diagonal sum and let A be a design matrix for the table. Then we have a system of equations

$$Ax = \boldsymbol{b},\ x \geq 0,\ x \in \mathbb{Z}^6. \tag{4}$$

Let H_{23} be the set of holes for the semigroup generated by columns of A. We saw that H_{23} is infinite. Suppose $\boldsymbol{b} \in H_{23}$, i.e., there exists a real solution but there does not exist an integer solution for the system (4). Let y be such a table with the right-hand-side $\boldsymbol{b}$ such that

$$\begin{matrix} y_{11} & y_{12} & y_{13} \\ y_{21} & y_{22} & y_{13} \end{matrix}$$

Now we consider a $R \times C$ table z where $\min\{R, C\} \geq 2$ and $\max\{R, C\} \geq 3$ such that

$$z_{ij} = \begin{cases} y_{ij} & \text{if } 1 \leq i \leq 2 \text{ and } 1 \leq j \leq 3, \\ 0 & \text{else.} \end{cases}$$

If we take the system of equations $A'x' = \boldsymbol{b}'$, $x' \geq 0$, where A' is the design matrix for a $R \times C$ table with fixed row sums, column sums, and the diagonal sum, then all solutions of this system x' have $x'_{ij} = 0$ for $i = 3, \cdots R$, $j = 4, \cdots, C$. Since $\boldsymbol{b} \in H_{23}$, there does not exist an integer solution (4). Thus, $\boldsymbol{b}'$ is a hole of the semigroup generated by columns of A'. Since there are infinitely many $\boldsymbol{b}$, there are infinitely many holes for a $R \times C$ table with fixed row sums, column sums, and the diagonal sum. Since the semigroup for a 2×3 table has infinitely many holes, we are done. □

Finally, we would like to investigate which faces of the polyhedral cone defined by the design matrix for a 3×3 table are almost saturated or nowhere saturated by Theorem 2.3. The results of our experiments are in Table 1. To enumerate all faces, we used `allfaces_gmp` from `cddlib`.

Dimension	# of faces	# of nowhere	# of almost
6	1	0	1
5	16	0	16
4	54	3	51
3	67	13	54
2	36	18	18
1	9	9	0

TABLE 1
Faces for 3×3 tables with fixed row, column sums and the diagonal sum. The first column represents the dimension of faces, the second column represents the number of faces, the third column represents the number of nowhere saturated faces, and the fourth column represents the number of almost saturated faces.

From Table 1 we see that 18 almost saturated 2 dimensional faces are minimal and 3 nowhere saturated 4 dimensional faces are the maximal nowhere saturated faces. Here "minimal" and "maximal" refer to the partial order of the face poset in terms of inclusion of faces.

4 Conclusion

In this paper we found a family of semigroups with infinitely many holes, namely two-way tables under the common diagonal effect model. Most theoretical studies on semigroups have been assuming normality. However, in practice, there are many cases where a semigroup is not normal. Therefore, we think that we need more research on semigroups with holes.

Also, it is known that non-normality of the semigroups causes difficulty for sequential importance sampling (SIS) [Chen et al., 2006]. A Markov basis has already been obtained for this model [Hara et al., 2008]. However, it is of interest to consider how to perform SIS for contingency tables under the CDEM.

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