

Three Counterexamples on Semi-graphoids

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Abstract

Semi-graphoids are combinatorial structures that arise in statistical learning theory. They are equivalent to convex rank tests and to polyhedral fans that coarsen the reflection arrangement of the symmetric group S_n . In this paper we resolve two problems on semi-graphoids posed in Studený's book [19], and we answer a related question of Postnikov, Reiner, and Williams on generalized permutohedra [18]. We also study the semigroup and the toric ideal associated with semi-graphoids.

1 Introduction

A *conditional independence (CI) statement* over a finite set of random variables, indexed by $[n] = \{1, 2, \dots, n\}$, is a formal symbol $[i \perp\!\!\!\perp j | K]$ where $K \subset [n]$ and $i, j \in [n] \setminus K$ are distinct. We identify the CI statements $[i \perp\!\!\!\perp j | K]$ and $[j \perp\!\!\!\perp i | K]$. The symbol $[i \perp\!\!\!\perp j | K]$ represents the statement that the random variables i and j are conditionally independent given the joint random variable K . For any joint probability distribution of the n random variables, the set \mathcal{M} of all CI statements that are valid for the given distribution satisfies the following property:

(SG) If $[i \perp\!\!\!\perp j | K \cup \ell]$ and $[i \perp\!\!\!\perp \ell | K]$ are in \mathcal{M} then so are $[i \perp\!\!\!\perp j | K]$ and $[i \perp\!\!\!\perp \ell | K \cup j]$.

A *semi-graphoid* is any set \mathcal{M} of CI statements which satisfies the axiom **(SG)**. Studený's book [19] gives an introduction to semi-graphoids and their role in statistical learning theory. For further details and references see also Matúš [12, 14]. In this paper we construct examples which answer two problems stated by Studený:

(Q1) *Is it true that every coatom of the lattice of (disjoint) semi-graphoids over $[n]$ is a structural independence model over $[n]$?* [19, Question 4, page 194]

(Q2) *Is every structural imset over $[n]$ already a combinatorial imset over $[n]$?* [19, Question 7, page 207]

Our approach is based on the geometric characterization of semi-graphoids in [16]. Let Π_{n-1} denote the $(n-1)$ -dimensional *permutohedron* [13, 22], which is the convex hull of all permutations of $(1, \dots, n)$. Each vertex of Π_{n-1} is labeled with a *descent permutation* $(\delta_1, \dots, \delta_n)$ as in [16]. Two descent permutations δ, δ' are *adjacent* if they differ by an adjacent transposition, i.e. for some index k we have $\delta_k = \delta'_{k+1}$, $\delta_{k+1} = \delta'_k$, and $\delta_i = \delta'_i$ for $i \notin \{k, k+1\}$. Adjacent permutations label

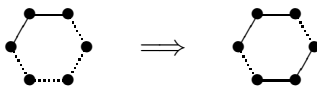
vertices which are adjacent in the edge graph of Π_{n-1} . We label the edge representing this unordered pair $\{\delta, \delta'\}$ with the conditional independence (CI) statement:

$$\delta_k \perp\!\!\!\perp \delta_{k+1} \mid \{\delta_1, \dots, \delta_{k-1}\}. \quad (1)$$

We also identify any set \mathcal{M} of CI statements with the set of edges of Π_{n-1} bearing it as a label, keeping in mind that opposite edges of a square have the same CI statement as their label.

Let $C_n = [0, 1]^n$ denote the standard n -dimensional cube. The vertices of Π_{n-1} are in bijection with the monotone edge paths from $(0, 0, \dots, 0)$ to $(1, 1, \dots, 1)$ on the cube C_n . A vertex of Π_{n-1} labeled $\delta_1, \dots, \delta_n$ corresponds to the monotone path $[\mathbf{e}_{\delta_1}, \mathbf{e}_{\delta_1} + \mathbf{e}_{\delta_2}, \dots, \sum_{i=1}^n \mathbf{e}_{\delta_i}]$ where \mathbf{e}_i denotes the i -th unit vector in \mathbb{R}^n . The 2-dimensional faces of C_n are in bijection with the CI statements on $[n]$. Namely, $[i \perp\!\!\!\perp j \mid K]$ represents the 2-face of C_n with $x_k = 1$ for $k \in K$ and $x_l = 0$ for $l \in [n] \setminus (K \cup \{i, j\})$. The number of these 2-cubes equals $\gamma_n := \binom{n}{2} 2^{n-2}$. There is a natural surjective mapping from the edges of Π_{n-1} onto the 2-faces of C_n , which as with the labeling by CI statements is not injective. Under this mapping, an edge of Π_{n-1} corresponds to a pair of adjacent monotone edge paths on C_n . These adjacent paths differ only along a 2-cube $[i \perp\!\!\!\perp j \mid K]$. In this manner, we identify any set \mathcal{M} of CI statements on $[n]$ with a set of 2-cubes on the boundary of C_n . Each 2-face of the permutohedron Π_{n-1} is either a square or a hexagon. By [16], the semi-graphoid axiom is equivalent to the following geometric condition on the edges of Π_{n-1} :

(SG') *If two adjacent edges of a hexagon are in \mathcal{M} then so are their two opposites.*



The normal fan of the permutohedron Π_{n-1} is the reflection arrangement of S_n . Theorem 3 in [16] identifies semi-graphoids with fans that coarsen this arrangement. Such fans are called *convex rank tests*. Namely, \mathcal{M} specifies the set of edges of Π_{n-1} whose dual walls in the normal fan are not present in the convex rank test.

A basic question about any semi-graphoid \mathcal{M} is whether its corresponding convex rank test is *submodular*, in other words, whether it is the normal fan of a polytope. That polytope would then be a *Minkowski summand* [22] of the permutohedron Π_{n-1} ; see [16] or [18, Proposition 3.2]. Polytopes that are Minkowski summands of Π_{n-1} are known as *generalized permutohedra* and they were studied in [17, 18].

Studený's first question has the following geometric translations:

(Q1) *Is every nontrivial coarsest convex rank test submodular?*

(Q1) *Is every nontrivial fan which maximally coarsens the S_n -arrangement the normal fan of a generalized permutohedron?*

In the first version of [18], Postnikov, Reiner and Williams asked a similar question:

(Q3) *Is every simplicial fan which coarsens the S_n -arrangement the normal fan of a simple generalized permutohedron?*

This paper answers all three questions. In Section 2 we derive and explain our counterexample for Question (Q3). That example is discussed in [18, Example 3.8]. By Studený's classification [20] of the 26424 semi-graphoids for $n = 4$, it had been

known that the answers to Questions **(Q1)** and **(Q2)** are affirmative for $n \leq 4$. In Sections 3 and 4 we construct counterexamples for **(Q1)** and **(Q2)** with $n = 5$.

Question **(Q2)** has the following reformulation in the setting of toric algebra [15, §7]. We represent the semi-graphoid axiom as an equation among formal symbols:

$$(\mathbf{SG}'') \quad [i \perp\!\!\!\perp j | K \cup \ell] + [i \perp\!\!\!\perp \ell | K] = [i \perp\!\!\!\perp j | K] + [i \perp\!\!\!\perp \ell | K \cup j]$$

for all i, j, l, K . These relations span the kernel of the linear map

$$\mathcal{A} : \mathbb{Z}^{\gamma_n} \rightarrow \mathbb{Z}^{2^n}, [i \perp\!\!\!\perp j | K] \mapsto e_{iK} + e_{jK} - e_K - e_{ijK}. \quad (2)$$

A semi-graphoid is a solution to the equations **(SG'')** in the semiring $\{0, \# \}$, representing “zero” and “positive”. In this semiring we have addition: $\# + x = \#$ and $0 + x = x$, as well as multiplication: $0 \cdot x = 0$ and $\# \cdot \# = \#$. A semi-graphoid is *submodular* if it is the set of zero coordinates of a solution to **(SG'')** over the non-negative real numbers. Then there exists a submodular function (i.e., a point in the *deformation cone* in the appendix of [18]) giving rise to the semi-graphoid as the normal fan of the polytope Q_w [16]. These definitions furnish us with an algebraic representation of a semi-graphoid \mathcal{M} and a systematic method for testing submodularity of \mathcal{M} by linear programming. Studený’s question **(Q2)** concerns the \mathbb{N} -linear span of the columns of the matrix \mathcal{A} :

(Q2) *Is the semigroup $\mathcal{A}(\mathbb{N}^{\gamma_n})$ normal, i.e., does it coincide with $\mathcal{A}(\mathbb{R}_{\geq 0}^{\gamma_n}) \cap \mathbb{Z}^{2^n}$?*

For more on normal semigroups and their interactions with polyhedral geometry and toric varieties, see [15]. In Section 5 we study the toric ideal [21] of \mathcal{A} in a polynomial ring in γ_n unknowns, and we examine how it differs from the subideal generated by the binomials

$$(\mathbf{SG}''') \quad [i \perp\!\!\!\perp j | K \cup \ell] \cdot [i \perp\!\!\!\perp \ell | K] - [i \perp\!\!\!\perp j | K] \cdot [i \perp\!\!\!\perp \ell | K \cup j].$$

Proposition 5.1 describes the primary decomposition of this binomial ideal for $n = 4$. We also discuss the problem of deriving the full Markov basis from **(SG''')**.

2 A non-submodular simplicial semi-graphoid

Let $n = 4$ and consider the 4-dimensional cube C_4 and the 3-dimensional permutohedron Π_3 . Each hexagon on Π_3 corresponds to one of the eight facets of C_4 . Each facet specifies three instances of the semi-graphoid axioms, written as in **(SG'')**:

$$\begin{array}{l}
 (*, *, *, 0) \quad \begin{array}{l}
 \llbracket 1 \perp\!\!\!\perp 2 | \emptyset \rrbracket + \llbracket 2 \perp\!\!\!\perp 3 | 1 \rrbracket = \llbracket 2 \perp\!\!\!\perp 3 | \emptyset \rrbracket + \llbracket 1 \perp\!\!\!\perp 2 | 3 \rrbracket \quad \Leftarrow \\
 \llbracket 1 \perp\!\!\!\perp 3 | \emptyset \rrbracket + \llbracket 1 \perp\!\!\!\perp 2 | 3 \rrbracket = \llbracket 1 \perp\!\!\!\perp 2 | \emptyset \rrbracket + \llbracket 1 \perp\!\!\!\perp 3 | 2 \rrbracket \\
 \llbracket 1 \perp\!\!\!\perp 3 | \emptyset \rrbracket + \llbracket 2 \perp\!\!\!\perp 3 | 1 \rrbracket = \llbracket 2 \perp\!\!\!\perp 3 | \emptyset \rrbracket + \llbracket 1 \perp\!\!\!\perp 3 | 2 \rrbracket
 \end{array} \\
 \\
 (*, *, 0, *) \quad \begin{array}{l}
 \llbracket 1 \perp\!\!\!\perp 2 | \emptyset \rrbracket + \llbracket 2 \perp\!\!\!\perp 4 | 1 \rrbracket = \llbracket 2 \perp\!\!\!\perp 4 | \emptyset \rrbracket + \llbracket 1 \perp\!\!\!\perp 2 | 4 \rrbracket \\
 \llbracket 1 \perp\!\!\!\perp 2 | \emptyset \rrbracket + \llbracket 1 \perp\!\!\!\perp 4 | 2 \rrbracket = \llbracket 1 \perp\!\!\!\perp 4 | \emptyset \rrbracket + \llbracket 1 \perp\!\!\!\perp 2 | 4 \rrbracket \\
 \llbracket 1 \perp\!\!\!\perp 4 | \emptyset \rrbracket + \llbracket 2 \perp\!\!\!\perp 4 | 1 \rrbracket = \llbracket 2 \perp\!\!\!\perp 4 | \emptyset \rrbracket + \llbracket 1 \perp\!\!\!\perp 4 | 2 \rrbracket
 \end{array}
 \end{array}$$

$$\begin{array}{l}
(*, 0, *, *) \quad \begin{array}{l} [1 \perp\!\!\!\perp 3 | \emptyset] + [1 \perp\!\!\!\perp 4 | 3] \\ \llbracket 3 \perp\!\!\!\perp 4 | \emptyset \rrbracket + [1 \perp\!\!\!\perp 3 | 4] \\ \llbracket 3 \perp\!\!\!\perp 4 | \emptyset \rrbracket + [1 \perp\!\!\!\perp 4 | 3] \end{array} = \begin{array}{l} [1 \perp\!\!\!\perp 4 | \emptyset] + [1 \perp\!\!\!\perp 3 | 4] \\ [1 \perp\!\!\!\perp 3 | \emptyset] + [3 \perp\!\!\!\perp 4 | 1] \\ [1 \perp\!\!\!\perp 4 | \emptyset] + [3 \perp\!\!\!\perp 4 | 1] \end{array} \quad \Leftarrow \\
(0, *, *, *) \quad \begin{array}{l} [2 \perp\!\!\!\perp 3 | \emptyset] + [3 \perp\!\!\!\perp 4 | 2] \\ [2 \perp\!\!\!\perp 4 | \emptyset] + [2 \perp\!\!\!\perp 3 | 4] \\ \llbracket 3 \perp\!\!\!\perp 4 | \emptyset \rrbracket + [2 \perp\!\!\!\perp 4 | 3] \end{array} = \begin{array}{l} \llbracket 3 \perp\!\!\!\perp 4 | \emptyset \rrbracket + [2 \perp\!\!\!\perp 3 | 4] \\ [2 \perp\!\!\!\perp 3 | \emptyset] + [2 \perp\!\!\!\perp 4 | 3] \\ [2 \perp\!\!\!\perp 4 | \emptyset] + [3 \perp\!\!\!\perp 4 | 2] \end{array} \\
(1, *, *, *) \quad \begin{array}{l} [3 \perp\!\!\!\perp 4 | 1] + \llbracket 2 \perp\!\!\!\perp 3 | 14 \rrbracket \\ [2 \perp\!\!\!\perp 4 | 1] + \llbracket 2 \perp\!\!\!\perp 3 | 14 \rrbracket \\ [2 \perp\!\!\!\perp 4 | 1] + [3 \perp\!\!\!\perp 4 | 12] \end{array} = \begin{array}{l} [2 \perp\!\!\!\perp 3 | 1] + [3 \perp\!\!\!\perp 4 | 12] \\ [2 \perp\!\!\!\perp 3 | 1] + [2 \perp\!\!\!\perp 4 | 13] \\ [3 \perp\!\!\!\perp 4 | 1] + [2 \perp\!\!\!\perp 4 | 13] \end{array} \quad \Leftarrow \\
(*, 1, *, *) \quad \begin{array}{l} [1 \perp\!\!\!\perp 3 | 2] + [3 \perp\!\!\!\perp 4 | 12] \\ [1 \perp\!\!\!\perp 3 | 2] + \llbracket 1 \perp\!\!\!\perp 4 | 23 \rrbracket \\ [3 \perp\!\!\!\perp 4 | 2] + \llbracket 1 \perp\!\!\!\perp 4 | 23 \rrbracket \end{array} = \begin{array}{l} [3 \perp\!\!\!\perp 4 | 2] + [1 \perp\!\!\!\perp 3 | 24] \\ [1 \perp\!\!\!\perp 4 | 2] + [1 \perp\!\!\!\perp 3 | 24] \\ [1 \perp\!\!\!\perp 4 | 2] + [3 \perp\!\!\!\perp 4 | 12] \end{array} \\
(*, *, 1, *) \quad \begin{array}{l} [1 \perp\!\!\!\perp 2 | 3] + \llbracket 1 \perp\!\!\!\perp 4 | 23 \rrbracket \\ [1 \perp\!\!\!\perp 4 | 3] + [2 \perp\!\!\!\perp 4 | 13] \\ [1 \perp\!\!\!\perp 2 | 3] + [2 \perp\!\!\!\perp 4 | 13] \end{array} = \begin{array}{l} [1 \perp\!\!\!\perp 4 | 3] + [1 \perp\!\!\!\perp 2 | 34] \\ [2 \perp\!\!\!\perp 4 | 3] + \llbracket 1 \perp\!\!\!\perp 4 | 23 \rrbracket \\ [2 \perp\!\!\!\perp 4 | 3] + [1 \perp\!\!\!\perp 2 | 34] \end{array} \quad \Leftarrow \\
(*, *, *, 1) \quad \begin{array}{l} [1 \perp\!\!\!\perp 3 | 4] + \llbracket 2 \perp\!\!\!\perp 3 | 14 \rrbracket \\ [1 \perp\!\!\!\perp 2 | 4] + [1 \perp\!\!\!\perp 3 | 24] \\ [1 \perp\!\!\!\perp 2 | 4] + \llbracket 2 \perp\!\!\!\perp 3 | 14 \rrbracket \end{array} = \begin{array}{l} [2 \perp\!\!\!\perp 3 | 4] + [1 \perp\!\!\!\perp 3 | 24] \\ [1 \perp\!\!\!\perp 3 | 4] + [1 \perp\!\!\!\perp 2 | 34] \\ [2 \perp\!\!\!\perp 3 | 4] + [1 \perp\!\!\!\perp 2 | 34] \end{array}
\end{array}$$

This is a system of 24 equations in $\gamma_4 = 24$ formal symbols $[i \perp\!\!\!\perp j | K]$.

A semi-graphoid is a solution to these equations over the semiring $\{0, +\}$. More precisely, given such a solution vector in $\{0, +\}^{24}$, the semi-graphoid \mathcal{M} consists of all coordinates $[i \perp\!\!\!\perp j | K]$ that have the value 0. There are 26424 semi-graphoids. They form a sublattice of the Boolean lattice $\{0, +\}^{24}$, with $+$ $<$ 0. Question **(Q1)** concerns the coatoms of this lattice. But let us first resolve Question **(Q3)**.

We consider the following collection of CI statements:

$$\mathcal{M} = \{ \llbracket 2 \perp\!\!\!\perp 3 | 14 \rrbracket, \llbracket 1 \perp\!\!\!\perp 4 | 23 \rrbracket, \llbracket 1 \perp\!\!\!\perp 2 | \emptyset \rrbracket, \llbracket 3 \perp\!\!\!\perp 4 | \emptyset \rrbracket \}. \quad (3)$$

These four symbols are highlighted in the 24 equations above by the use of double brackets $\llbracket \dots \rrbracket$. Each equation (individually) can be solved among the positive reals after these four symbols have been set to zero, or equivalently they can be solved as a system over $\{0, +\}$. This shows that \mathcal{M} is a semi-graphoid.

The semi-graphoid \mathcal{M} is represented geometrically by the three-dimensional polytope in Figure 1. This polytope is *simple*, i.e., each of the 16 vertices is adjacent to three other vertices. The eight vertices whose labels include three bars (such as $4|2|1|3$) correspond to unique permutations in S_4 (namely the descent permutation 4213), while the eight vertices whose labels have two bars (such as $4|1|23$) correspond to pairs of permutations in S_4 (namely descent permutations 4123 and 4132). This partition of S_4 into eight singletons and eight pairs is the convex rank test corresponding to the semi-graphoid \mathcal{M} under the bijection of [16]. The normal fan of the polytope in Figure 1 is a simplicial fan which is combinatorially (but not geometrically) isomorphic to a fan that coarsens the hyperplane arrangement of S_4 .

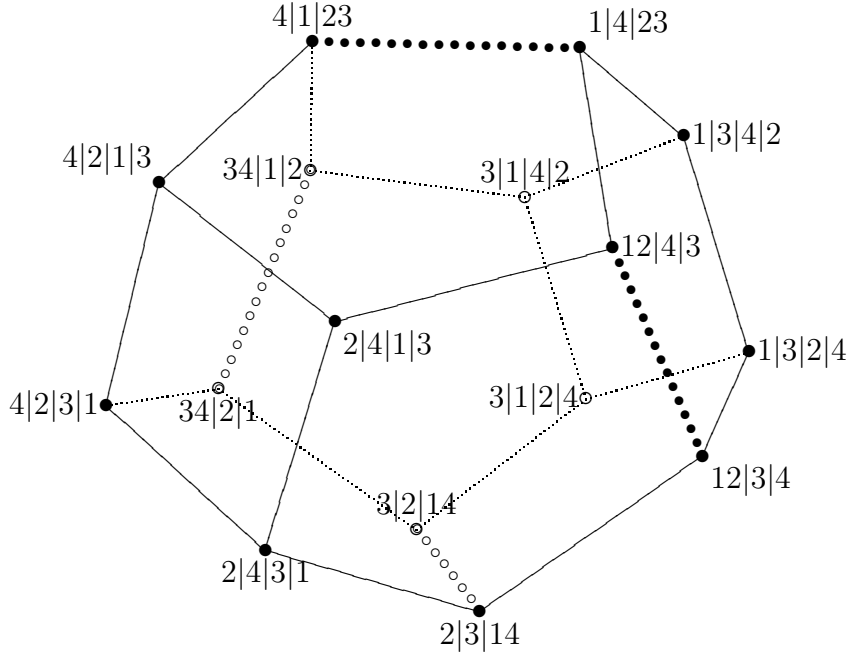


Figure 1: A simple 3-dimensional polytope with 16 vertices and 10 facets

Proposition 2.1. *The simplicial semi-graphoid \mathcal{M} is not submodular.*

Proof. Suppose that \mathcal{M} were submodular. Then the above equations have a solution in $(\mathbb{R}_{\geq 0})^{24}$ whose coordinates in \mathcal{M} are zero and whose other 20 coordinates are positive. The four equations marked by an “ \leftarrow ” give the following four equations:

$$\begin{aligned}
 [2 \perp\!\!\!\perp 3 | 1] &= [2 \perp\!\!\!\perp 3 | \emptyset] + [1 \perp\!\!\!\perp 2 | 3] \\
 [1 \perp\!\!\!\perp 4 | 3] &= [1 \perp\!\!\!\perp 4 | \emptyset] + [3 \perp\!\!\!\perp 4 | 1] \\
 [3 \perp\!\!\!\perp 4 | 1] &= [2 \perp\!\!\!\perp 3 | 1] + [3 \perp\!\!\!\perp 4 | 12] \\
 [1 \perp\!\!\!\perp 2 | 3] &= [1 \perp\!\!\!\perp 4 | 3] + [1 \perp\!\!\!\perp 2 | 34].
 \end{aligned}$$

Adding the left hand sides and the right hand sides of the four equations yields

$$[2 \perp\!\!\!\perp 3 | \emptyset] + [1 \perp\!\!\!\perp 4 | \emptyset] + [3 \perp\!\!\!\perp 4 | 12] + [1 \perp\!\!\!\perp 2 | 34] = 0.$$

This contradicts the assumption that these four values are strictly positive. \square

The set of non-negative solutions to the 24 equations (\mathbf{SG}'') is an 11-dimensional cone in $(\mathbb{R}_{\geq 0})^{24}$. This cone is isomorphic to the 16-dimensional cone of submodular functions on $2^{[4]}$, modulo its 5-dimensional lineality space. Its 22108 faces are in bijection with the submodular semi-graphoids, or, equivalently, with the generalized permutohedra for $n = 4$. In addition to these, there are 4316 semi-graphoids that are not submodular. Each of the latter can be represented by a polytope of dimension ≤ 3 as in Figure 1. These polytopes have the combinatorial properties of generalized permutohedra [18], but they cannot be realized as Minkowski summands of Π_3 . For example, see [11, Figure 5] for a polytope that represents Studený’s example of a semi-graphoid that is not submodular (see [16] and [19, Section 2.2.4]).

We now give a classification of non-submodular semi-graphoids for $n = 4$ and $|\mathcal{M}|$ small. All simplicial examples are coarsenings (up to relabeling) of the particular semi-graphoid \mathcal{M} in Proposition 2.1. The following table lists the number of semi-graphoids classified by number of CI statements, their type, and whether they are simplicial. Here, the *type* of a semi-graphoid is the triple (m_0, m_1, m_2) where m_t is the number of CI statements $[i \perp\!\!\!\perp j | K]$ in \mathcal{M} such that $|K| = m_t$.

$ \mathcal{M} $	type	non-simplicial	simplicial	total
3	(0, 3, 0)	8	0	8
4	(0, 4, 0)	78	0	78
4	(1, 2, 1)	30	0	30
4	(2, 0, 2)	0	6	6
5	(0, 5, 0)	300	0	300
5	(1, 2, 2)	30	0	30
5	(1, 3, 1)	84	0	84
5	(2, 0, 3)	12	12	24
5	(2, 2, 1)	30	0	30
5	(3, 0, 2)	24	0	24
6	(0, 6, 0)	604	0	604
6	(1, 3, 2)	84	0	84
6	(1, 4, 1)	78	0	78
6	(2, 0, 4)	30	3	33
6	(2, 2, 2)	30	0	30
6	(2, 3, 1)	84	0	84
6	(3, 0, 3)	74	12	96
6	(4, 0, 2)	30	3	33
7	(0, 7, 0)	684	0	684
7	(1, 4, 2)	78	0	78
7	(1, 5, 1)	24	0	24
7	(2, 0, 5)	18	0	18
7	(2, 3, 2)	84	0	84
7	(2, 4, 1)	78	0	78
7	(3, 0, 4)	132	0	132
7	(4, 0, 3)	132	0	132
7	(5, 0, 2)	18	0	18
8	(0, 8, 0)	450	0	450
8	(1, 5, 2)	24	0	24
8	(2, 0, 6)	3	0	3
8	(2, 4, 2)	48	0	48
8	(2, 5, 1)	24	0	24
8	(3, 0, 5)	72	0	72
8	(4, 0, 4)	174	0	174
8	(5, 0, 3)	72	0	72
8	(6, 0, 2)	3	0	3

$ \mathcal{M} $	type	non-simplicial	simplicial	total
9	(0 , 9 , 0)	212	0	212
9	(3 , 0 , 6)	12	0	12
9	(4 , 0 , 5)	84	0	84
9	(5 , 0 , 4)	84	0	84
9	(6 , 0 , 3)	12	0	12
10	(0 , 10 , 0)	60	0	60
10	(4 , 0 , 6)	15	0	15
10	(5 , 0 , 5)	24	0	24
10	(6 , 0 , 4)	15	0	15
11	(0 , 11 , 0)	12	0	12
11	(5 , 0 , 6)	6	0	6
11	(6 , 0 , 5)	6	0	6

3 A non-submodular coarsest semi-graphoid

We now consider the case $n = 5$. There are $\gamma_5 = 80$ CI statements, one for each two-dimensional face of the 5-cube C_5 . There are 120 instances of the semi-graphoid axioms (\mathbf{SG}''), three for each of the 40 three-dimensional faces of C_5 , listed as additive equations in the Appendix. The semi-graphoids are the solutions of these equations over $\{0, \# \}^{80}$. These solutions include the all-zero vector $\mathbf{0}$ which represents the semi-graphoid that consists of all 80 CI statements, and which is the maximal element in the lattice of semi-graphoids. A semi-graphoid is said to be *coarsest* if it is maximal among non- $\mathbf{0}$ semi-graphoids. Geometrically, such a semi-graphoid corresponds to a fan which coarsens the S_5 -arrangement but cannot be coarsened to a non-trivial fan.

We now present the counterexample which answers question (**Q1**). Our constructions make use of the identification of semi-graphoids with convex rank tests that was derived in [16]. Let Γ denote the partition of the symmetric group S_5 into fourteen classes as follows. There are eight classes containing 12 permutations each:

$$\begin{array}{cccc} 15|234 & 234|15 & 123|45 & 235|14 \\ 124|35 & 245|13 & 134|25 & 345|12. \end{array}$$

And there are six classes containing four permutations each:

$$\begin{array}{ccc} 12|5|34 & 25|1|34 & 13|5|24 \\ 35|1|24 & 14|5|23 & 45|1|23. \end{array}$$

Here $15|234$ denotes the class of all descent permutations $ijklm$ with $\{i, j\} = \{1, 5\}$ and $\{k, l, m\} = \{2, 3, 4\}$. Similarly, $45|1|23$ denotes the class of all permutations $ijklm$ with $\{i, j\} = \{4, 5\}$, $k = 1$, and $\{l, m\} = \{2, 3\}$. Clearly, Γ is a pre-convex rank test, as each of the 14 classes is the set of all linear extensions of a poset on $\{1, 2, 3, 4, 5\}$. Note that the subgroup of S_5 fixing the pre-convex rank test Γ has order 12, because Γ is fixed under permutations of $\{1, 5\}$ and of $\{2, 3, 4\}$. The 14 classes of Γ are represented by the 14 vertices of the polytope depicted in Figure 2.

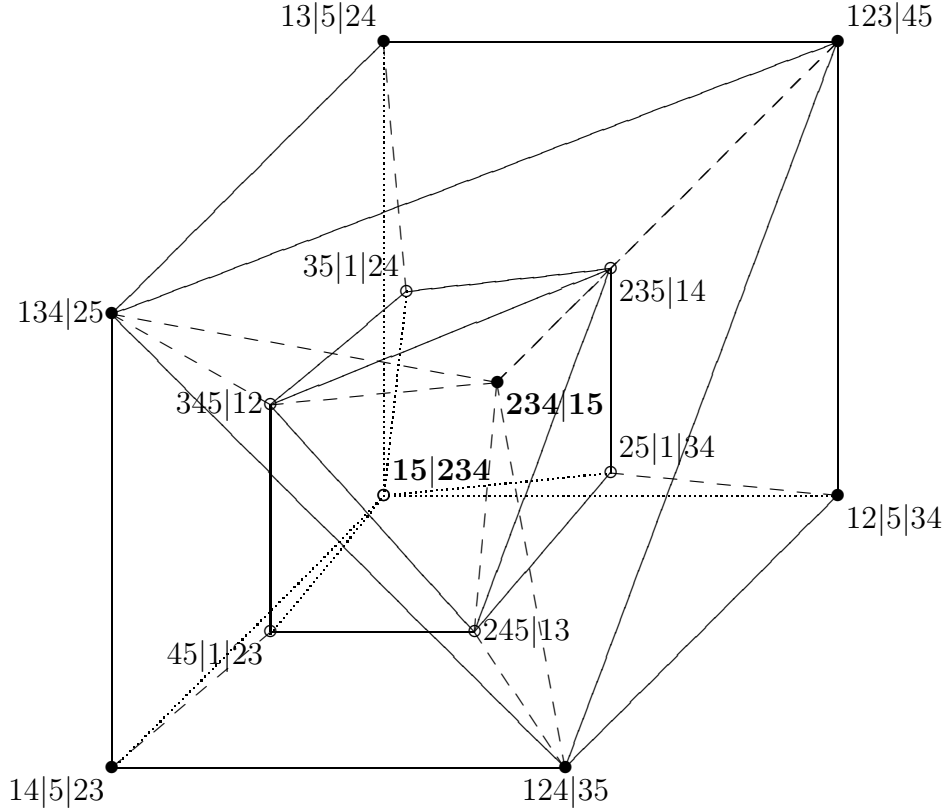


Figure 2: Schlegel diagram [22] of a 4-dimensional polytope with 10 facets

Each pair of permutations in a given class of Γ which differ by an adjacent transposition specifies a CI statement. For instance, the four-element class $45|1|23$ specifies the two CI statements $[[4\perp\perp 5|\emptyset]]$ and $[[2\perp\perp 3|145]]$, while the 12-element class $15|234$ specifies the seven CI statements

$$[[1\perp\perp 5|\emptyset]], [[2\perp\perp 3|15]], [[2\perp\perp 3|145]], [[2\perp\perp 4|15]], [[2\perp\perp 4|135]], [[3\perp\perp 4|15]], [[3\perp\perp 4|125]].$$

Altogether, we obtain 44 CI statements $[[\cdot|\cdot]]$ from the 14 classes, and we identify the pre-convex rank test Γ with the set of these 44 CI statements. We now prove:

Theorem 3.1. Γ is a coarsest convex rank test which is not submodular.

Proof. To establish this theorem, we must prove the following three claims:

- Γ is a convex rank test, i.e. it satisfies the semi-graphoid axiom (**SG**).
- There is no proper convex rank test which is coarser than Γ .
- The convex rank test Γ is not submodular.

We shall prove all three statements at once, by examining the semi-graphoid equations (**SG''**). As in Section 2, the 44 symbols in Γ are denoted with double brackets $[[\cdot|\cdot]]$, while the 36 symbols not in Γ are denoted with brackets $[\cdot|\cdot]$. With this

distinction, there are four symmetry types of semi-graphoid equations that involve the 36 positive unknowns $[\cdot|\cdot]$. The full list is given in the Appendix:

$$\begin{array}{lll}
\text{Type I} & [3\perp\perp 5|12] + \llbracket 3\perp\perp 4|125 \rrbracket & = [3\perp\perp 4|12] + \llbracket 3\perp\perp 5|124 \rrbracket \\
\text{Type II} & [1\perp\perp 5|2] + [1\perp\perp 3|25] & = \llbracket 1\perp\perp 3|2 \rrbracket + [1\perp\perp 5|23] \\
\text{Type III} & [4\perp\perp 5|1] + [2\perp\perp 5|14] & = [2\perp\perp 5|1] + [4\perp\perp 5|12] \\
\text{Type IV} & [1\perp\perp 2|5] + \llbracket 2\perp\perp 3|15 \rrbracket & = \llbracket 2\perp\perp 3|5 \rrbracket + [1\perp\perp 2|35]
\end{array}$$

After setting the 44 unknowns $\llbracket \cdot|\cdot \rrbracket$ to zero, we are left with 120 equations in the 36 strictly positive unknowns. For instance, the first three types give

$$\begin{array}{lll}
\text{Type I} & [3\perp\perp 5|12] & = [3\perp\perp 4|12] \\
\text{Type II} & [1\perp\perp 5|2] + [1\perp\perp 3|25] & = [1\perp\perp 5|23] \\
\text{Type III} & [4\perp\perp 5|1] + [2\perp\perp 5|14] & = [2\perp\perp 5|1] + [4\perp\perp 5|12]
\end{array}$$

The axiom (**SG''**) merely requires that each of these equations is *individually* solvable. This is obviously the case. Hence Γ is a semi-graphoid.

The 78 equations of Type I listed in the Appendix imply that all 36 positive unknowns must be equal. So, if another CI statement is added to the semi-graphoid Γ , then all others must be added in order for (**SG**) to remain valid. This proves our second claim that Γ is a coarsest convex rank test.

Given that the 36 unknowns $[\cdot|\cdot]$ must be equal, the 12 Type II equations imply that their common value is zero, contradicting the requirement that they be positive. Hence the 120 original equations *altogether* have no non-negative real solution that is consistent with Γ . This proves our third claim that Γ is not submodular. \square

Every semi-graphoid for $n = 5$ corresponds to a 4-dimensional fan. Intersecting this fan with a sphere around the origin, we obtain a polyhedral cell decomposition of the 3-dimensional sphere. We do not know whether each of these 3-spheres can be realized as the boundary of a 4-dimensional polytope. However, using [22, §5], every semi-graphoid can be represented by a 3-dimensional diagram as in Figure 2.

For the specific semi-graphoid Γ of Theorem 3.1, the diagram in Figure 2 is indeed the boundary of a 4-polytope with f -vector [22] (14, 36, 32, 10). As with the polytope of Section 3, this polytope only combinatorially rather than geometrically represents Γ because Γ is not submodular. The following coordinates for this polytope were found by a direct calculation, using the techniques described in [3]. Each of the following ten row vectors represents a facet of our polytope:

POINTS

1	1/4	0	0	0	0
1	0	1	0	0	0
1	0	0	1	0	0
1	0	0	0	1	0
1	0	0	0	0	1
1	-1/4	1/4	1/4	5/4	1/4
1	280/893	-280/893	25/893	0	28/893
1	1/57	1/57	-1/57	17/19	2/57
1	1	1	0	-5	1

1 2/37 20/37 1/37 10/37 -2/37

For instance, the last row represents the facet-defining inequality

$$\frac{2}{37} \cdot x_1 + \frac{20}{37} \cdot x_2 + \frac{1}{37} \cdot x_3 + \frac{10}{37} \cdot x_4 - \frac{2}{37} \cdot x_5 \leq 1.$$

Here, we are considering the vectors $(x_1, x_2, x_3, x_4, x_5)$ to be elements in the quotient of \mathbb{R}^5 modulo the one-dimensional linear subspace spanned by $(4, 1, 1, 1, 1)$. Our format is that of the software `Polymake` [9]. If the above eleven lines are put in a file named `mypolytope` then the following command in `Polymake` will verify that this polytope does indeed have the combinatorial structure displayed in Figure 2:

```
polymake mypolytope F_VECTOR VERTICES_IN_FACETS
```

The 10 facets of our 4-polytope correspond to the facets of the 5-cube, and they comprise all classes of permutations in S_5 in which the first or last coordinate is fixed. The facets corresponding to permutations with 1 *or* 5 in the *first* coordinate have seven vertices, twelve edges, and eight 2-faces. The facets corresponding to permutations with 2, 3 *or* 4 *first* have seven vertices, 13 edges, and eight 2-faces. The facets for 1 *or* 5 *last* are tetrahedra. The facets for 2, 3 *or* 4 *last* are cubes in which one edge has been contracted; they have seven vertices and 11 edges.

4 The semi-graphoid semigroup is not normal

Continuing to assume $n = 5$, we now consider the linear map \mathcal{A} in the Introduction. It maps the free abelian group \mathbb{Z}^{80} spanned by the CI statements to the free abelian group \mathbb{Z}^{32} with basis $\{e_K : K \subseteq [5]\}$ as specified in (2). The matrix representing \mathcal{A} has 32 rows and 80 columns; each column has four non-zero entries: two $+1$'s and two -1 's. The rank of \mathcal{A} is 26. The *semi-graphoid semigroup* is $\mathcal{A}(\mathbb{N}^{80})$, the non-negative integer span of the columns of this 32×80 -matrix. This is a subsemigroup of \mathbb{Z}^{32} . Equivalently, the semi-graphoid semigroup is the affine semigroup with 80 generators and 120 relations (given in the Appendix). Note that the polyhedral cone dual to the semi-graphoid semigroup is the cone of submodular functions.

In the paper [19] (up to a sign change), the vectors in \mathbb{Z}^{32} are called *imsets*, the columns of \mathcal{A} are *elementary imsets*, and the elements of $\mathcal{A}(\mathbb{N}^{80})$ are *combinatorial imsets*. A *structural imset* is a lattice point which lies in the polyhedral cone spanned by the elementary imsets. Studený's question (**Q2**) whether each structural imset is combinatorial translates into the question whether the semigroup $\mathcal{A}(\mathbb{N}^{80})$ is normal.

Theorem 4.1. *The semi-graphoid semigroup is not normal for $n = 5$.*

Proof. Consider the following element in the free abelian group \mathbb{Z}^{80} :

$$\begin{aligned} & [1\perp\perp 5|2] + [1\perp\perp 4|3] + [2\perp\perp 3|4] + [2\perp\perp 3|5] + [3\perp\perp 4|12] \\ & + [2\perp\perp 5|13] + [1\perp\perp 2|45] + [1\perp\perp 3|45] + [4\perp\perp 5|23] - [2\perp\perp 3|45]. \end{aligned} \tag{4}$$

The image of this element under the map $\mathcal{A} : \mathbb{Z}^{80} \rightarrow \mathbb{Z}^{32}$ is the imset

$$\begin{aligned} \mathbf{b} := & -e_2 - e_3 - e_4 - e_5 - e_{23} + e_{24} + 2e_{25} + 2e_{34} + e_{35} - e_{45} + 2e_{123} \\ & + e_{124} - e_{125} - e_{134} + e_{135} + 2e_{145} - e_{1234} - e_{1235} - e_{1245} - e_{1345}. \end{aligned} \tag{5}$$

The imset \mathbf{b} is structural because $2 \cdot \mathbf{b}$ is a combinatorial imset. It is the image of

$$\begin{aligned} & [4\perp\perp 5|2] + [4\perp\perp 5|3] + [1\perp\perp 3|4] + [1\perp\perp 2|5] + [2\perp\perp 5|14] + [3\perp\perp 4|15] \\ & + [1\perp\perp 4|23] + [1\perp\perp 5|23] + [1\perp\perp 5|2] + [1\perp\perp 4|3] + [2\perp\perp 3|4] \\ & + [2\perp\perp 3|5] + [3\perp\perp 4|12] + [2\perp\perp 5|13] + [1\perp\perp 2|45] + [1\perp\perp 3|45] \quad \in \mathbb{N}^{80} \end{aligned} \quad (6)$$

under the linear map \mathcal{A} .

Suppose that \mathbf{b} were a combinatorial imset. Then there exists $\mathbf{x} \in \mathbb{N}^{80}$ such that $\mathcal{A} \cdot \mathbf{x} = \mathbf{b}$. We write $\mathbf{x} = \sum_i [a_i \perp\perp b_i | K_i]$, where we allow repetition in the sum. In any elementary imset, the basis vector e_\emptyset occurs with coefficient -1 or 0 , and the basis vector e_{12345} occurs with coefficient -1 or 0 . However, neither e_\emptyset nor e_{12345} appears in the imset \mathbf{b} , so we conclude that $|K_i| = 1$ or $|K_i| = 2$ for all terms $[a_i \perp\perp b_i | K_i]$ in the representation of \mathbf{x} . The first four terms $-e_2 - e_3 - e_4 - e_5$ in \mathbf{b} imply that \mathbf{x} has precisely four terms $[a_i \perp\perp b_i | K_i]$ with $|K_i| = 1$, and the terms $-e_{1234} - e_{1235} - e_{1245} - e_{1345}$ imply that \mathbf{x} has precisely four terms with $|K_i| = 2$.

Each of the eight terms in \mathbf{x} evaluates to an alternating sum of 4 terms under the map \mathcal{A} . Some cancellation occurs among the resulting 32 terms. Prior to that cancellation, our imset had been written as the sum of two subsums, $\mathbf{b} = \mathcal{A} \cdot \mathbf{x} =$

$$\begin{aligned} & -e_2 - e_3 - e_4 - e_5 + e_{24} + 2e_{25} + 2e_{34} + e_{35} + e_{A_1} + e_{A_2} - e_{125} - e_{134} - e_{B_1} - e_{B_2} \\ & -e_{23} - e_{45} - e_{A_1} - e_{A_2} + 2e_{123} + e_{124} + e_{135} + 2e_{145} + e_{B_1} + e_{B_2} - e_{1234} - e_{1235} - e_{1245} - e_{1345}, \end{aligned}$$

where $|A_1| = |A_2| = 2$ and $|B_1| = |B_2| = 3$. The first line is the sum of the four elementary imsets $\mathcal{A}([a_i \perp\perp b_i | K_i])$ with $|K_i| = 1$, and the second line is the sum of the four elementary imsets with $|K_i| = 2$. A contradiction will arise when we try to determine the unknown pairs A_1 and A_2 . The term $-e_{125}$ in the first line must come from $K_i = \{2\}$ or $K_i = \{5\}$. This implies that either $\{1, 2\}$ or $\{1, 5\}$ is in $A_* = \{A_1, A_2\}$. Similarly, the term $-e_{134}$ shows that either $\{1, 3\}$ or $\{1, 4\}$ is in A_* . Now consider the second line. The presence of the term $2e_{123}$ implies that $\{1, 2\}$ or $\{1, 3\}$ is in A_* , and the term $2e_{145}$ implies that $\{1, 4\}$ or $\{1, 5\}$ is in A_* . The term e_{124} shows that $\{1, 2\}$, $\{1, 4\}$, or $\{2, 4\}$ is in A_* , and, finally, the term e_{135} shows that $\{1, 3\}$, $\{1, 5\}$, or $\{3, 5\}$ is in A_* . However, no such pair of pairs A_* satisfies these six restrictions. This proves that \mathbf{b} is not a combinatorial imset. \square

The main point of the above proof was to show that the linear system $\mathcal{A} \cdot \mathbf{x} = \mathbf{b}$ has no solution with non-negative *integer* coordinates. This can also be verified automatically using integer programming software. In fact, using such software we found that $\mathcal{A} \cdot \mathbf{x} = \mathbf{b}$ has only one solution with non-negative *real* coordinates, namely, that unique solution $\mathbf{x} \in (\mathbb{R}_{\geq 0})^{80}$ is the expression in (6) scaled by $1/2$.

The reader might now inquire how the imset \mathbf{b} was found. There are several algorithms that test whether a given affine semigroup is normal, including one recently proposed by Takemura, Yoshida and the first author [10], and the method of Bruns and Koch [4] which is implemented in their software `normaliz`.

Our original attempts to apply these methods directly to the 32×80 -matrix \mathcal{A} were unsuccessful. Instead we succeeded by partially computing a *Markov basis* for the matrix \mathcal{A} using the software `4ti2` [1]. The imset \mathbf{b} was found by inspecting the partial results produced by `4ti2`. By now, we have computed the full Markov using an improved version of `4ti2`. We explain the details in the next section.

5 Computations in toric algebra

Let $\mathbb{Q}[\text{CI}_n]$ denote the polynomial ring over the field of rational numbers \mathbb{Q} generated by the symbols $[i \perp\!\!\!\perp j | K]$. Thus $\mathbb{Q}[\text{CI}_n]$ is a polynomial ring in γ_n unknowns, one for each 2-face of the n -cube C_n . We write $\prod \text{CI}_n$ for the product of all the unknowns. We define the *semi-graphoid ideal* to be the ideal I_{SG} generated by the binomials in (SG''') . Thus the generators of I_{SG} represent the semi-graphoid axioms. Following [15, §7], we introduce the *toric ideal* $I_{\mathcal{A}}$ which is a prime ideal obtained from I_{SG} by saturation:

$$I_{\mathcal{A}} := (I_{\text{SG}} : (\prod \text{CI}_n)^\infty). \quad (7)$$

The binomials in $I_{\mathcal{A}}$ represent the vectors in the kernel of the linear map $\mathcal{A} : \mathbb{Z}^{\gamma_n} \rightarrow \mathbb{Z}^{2^n}$. A minimal set of binomials which generates $I_{\mathcal{A}}$ is said to be a *Markov basis* for the matrix \mathcal{A} . See [5] for a discussion of Markov bases in the context of statistics.

Let us illustrate these concepts for $n = 3$. The polynomial ring $\mathbb{Q}[\text{CI}_3]$ has six unknowns, one for each facet of the 3-cube. They are the entries of the 2×3 -matrix

$$\begin{pmatrix} [1 \perp\!\!\!\perp 2 | \emptyset] & [1 \perp\!\!\!\perp 3 | \emptyset] & [2 \perp\!\!\!\perp 3 | \emptyset] \\ [1 \perp\!\!\!\perp 2 | 3] & [1 \perp\!\!\!\perp 3 | 2] & [2 \perp\!\!\!\perp 3 | 1] \end{pmatrix}. \quad (8)$$

The semi-graphoid ideal I_{SG} is generated by the three 2×2 -minors of the matrix (8). This is a prime ideal of codimension 2 and degree 3, and hence we have $I_{\text{SG}} = I_{\mathcal{A}}$. See e.g. Eisenbud [6] for definitions of these concepts. Here the Markov basis for \mathcal{A} consists precisely of the three semi-graphoid axiom instances.

We next consider the case $n = 4$. The polynomial ring $\mathbb{Q}[\text{CI}_4]$ has 24 unknowns, one for each 2-face of the 4-cube. They are the entries of eight 2×3 -matrices as in (8), one for each of the eight facets of the 4-cube. Thus the semi-graphoid ideal I_{SG} is generated by 24 quadrics, one for each of the 24 axiom instances (SG'') in the list given in Section 2. For instance, the last instance in that list translates into the quadric $[1 \perp\!\!\!\perp 2 | 4] \cdot [2 \perp\!\!\!\perp 3 | 14] - [2 \perp\!\!\!\perp 3 | 4] \cdot [1 \perp\!\!\!\perp 2 | 34]$, which is one of the 24 generators of I_{SG} . Using the software `Macaulay2` [8] we derived the following result:

Proposition 5.1. *The semi-graphoid ideal I_{SG} for $n = 4$ is a radical ideal which is the intersection of the toric ideal $I_{\mathcal{A}}$ and 17 additional associated monomial prime ideals.*

Before discussing this prime decomposition in detail, let us make a few general remarks. We wish to argue that toric algebra and algebraic geometry provide useful algorithmic tools for the research directions presented in [19]. For any ideal I of $\mathbb{Q}[\text{CI}_n]$ and any subset Ω of \mathbb{C} , the *variety* $V_\Omega(I)$ is defined as the set of all vectors in Ω^{γ_n} which are common zeros of all the polynomials in I . Then $V_{\mathbb{C}}(I_{\text{SG}})$ is a complex variety, reducible for $n \geq 4$, one of whose irreducible components is the complex toric variety $V_{\mathbb{C}}(I_{\mathcal{A}})$. Inside this toric variety are the real toric variety $V_{\mathbb{R}}(I_{\mathcal{A}})$. Its non-negative part $V_{\mathbb{R}_{\geq 0}}(I_{\mathcal{A}})$ is homeomorphic to the cone spanned by the elementary insets. Our next result shows that the semi-graphoids are precisely the points on these varieties whose coordinates are 0 or 1.

Theorem 5.2. *The semi-graphoids on the set $[n]$ are in bijection with the points in $V_{\{0,1\}}(I_{\text{SG}})$. The submodular semi-graphoids on $[n]$ are in bijection with the points in $V_{\{0,1\}}(I_{\mathcal{A}})$.*

Proof. We replace the additive semiring $\{0, +\}$ with the multiplicative semiring $\{1, 0\}$. This translates from the additive notation (\mathbf{SG}'') to the multiplicative notation (\mathbf{SG}''') . With this translation, the first statement in Theorem 5.2 is obvious.

The second statement is less obvious and is based on the geometry of toric varieties. Specifically, we shall use the characterization of *facial* index sets which is developed in [7]. If we consider our specific $2^n \times \gamma_n$ -matrix \mathcal{A} then the role of the set $\{1, \dots, m\}$ in [7] is played by the set of CI statements, and a subset of CI statements is facial for \mathcal{A} if and only if it is submodular semi-graphoid. With this observation, our second assertion follows from Lemma A.2 in the Appendix of [7]. \square

Using Theorem 5.2, we can study semi-graphoids by studying the zero-dimensional ideals obtained by adding $\langle x^2 - x : x \in \text{CI}_n \rangle$ to the ideal $I_{\mathbf{SG}}$ or $I_{\mathcal{A}}$. With the command `degree` in `Macaulay2` [8], it takes only a few seconds to compute

$$\#V_{\{0,1\}}(I_{\mathbf{SG}}) = 26424 \quad \text{and} \quad \#V_{\{0,1\}}(I_{\mathcal{A}}) = 22108. \quad (9)$$

The difference between these numbers is explained geometrically by the prime decomposition in Proposition 5.1, which we shall now describe in explicit terms.

The 17 associated monomial primes of $I_{\mathbf{SG}}$ come in three symmetry classes. First there are two primes of codimension 12. A representative is the ideal

$$\left\langle \begin{array}{l} [1\perp\perp 2|\emptyset], [1\perp\perp 3|\emptyset], [1\perp\perp 4|\emptyset], [2\perp\perp 3|\emptyset], [2\perp\perp 4|\emptyset], [3\perp\perp 4|\emptyset], \\ [3\perp\perp 4|12], [2\perp\perp 4|13], [2\perp\perp 3|14], [1\perp\perp 4|23], [1\perp\perp 3|24], [1\perp\perp 2|34] \end{array} \right\rangle.$$

The semi-graphoid ideal $I_{\mathbf{SG}}$ has 12 associated primes of codimension 15, such as

$$\left\langle \begin{array}{l} [1\perp\perp 2|\emptyset], [1\perp\perp 3|\emptyset], [1\perp\perp 4|\emptyset], [3\perp\perp 4|\emptyset], [1\perp\perp 3|2], [1\perp\perp 4|2], [3\perp\perp 4|2], [1\perp\perp 2|3], \\ [2\perp\perp 4|3], [1\perp\perp 2|4], [2\perp\perp 3|4], [3\perp\perp 4|12], [2\perp\perp 4|13], [2\perp\perp 3|14], [1\perp\perp 2|34] \end{array} \right\rangle.$$

Next, $I_{\mathbf{SG}}$ has three associated primes of codimension 16. A representative is

$$\left\langle \begin{array}{l} [1\perp\perp 2|\emptyset], [1\perp\perp 3|\emptyset], [2\perp\perp 4|\emptyset], [3\perp\perp 4|\emptyset], [2\perp\perp 4|1], [3\perp\perp 4|1], [1\perp\perp 3|2], [3\perp\perp 4|2], \\ [1\perp\perp 2|3], [2\perp\perp 4|3], [1\perp\perp 2|4], [1\perp\perp 3|4], [3\perp\perp 4|12], [2\perp\perp 4|13], [1\perp\perp 3|24], [1\perp\perp 2|34] \end{array} \right\rangle.$$

Each of the 4316 non-submodular semi-graphoids is a $\{0, 1\}$ -valued point not in $V(I_{\mathcal{A}})$ but in one of the 17 coordinate subspaces corresponding to these primes.

The last associated prime of $I_{\mathbf{SG}}$ is the toric ideal $I_{\mathcal{A}}$. This ideal has codimension 13 and degree 396. Its minimal generating set consists of 52 binomials. Besides the 24 quadratics (axiom instances), the Markov basis of \mathcal{A} contains four cubics

$$\begin{aligned} & [2\perp\perp 3|1] \cdot [3\perp\perp 4|2] \cdot [1\perp\perp 3|4] - [3\perp\perp 4|1] \cdot [1\perp\perp 3|2] \cdot [2\perp\perp 3|4], \\ & [2\perp\perp 3|1] \cdot [2\perp\perp 4|3] \cdot [1\perp\perp 2|4] - [2\perp\perp 4|1] \cdot [1\perp\perp 2|3] \cdot [2\perp\perp 3|4], \\ & [1\perp\perp 3|2] \cdot [1\perp\perp 4|3] \cdot [1\perp\perp 2|4] - [1\perp\perp 4|2] \cdot [1\perp\perp 2|3] \cdot [1\perp\perp 3|4], \\ & [2\perp\perp 4|1] \cdot [3\perp\perp 4|2] \cdot [1\perp\perp 4|3] - [3\perp\perp 4|1] \cdot [1\perp\perp 4|2] \cdot [2\perp\perp 4|3], \end{aligned}$$

and 24 quartics such as

$$[1\perp\perp 2|\emptyset] \cdot [3\perp\perp 4|\emptyset] \cdot [2\perp\perp 4|13] \cdot [1\perp\perp 3|24] - [1\perp\perp 3|\emptyset] \cdot [2\perp\perp 4|\emptyset] \cdot [3\perp\perp 4|12] \cdot [1\perp\perp 2|34].$$

These cubics and quartics correspond to the non-semi-graphoid properties (A.6) and (A.7) in [20].

We now come to the case $n = 5$. It will be a challenge for future commutative algebra software to compute a primary decomposition of the semi-graphoid ideal $I_{\mathbf{SG}}$ for $n = 5$. At present we do not know even whether $I_{\mathbf{SG}}$ is radical. Let us therefore focus on the main component of this ideal, namely, the toric ideal $I_{\mathcal{A}}$.

We succeeded in computing its minimal generators, that is, the Markov basis of \mathcal{A} . This was accomplished using the software `4ti2` [1], and we now state the result:

Theorem 5.3. *The toric ideal $I_{\mathcal{A}}$ representing semi-graphoids on $n = 5$ has codimension 54. The reduced Gröbner basis of $I_{\mathcal{A}}$ in the reverse lexicographic term order consists of 958,202 binomials of degree up to 30. The minimal Markov basis we found consists of 75,889 binomials of degrees ranging from 2 to 12. They come in 613 symmetry classes which are explained in Table 1 below. The minimal Markov basis of $I_{\mathcal{A}}$ is not unique. Moreover, the semigroup of \mathcal{A} is not normal.*

degree	Markov basis elements	symmetry classes
2	120	2
3	40	1
4	270	6
5	984	9
6	12,630	126
7	26,280	195
8	26,925	193
9	3,600	33
10	3,420	35
11	240	2
12	1,380	11

Table 1: Degrees of Markov basis elements of $I_{\mathcal{A}}$ for $n = 5$; representatives of the 613 symmetry classes are available from <http://www.4ti2.de/articles/data/>

Proof. The Markov basis and the Gröbner basis of $I_{\mathcal{A}}$ were computed with `4ti2` and the above numbers of elements correspond to the output sizes when invoking the functions `markov` and `groebner` in `4ti2`. The Markov basis of $I_{\mathcal{A}}$ is not unique, since the Markov move

$$\begin{aligned}
& [2\perp\perp 3|1] + [1\perp\perp 3|5] + [3\perp\perp 4|12] + [3\perp\perp 5|24] \\
& - [3\perp\perp 5|1] - [2\perp\perp 3|5] - [1\perp\perp 3|24] - [3\perp\perp 4|25]
\end{aligned} \tag{10}$$

is not indispensable. Recall (e.g. from [2]) that a binomial $\mathbf{x}^{\mathbf{g}^+} - \mathbf{x}^{\mathbf{g}^-}$ in the toric ideal $I_{\mathcal{A}}$ is called *indispensable* if

$$\{\mathbf{z} \in \mathbb{N}^{80} : \mathcal{A} \cdot \mathbf{z} = \mathcal{A} \cdot \mathbf{g}^+\} = \{\mathbf{g}^+, \mathbf{g}^-\}.$$

This means that the Markov move $\mathbf{g} = \mathbf{g}^+ - \mathbf{g}^-$ corresponds to a 2-element fiber given by the right-hand side $\mathcal{A} \cdot \mathbf{g}^+$ and consequently, \mathbf{g} must belong to *every* Markov

basis of $I_{\mathcal{A}}$. To see that the Markov move from (10) is not indispensable, we enumerate the full fiber of $[2 \perp\!\!\!\perp 3|1] + [1 \perp\!\!\!\perp 3|5] + [3 \perp\!\!\!\perp 4|12] + [3 \perp\!\!\!\perp 5|24]$ using the moves from the computed Markov basis. In addition to the two known elements, we obtain exactly two more elements, namely $[3 \perp\!\!\!\perp 4|1] + [1 \perp\!\!\!\perp 3|5] + [2 \perp\!\!\!\perp 3|14] + [3 \perp\!\!\!\perp 5|24]$ and $[3 \perp\!\!\!\perp 5|1] + [3 \perp\!\!\!\perp 4|5] + [1 \perp\!\!\!\perp 3|24] + [2 \perp\!\!\!\perp 3|45]$. In fact, we obtain a different minimal Markov basis of $I_{\mathcal{A}}$ by replacing the Markov move from (10) with the move

$$[3 \perp\!\!\!\perp 4|1] + [1 \perp\!\!\!\perp 3|5] + [2 \perp\!\!\!\perp 3|14] + [3 \perp\!\!\!\perp 5|24] - [3 \perp\!\!\!\perp 5|1] - [3 \perp\!\!\!\perp 4|5] - [1 \perp\!\!\!\perp 3|24] - [2 \perp\!\!\!\perp 3|45].$$

To show that the semigroup of \mathcal{A} is not normal, consider the Markov basis move

$$\mathbf{g} := (\alpha + 2 \cdot [2 \perp\!\!\!\perp 3|45]) - (\beta + 2 \cdot [4 \perp\!\!\!\perp 5|23]) \in \mathbb{Z}^{80}, \quad \text{where}$$

$$\alpha = [4 \perp\!\!\!\perp 5|2] + [4 \perp\!\!\!\perp 5|3] + [1 \perp\!\!\!\perp 3|4] + [1 \perp\!\!\!\perp 2|5] + [2 \perp\!\!\!\perp 5|14] + [3 \perp\!\!\!\perp 4|15] + [1 \perp\!\!\!\perp 4|23] + [1 \perp\!\!\!\perp 5|23],$$

$$\beta = [1 \perp\!\!\!\perp 5|2] + [1 \perp\!\!\!\perp 4|3] + [2 \perp\!\!\!\perp 3|4] + [2 \perp\!\!\!\perp 3|5] + [3 \perp\!\!\!\perp 4|12] + [2 \perp\!\!\!\perp 5|13] + [1 \perp\!\!\!\perp 2|45] + [1 \perp\!\!\!\perp 3|45].$$

This lattice vector corresponds to a binomial $\mathbf{x}^{\mathbf{g}^+} - \mathbf{x}^{\mathbf{g}^-}$ which is in the toric ideal $I_{\mathcal{A}}$ and has the property that both of its monomials are not square-free. We verified that $\mathbf{x}^{\mathbf{g}^+} - \mathbf{x}^{\mathbf{g}^-}$ is indispensable for $I_{\mathcal{A}}$ by computing the minimal Hilbert basis (that is, the \leq -minimal integer solutions) of the cone

$$\{(\mathbf{z}, u) \in \mathbb{R}^{81} : \mathcal{A} \cdot \mathbf{z} - (\mathcal{A} \cdot \mathbf{g}^+) \cdot u = 0, (\mathbf{z}, u) \geq 0\}.$$

This was done using the function `hilbert` of `4ti2` which produced precisely the two expected elements $(\mathbf{g}^+, 1)$ and $(\mathbf{g}^-, 1)$ within a few seconds. Again, one could also use \mathbf{g}^+ and the computed Markov basis to enumerate all elements in this fiber.

From our indispensable Markov move $\mathbf{g} = (\alpha + 2 \cdot [2 \perp\!\!\!\perp 3|45]) - (\beta + 2 \cdot [4 \perp\!\!\!\perp 5|23])$, we now construct the imset \mathbf{b} presented in Section 4. We first check that \mathbf{b} was not a combinatorial imset by showing that $\mathcal{A}\mathbf{x} = \mathbf{b}$ has no solutions with non-negative integer coordinates. Using the functions `hilbert` and `rays` of the program `4ti2`, we computed the Hilbert basis and the extreme rays of the cone

$$\{(\mathbf{z}, u) \in \mathbb{R}^{81} : \mathcal{A} \cdot \mathbf{z} = \mathbf{b} \cdot u \text{ and } (\mathbf{z}, u) \geq 0\}.$$

Both computations quickly finished. They show that this cone has dimension one and is generated by the single vector $(\alpha + \beta, 2)$. Consequently, the only non-negative real solution to $\mathcal{A} \cdot \mathbf{x} = \mathbf{b}$ is $(\alpha + \beta)/2$, which is not an integer solution.

For the benefit of the reader, we complete this proof by presenting a degree 12 Markov basis element, which can easily be proved to be indispensable, too:

$$\begin{aligned} & [1 \perp\!\!\!\perp 5|2] + [2 \perp\!\!\!\perp 5|3] + 2 \cdot [2 \perp\!\!\!\perp 3|4] + [1 \perp\!\!\!\perp 2|5] + [3 \perp\!\!\!\perp 4|5] + [3 \perp\!\!\!\perp 4|12] + [3 \perp\!\!\!\perp 4|15] + \\ & 2 \cdot [2 \perp\!\!\!\perp 5|134] + [3 \perp\!\!\!\perp 4|5] + [3 \perp\!\!\!\perp 4|12] - [3 \perp\!\!\!\perp 4|2] - [1 \perp\!\!\!\perp 4|3] - [1 \perp\!\!\!\perp 3|4] - [2 \perp\!\!\!\perp 5|4] - \\ & 2 \cdot [2 \perp\!\!\!\perp 3|5] - [2 \perp\!\!\!\perp 5|13] - [2 \perp\!\!\!\perp 5|14] - 2 \cdot [3 \perp\!\!\!\perp 4|125] - [1 \perp\!\!\!\perp 5|234] - [1 \perp\!\!\!\perp 2|345]. \end{aligned}$$

□

Finally, let us remark that the computations of the 75, 889 Markov basis elements and of the 959, 202 Gröbner basis elements were both started independently from the given matrix using the `markov` and the `groebner` commands of `4ti2` version 1.3.1. They took about 20 and 17.75 days, respectively, on an AMD Opteron 2.4 GHz CPU running SuSE Linux 10.0. The input and output files are available from <http://www.4ti2.de/articles/data/>.

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