

CHALLENGING COMPUTATIONS OF HILBERT BASES OF CONES ASSOCIATED WITH ALGEBRAIC STATISTICS

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ABSTRACT. In this paper we present two independent computational proofs that the monoid derived from $5 \times 5 \times 3$ contingency tables is normal, completing the classification by Hibi and Ohsugi. We show that Vlach's vector disproving normality for the monoid derived from $6 \times 4 \times 3$ contingency tables is the unique minimal such vector up to symmetry. Finally, we compute the full Hilbert basis of the cone associated with the non-normal monoid of the semi-graphoid for $|N| = 5$. The computations are based on extensions of the packages LattE-4ti2 and Normaliz.

1. INTRODUCTION

Let $S = \text{monoid}(G)$ be an affine monoid generated by a finite set $G \subseteq \mathbb{Z}^n$ of integer vectors. We call S *normal* if $S = \text{cone}(G) \cap \text{lattice}(G)$, where $\text{cone}(G) = \{\mathbf{x} \in \mathbb{R}^n : \mathbf{x} = \sum \lambda_i \mathbf{g}_i, \lambda_i \in \mathbb{R}_+, \mathbf{g}_i \in G\}$ denotes the rational polyhedral cone generated by G and where $\text{lattice}(G) = \{\mathbf{x} \in \mathbb{R}^n : \mathbf{x} = \sum \lambda_i \mathbf{g}_i, \lambda_i \in \mathbb{Z}, \mathbf{g}_i \in G\}$ denotes the sublattice of \mathbb{Z}^n generated by G . In this paper, we will stick to the case that $\text{lattice}(G) = \mathbb{Z}^n$. Then, normality of S is equivalent to saying that G contains the Hilbert basis of $\text{cone}(G)$, i.e., every lattice point in $\text{cone}(G)$ can be written as a nonnegative integer linear combination of elements in G . Lattice points in $\text{cone}(G) \setminus \text{monoid}(G)$ are called *holes* (or *gaps*). Clearly, $\text{monoid}(G)$ is nonnormal if and only there exists at least one hole.

By the *Hilbert basis* $\mathcal{H}(C)$ of a pointed rational cone C we mean the unique minimal system of generators of the monoid M of lattice points in C . The Hilbert basis of C consists of the *irreducible elements* of M , i.e., those elements of M that do not have a nontrivial representation as a sum of two elements of M (see [2, Ch. 2] for a comprehensive discussion). Note that deciding normality of an affine monoid is NP-hard [6].

An $r_1 \times r_2 \times \cdots \times r_N$ *contingency table* is a function $T : \{1, \dots, r_1\} \times \cdots \times \{1, \dots, r_N\} \rightarrow \mathbb{Z}_+$ where \mathbb{Z}_+ denotes the nonnegative integers. It can be imagined as an N -dimensional

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Lemma 1. *The monoid derived from $5 \times 5 \times 3$ contingency tables by taking line sums (= two-marginals) is normal.*

This completes the normality classification of the monoids derived from $r_1 \times r_2 \times \cdots \times r_N$ contingency tables by taking line sums as given in [12]:

Theorem 2. *Let $r_1 \geq r_2 \geq \dots \geq r_N \geq 2$ be integer numbers. Then the monoid derived from $r_1 \times r_2 \times \cdots \times r_N$ contingency tables by taking line sums is normal if and only if the contingency table is of size*

- $r_1 \times r_2$, $r_1 \times r_2 \times 2 \times \dots \times 2$, or
- $r_1 \times 3 \times 3$, or
- $4 \times 4 \times 3$, $5 \times 4 \times 3$, or $5 \times 5 \times 3$.

For the monoid of $6 \times 4 \times 3$ contingency tables, a vector disproving normality was presented by Vlach [16]. Let M be the monoid derived from $6 \times 4 \times 3$ contingency tables and \mathbf{f} be the vector in $\mathbb{R}^{4 \times 3} \oplus \mathbb{R}^{6 \times 3} \oplus \mathbb{R}^{6 \times 4}$ given by the following three matrices:

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix} \text{ and } \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{pmatrix}.$$

The unique point in the $6 \times 4 \times 3$ (transportation) polytope $\{\mathbf{z} \in \mathbb{R}^{6 \times 4 \times 3} : A\mathbf{z} = \mathbf{f}, \mathbf{z} \geq \mathbf{0}\}$ is

$$\mathbf{z}^* = \frac{1}{2} \left(\begin{array}{ccc|ccc|ccc|ccc|ccc} 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \end{array} \right).$$

(We have written the $6 \times 4 \times 3$ contingency table \mathbf{z}^* as a sequence of 6 matrices of size 4×3 .) This equation shows on the one hand that \mathbf{f} indeed belongs to the cone C generated by M (since $2\mathbf{f} \in M$), and on the other hand, by the uniqueness of the solution, that $\mathbf{f} \notin M$. Since $\mathbb{Z}^{6 \times 4 \times 3} / \text{lattice}(M)$ is torsionfree (as one can verify computationally), \mathbf{f} lies in $\text{lattice}(M)$, and it follows that M is not normal. We can show the following more precise result.

Lemma 3. *The vector \mathbf{f} presented by Vlach [16] is the unique vector (up to the underlying $S_6 \times S_4 \times S_3$ symmetry) in the Hilbert basis of the cone of $6 \times 4 \times 3$ contingency tables that is not an extreme ray.*

The treatment in [8] now completely describes *all* holes of the cone, that is, all lattice points in $\text{cone}(A_{6 \times 4 \times 3})$ that cannot be written as a nonnegative linear integer combination of the (integer) generators of the cone:

One approach to find the Hilbert basis of C is to find a regular triangulation of C into simplicial cones C_1, \dots, C_k and to compute the Hilbert bases of the simplicial cones C_1, \dots, C_k . Clearly, the union of these Hilbert bases is a (typically non-minimal) system of generators of the monoid of lattice points in C . The drawback of this approach is that a complete triangulation of C is often too hard to accomplish.

Instead of computing a full triangulation, we compute only a (regular) subdivision of C into few cones. To this end we remove one of the generators of the cones, say \mathbf{r}_s , compute the convex hull of the cone $C' = \text{cone}(\mathbf{r}_1, \dots, \mathbf{r}_{s-1})$, and find all facets \mathcal{F} of C' that are visible from \mathbf{r}_s . By \mathcal{F}' we denote the set of all cones that we get as the convex hull of a facet in \mathcal{F} with the ray generated by \mathbf{r}_s . Then $\mathcal{F}' \cup \{C'\}$ gives a regular subdivision of C , called the *subdivision with distinguished generator* \mathbf{r}_s . Before we now subdivide those cones in \mathcal{F}' further into smaller cones, we use the following simple observation to remove cones that can be avoided due to the underlying symmetry given by S .

Lemma 6. *Let $C, C_1, \dots, C_k \subseteq \mathbb{R}^n$ be rational polyhedral cones such that $C = \bigcup_{i=1}^k C_i$ (not necessarily a disjoint union). Suppose that there is a permutation σ and indices i and j such that $C_i \subseteq \sigma(C_j) \subseteq C$. Then the Hilbert basis of C is contained in the union of the Hilbert bases of the cones $C_1, \dots, C_{i-1}, \sigma(C_j), C_{i+1}, \dots, C_k$.*

Proof. The result follows by observing that all lattice points in C_i also belong to $\sigma(C_j)$ and thus can be written as a nonnegative integer linear combination of the Hilbert basis of $\sigma(C_j)$. \square

If successful, this test whether C_i can be dropped is a very efficient way of removing unnecessary cones. However, the fewer generators are present in the cones C_1, \dots, C_k , the higher the chance that this test fails. So one has to make a trade-off between a simple test (that may fail more and more often) and a direct treatment of each cone C_i . As we compute only regular subdivisions whose cones are spanned by some of the vectors $\mathbf{r}_1, \dots, \mathbf{r}_s$, each of the cones C_1, \dots, C_k can be represented by a characteristic 0-1-vector $\chi(C_1), \dots, \chi(C_k)$ of length s that encodes which of the generators of C are present in this cone. This makes the test $C_i \subseteq \sigma(C_j)$ comparatively cheap, as we only need to check whether $\chi(C_i) \leq \sigma(\chi(C_j))$.

Summarizing these ideas, the symmetry-exploiting approach can be stated as follows:

- (1) Let $C = \text{cone}(\mathbf{r}_1, \dots, \mathbf{r}_s) \subseteq \mathbb{R}^n$ and $\mathcal{C} = \{C\}$.
- (2) $i := 0$
- (3) While $\mathcal{C} \neq \emptyset$ do
 - (a) $i := i + 1$
 - (b) For all $K \in \mathcal{C}$ that contain the i -th generator compute a subdivision with distinguished i th generator.
 - (c) Let \mathcal{T} be the set of all cones in these subdivisions.
 - (d) Let \mathcal{M} be the set of those cones with a maximum number of rays.
 - (e) Let $\mathcal{C} \neq \emptyset$ be the set \mathcal{M} together with all cones $T \in \mathcal{T}$ that are not covered by a cone $\sigma(M)$ with $M \in \mathcal{M}$ and $\sigma \in S$, see Lemma 6.

- (f) Remove from \mathcal{C} all simplicial cones and compute their Hilbert bases.
- (4) For each computed Hilbert basis element \mathbf{h} compute its full orbit $\{\sigma(\mathbf{h}) : \sigma \in S\}$ and collect them in a set \mathcal{H} .
- (5) Remove the reducible elements from \mathcal{H} .
- (6) Return the set of irreducible elements as the minimal Hilbert basis of C .

This quite simple approach via triangulations and elimination of cones by symmetric covering already solves all three presented examples. In particular, it gives a computational proof to Lemma 1. The candidates for the representatives of Hilbert basis elements can be computed using “LattE for tea, too” by calling

```
dest/bin/hilbert-from-rays-symm --hilbert-from-rays="dest/bin/hilbert-from-rays"
                                --dimension=26 S5.rays
dest/bin/hilbert-from-rays-symm --hilbert-from-rays="dest/bin/hilbert-from-rays"
                                --dimension=43 355.short.rays
dest/bin/hilbert-from-rays-symm --hilbert-from-rays="dest/bin/hilbert-from-rays"
                                --dimension=42 346.short.rays
```

The data files can be found on <http://www.latte-4ti2.de>. (For typographical reasons each command has been printed in two lines.)

3.2. Second approach: partial triangulation. In the second approach, we build up a triangulation of the given cone $C = \text{cone}(\mathbf{r}_1, \dots, \mathbf{r}_s) \subseteq \mathbb{R}^n$. However, by using the following Lemma 7 and its Corollary 8, we can avoid regions of the triangulation that consist only of unimodular cones (for which the extreme ray generators already constitute a Hilbert basis). More precisely, we try to omit simplicial cones whose non-extreme Hilbert basis elements are contained in previously computed simplicial cones.

In the following we describe the facets of a full-dimensional rational cone by (uniquely determined) primitive integral exterior normal vectors. In other words, $F = \{\mathbf{x} \in C : \mathbf{c}^\top \mathbf{x} = 0\}$ where \mathbf{c} has coprime integer entries and $\mathbf{c}^\top \mathbf{y} \leq 0$ for all $\mathbf{y} \in C$.

Lemma 7. *Let $C = \text{cone}(\mathbf{r}_1, \dots, \mathbf{r}_k) \subseteq \mathbb{R}^n$ be a rational polyhedral cone such that*

- $\mathbf{r}_1, \dots, \mathbf{r}_k \in \mathbb{Z}^n$,
- $\mathbf{r}_1, \dots, \mathbf{r}_{k-1}$ lie in a facet of C defined by the hyperplane $\mathbf{c}^\top \mathbf{x} = 0$,
- $\mathbf{c}^\top \mathbf{r}_k = 1$.

Then the Hilbert basis of C is the union of $\{\mathbf{r}_k\}$ and the Hilbert basis of $\text{cone}(\mathbf{r}_1, \dots, \mathbf{r}_{k-1})$.

Proof. Let $\mathbf{z} \in C \cap \mathbb{Z}^n$. Then $\mathbf{z} = \sum_{i=1}^k \lambda_i \mathbf{r}_i$ for some nonnegative real numbers $\lambda_1, \dots, \lambda_k$. Multiplying by \mathbf{c}^\top , we obtain

$$\mathbf{c}^\top \mathbf{z} = \sum_{i=1}^k \lambda_i \mathbf{c}^\top \mathbf{r}_i = \lambda_k \mathbf{c}^\top \mathbf{r}_k = \lambda_k.$$

As $\mathbf{c}, \mathbf{z} \in \mathbb{Z}^n$, we obtain $\lambda_k \in \mathbb{Z}$. Hence, \mathbf{z} is the sum of a nonnegative integer multiple of \mathbf{r}_k and a lattice point $\mathbf{z} - \lambda_k \mathbf{r}_k \in \text{cone}(\mathbf{r}_1, \dots, \mathbf{r}_{k-1})$, which can be written as a nonnegative integer linear combination of elements from the Hilbert basis of this cone. The result now follows. \square

This lemma implies the following fact, which excludes many regions when searching for missing Hilbert basis elements.

Corollary 8. *Let $\mathbf{r}_1, \dots, \mathbf{r}_k \in \mathbb{Z}^n$ such that $C' = \text{cone}(\mathbf{r}_1, \dots, \mathbf{r}_{k-1})$ has dimension n , and $C = C' + \text{cone}(\mathbf{r}_k)$. Suppose that $\mathbf{r}_k \notin C'$. Moreover, let F_1, \dots, F_q be the facets of C' visible from \mathbf{r}_k and let $\mathbf{c}_1, \dots, \mathbf{c}_q$ the normal vectors of these facets as introduced above. Then*

$$\mathcal{H}(C') \cup \{\mathbf{r}_k\} \cup \bigcup \{\mathcal{H}(F_i + \text{cone}(\mathbf{r}_k)) : |\mathbf{c}_i^\top \mathbf{r}_k| \geq 2, i = 1, \dots, q\}$$

generates $C \cap \mathbb{Z}^n$.

Proof. Evidently we obtain a system of generators of $C \cap \mathbb{Z}^n$ if we extend the union in the Corollary over all facets F_i , $i = 1, \dots, q$. It remains to observe that

$$\mathcal{H}(F_i + \text{cone}(\mathbf{r}_k)) = \{\mathbf{r}_k\} \cup \mathcal{H}(C' \cap F_i)$$

if $|\mathbf{c}_i^\top \mathbf{r}_k| = 1$. But this is the statement of Lemma 7. \square

Corollary 8 yields an extremely efficient computation of Hilbert bases—provided the case $|\mathbf{c}_i^\top \mathbf{r}_k| \geq 2$ occurs only rarely, or, in other words, the system $\mathbf{r}_1, \dots, \mathbf{r}_k$ of generators is not too far from a Hilbert basis.

A thoroughly consequent application of Corollary 8 could be realized as follows, collecting the list $\mathcal{A}(C)$ of critical simplicial cones in a recursive algorithm.

- (1) Initially $\mathcal{A}(C)$ is empty.
- (2) One searches lexicographically for the first linearly independent subset $\{\mathbf{r}_{i_1}, \dots, \mathbf{r}_{i_d}\}$. If the cone generated by these elements is not unimodular, it is added to $\mathcal{A}(C)$.
- (3) Now the remaining elements among $\mathbf{r}_1, \dots, \mathbf{r}_s$ (if any) are inserted into the algorithm in ascending order. Suppose that C' is the cone generated by the elements processed already, and let \mathbf{r}_j be the next element to be inserted. Then for all facets F_i of C' such that $\mathbf{c}_i^\top \mathbf{r}_k \geq 2$ the list $\mathcal{A}(C)$ is augmented by $\mathcal{A}(F_i + \text{cone}(\mathbf{r}_j))$.

After all the critical simplicial cones have been collected, it remains to compute their Hilbert bases and to reduce their union globally, together with $\{\mathbf{r}_1, \dots, \mathbf{r}_s\}$.

Let us add some remarks on this approach.

- (a) It is not hard to see that the list $\mathcal{A}(C)$ constitutes a subcomplex of the lexicographical triangulation obtained by inserting $\mathbf{r}_1, \dots, \mathbf{r}_s$. However, this fact is irrelevant for the computation of Hilbert bases.

- (b) In an optimal list of simplicial cones each candidate for the Hilbert basis of C would appear exactly once. (The candidates are the elements of the Hilbert bases of the simplicial cones.) The algorithm above cannot achieve this goal since the cones $F + \text{cone}(\mathbf{r}_j)$ for fixed j are treated independently of each other.
- (c) The drawback of the algorithm above is that it uses the Fourier-Motzkin elimination recursively for subcones. Therefore `Normaliz` applies the algorithm above only on the top level and produces a full triangulation of the cones $F_i + \text{cone}(\mathbf{r}_k)$ for which $\mathbf{c}_i^\top \mathbf{r}_k \geq 2$ (instead of the list $\mathcal{A}(F_i + \text{cone}(\mathbf{r}_j))$).
- (d) It is a crucial feature of the partial triangulation that it reduces memory usage drastically.

	Contingency tables				Semigraphoid
	$4 \times 4 \times 3$	$5 \times 4 \times 3$	$5 \times 5 \times 3$	$6 \times 4 \times 3$	$N = 5$
emb-dim	40	47	55	54	32
dim	30	36	43	42	26
# rays	48	60	75	72	80
# HB	48	60	75	4,392	1,300
# supp hyp	4,948	29,387	306,955	153,858	117,978
# full tri	2,654,000	102,538,980	9,248,466,183	3,100,617,276	1,045,346,320
# partial tri	48	4,320	775,800	206,064	3,109,495
# cand	96	1,260	41,593	10,872	168,014
real time par.	< 0.1	0.2	38	9	14
real time ser.	< 0.1	1.5	813	201	225

TABLE 1. Data of challenging Hilbert basis computations

We illustrate the size of the computation and the gain of the improved algorithm by the data in Table 1. In the table we use the following abbreviations: `emb-dim` is the dimension of the space in which the cone (or monoid) is embedded, `dim` denotes its dimension, `# rays` is the number of extreme rays, `# HB` is the number of elements in the Hilbert basis, `# full tri` is the number of simplicial cones in a full triangulation computed by `Normaliz`, `# partial tri` is the number of cones in the partial triangulation, `# cand` is the number of candidates for the Hilbert basis, and `# supp hyp` is the number of support hyperplanes.

In addition to the improved algorithm just presented, parallelization has contributed substantially to the rather short computation times (given in minutes) that (the experimental version of) `Normaliz` needs for the cones considered. The computation times were measured on a SUN Fire X4450 with 24 Xeon cores where we had limited the

number of threads to 1 for the strictly serial computation. Even on a single processor machine computation times are moderate, as the last line of Table 1 shows.

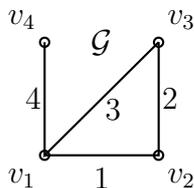
We should add that `Normaliz` cannot compute the full triangulations for $5 \times 5 \times 3$, $6 \times 4 \times 3$ and the semi-graphoid. The numbers were determined by a special program that just produced and counted the simplicial cones.

4. ON A CONJECTURE OF STURMFELS AND SULLIVANT

In this short section we report on a partial verification of a conjecture of Sturmfels and Sullivant on the normality of cut monoids of graphs.

Let \mathcal{G} be a simple, undirected graph without loops on the vertex set V with edge set E . We label the edges $1, \dots, e$. A *cut* of \mathcal{G} is a decomposition $V = A \cup B$ into disjoint subsets. Each cut defines a 0-1-vector $\mathbf{c}_{\{A,B\}}$ in \mathbb{Z}^{2e} as follows: (i) for $j = 1, \dots, e$ the j -th entry of $\mathbf{c}_{\{A,B\}}$ is 1 if and only if the vertices x, y of edge j satisfy $\{x, y\} \subset A$ or $\{x, y\} \subset B$; (ii) for $j = e + 1, \dots, 2e$ the j -th entry of $\mathbf{c}_{\{A,B\}}$ is 1 if and only if the vertices of edge $j - e$ belong to different sets in the decomposition.

The *cut monoid* of \mathcal{G} is the submonoid of \mathbb{Z}^{2e} generated by the vectors $\mathbf{c}_{\{A,B\}}$ where $\{A, B\}$ runs through the cuts of \mathcal{G} . The eight 0-1-vectors below the figure generate the cut monoid of the graph \mathcal{G} :



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

Cut monoids have been introduced to the algebraic statistics literature by Sturmfels and Sullivant [14]. They stated the very interesting conjecture that cut monoids of graphs without K_5 -minors are normal. (A minor of a graph \mathcal{G} is a graph \mathcal{H} that can be produced from \mathcal{G} by a composition of (i) deletion of a vertex and (ii) contraction of an edge.) In fact, the cut monoid of K_5 is nonnormal, this implies nonnormality for every graph with a K_5 -minor. Sturmfels and Sullivant verified their conjecture for graphs with at most 6 vertices.

For graphs with 7 and 8 vertices we used the approach via partial triangulations (and parallelization) in order to verify the conjecture. We generated all these graphs (up to

symmetry) with the help of nauty [10] and then excluded the graphs which have a K_5 -minor. For the remaining graphs no counterexample could be found. The computations took 1 minute for 689 graphs with 7 vertices and 20 hours for 6708 graphs with 8 vertices.

For recent progress on this problem we refer the reader to Ohsugi [11].

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