Toric Varieties in Statistics

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Outline

1. Algebraic Statistics: Log-Linear Models
   - Warm-up Example
   - General Theory
2. Hierarchical Models - Current Research
   - What is a Hierarchical Model?
   - Unimodularity
   - Normality

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2 Hierarchical Models - Current Research
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Example

	Death Penalty		
Defendant's Race	Yes	No	Total
White	19	141	160
Black	17	149	166
Total	36	290	326

Table: Homicide indictments in Florida in the 1970s [4]

- Did race play a role in determining whether someone received the death penalty?
- Let p_{wy} be the probability that a defendant is white, and is given the death penalty
- Define p_{wn}, p_{by}, p_{bn} analogously
- Race and sentencing are independent iff $p_{wy}p_{bn} - p_{wn}p_{by} = 0$

Are they independent?

- Let S be the set of tables with the same row and column sums as data
- If $p_{wy}p_{bn} - p_{wn}p_{by} = 0$ then

$$Pr(U = u | U \in S) = \frac{1}{u_{wy}!u_{wn}!u_{by}!u_{bn}! \sum_{v \in S} \frac{1}{v_{wy}!v_{wn}!v_{by}!v_{bn}!}}$$

- The χ^2 test statistic for our data u should be "small"

$$\chi^2(U) = \frac{(U_{wy} - \hat{u}_{wy})^2}{\hat{u}_{wy}} + \frac{(U_{wn} - \hat{u}_{wn})^2}{\hat{u}_{wn}} + \frac{(U_{by} - \hat{u}_{by})^2}{\hat{u}_{by}} + \frac{(U_{bn} - \hat{u}_{bn})^2}{\hat{u}_{bn}}$$

  where the $\hat{u}$s are the expected values
- Compute the p-value $p = Pr(\chi^2(U) \geq \chi^2(u) | U \in S)$
- If p value is small, then independence is unlikely

Enumerating S

- S is set of nonnegative integer matrices with row and column sums

$$r = \begin{pmatrix} 160 \\ 166 \end{pmatrix} \qquad \text{and} \qquad c = \begin{pmatrix} 36 & 290 \end{pmatrix}$$

- Each matrix in S is $u + \lambda m$ for some $\lambda \in \mathbb{Z}$ where

$$m = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

$$u = \begin{pmatrix} 19 & 141 \\ 17 & 149 \end{pmatrix} \qquad u + 6m = \begin{pmatrix} 25 & 135 \\ 11 & 155 \end{pmatrix}$$

- Enumeration in most other models is infeasible, so use random sample

Log-Linear Models

Definition

A *statistical model* is a collection of probability distributions that satisfy some given conditions.

Many statistical models can be defined algebraically.

Definition

Let $\mathcal{A} \in \mathbb{Z}^{d \times n}$ be an integer matrix. We define the *toric ideal* associated to $\mathcal{A}$ to be

$$I_{\mathcal{A}} = \langle \mathbf{x}^{\mathbf{u}} - \mathbf{x}^{\mathbf{v}} | \mathbf{u}, \mathbf{v} \in \mathbb{N}^n \text{ with } \mathcal{A}\mathbf{u} = \mathcal{A}\mathbf{v} \rangle \subseteq \mathbb{K}[x_1, \dots, x_n].$$

We define the *log-linear model associated to $\mathcal{A}$* to be

$$\mathcal{M}_{\mathcal{A}} = \text{int}(\Delta_{n-1}) \cap V(I_{\mathcal{A}})$$

where $\Delta_{n-1} = \{p \in \mathbb{R}^n | p_i \geq 0 \text{ and } \sum_{i=1}^n p_i = 1\}$.

Example

The independence model can be realized as a log-linear model.

$$\mathcal{A} = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{pmatrix} \qquad \ker \mathcal{A} = \mathrm{Span}_{\mathbb{R}} \begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \end{pmatrix}$$

$$I_{\mathcal{A}} = \langle x_1 x_4 - x_2 x_3 \rangle \qquad \mathcal{M}_{\mathcal{A}} = V(I_{\mathcal{A}}) \cap \mathrm{int}(\Delta_3)$$

Hypothesis Testing for Log Linear Models

- $u \in \mathbb{N}^n$ is data, randomly generated according to some (unknown) distribution $p = (p_1, \ldots, p_n)$
- Null hypothesis: $p \in \mathcal{M}_\mathcal{A}$
- In this case, distribution on $\{v \in \mathbb{N}^n | \mathcal{A}v = \mathcal{A}u\}$ is

$$\Pr(U = u | AU = Au) = \frac{1/\left(\prod_{i=1}^n u_i!\right)}{\sum_{v \in \mathbb{N}^n : Av = Au} 1/\left(\prod_{i=1}^n v_i!\right)}$$

- Test statistic

$$\chi^2(U) := \sum_{i=1}^n \frac{(U_i - \hat{u}_i)^2}{\hat{u}_i}$$

  where $\hat{u}_i$ are the expected values
- If $p = Pr(\chi^2(U) \geq \chi^2(u) | \mathcal{A}U = \mathcal{A}u)$ is small, then our null hypothesis is probably wrong

Monte Carlo Method for Computing $\chi^2(u)$

- Define $\mathcal{F}_{\mathcal{A},b} := \{v \in \mathbb{N}^n | \mathcal{A}v = b\}$. Usually finite for all b
- Create graph on $\mathcal{F}_{\mathcal{A},b}$
  - Select $\{m_1, \ldots, m_k\} \subset \ker_{\mathbb{Z}} \mathcal{A}$
  - Edge between $u, v \in \mathcal{F}_{\mathcal{A},b}$ iff $u = v \pm m_i$, some i

Theorem (Diaconis-Sturmfels 1998)

If the graph on $\mathcal{F}_{\mathcal{A},b}$ is connected, then a certain random walk on $\mathcal{F}$ produces a sequence $v_1, v_2, \ldots$ such that with probability 1,

$$\lim_{M\to\infty} \frac{1}{M} \sum_{t=1}^{M} 1_{\{\chi^2(v_i)\geq\chi^2(u)\}} = Pr(\chi^2(U) \geq \chi^2(u) | AU = Au)$$

Theorem (Diaconis-Sturmfels 1998)

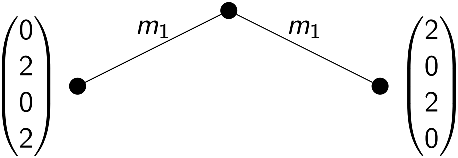
Let $\{m_1, \ldots, m_k\} \subset \ker_{\mathbb{Z}} \mathcal{A}$. The graph on $\mathcal{F}_{\mathcal{A},b}$ is connected for all $b \in \mathbb{N}^d$ iff

$$I_{\mathcal{A}} = \langle \mathbf{x}^{m_i^+} - \mathbf{x}^{m_i^-} | i = 1, \ldots, k\rangle.$$

Example

$$\mathcal{A} = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{pmatrix} \quad m_1 = \begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \end{pmatrix} \quad m_1^+ = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} \quad m_1^- = \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}$$

$$b = \begin{pmatrix} 2 \\ 2 \\ 2 \\ 2 \end{pmatrix} \qquad \mathcal{F}_{\mathcal{A},b} = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \qquad I_{\mathcal{A}} = \langle x_1x_4 - x_2x_3 \rangle$$



Markov Bases

Definition

We call $M := \{m_1, \ldots, m_k\} \subset \ker_{\mathbb{Z}} \mathcal{A}$ a *Markov basis* if

$$I_{\mathcal{A}} = \langle \mathbf{x}^{m_i^+} - \mathbf{x}^{m_i^-} | i = 1, \ldots, k \rangle.$$

Question

Given $\mathcal{A}$, can we efficiently compute a Markov basis?

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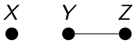
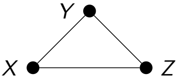
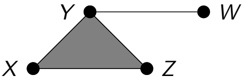
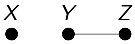
Hierarchical Models

Definition (Hierarchical Model)

Let $X_1, \ldots, X_n$ be discrete random variables. A simplicial complex $\mathcal{C}$ on $X_1, \ldots, X_n$ specifies independence relations among the X_is. The collection of probability distributions on $X_1, \ldots, X_n$ satisfying these relations is called a *hierarchical model*.

X is independent of Y and Z, but Y and Z are dependent	
There is no 3-way dependence	
X and Z are independent of W given Y	

Hierarchical Models as Log-Linear Models - Example

- Assume X, Y, and Z have 3, 2, and 2 states.
- Independence relationship: 

- The matrix that maps $3 \times 2 \times 2$ tables to the "down" and "left and back" margins realizes this as a log-linear model

$$\begin{matrix} \text{front} & & \text{back} \\ \begin{pmatrix} 1 & 1 \\ 2 & 0 \\ 3 & 1 \end{pmatrix} & & \begin{pmatrix} 2 & 1 \\ 1 & 3 \\ 0 & 2 \end{pmatrix} \end{matrix}$$

$$\text{sum going down: } \begin{pmatrix} 3 & 6 \\ 6 & 2 \end{pmatrix} \qquad \text{sum going left and back: } \begin{pmatrix} 5 \\ 6 \\ 6 \end{pmatrix}$$

Hierarchical Models as Log Linear Models

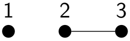
- Discrete random variables $X_1, \ldots, X_n$
- X_i has d_i states. Notation: $\mathbf{d} = (d_1, \ldots, d_n)$
- $\mathcal{C}$ denotes a simplicial complex on $[n]$
- The corresponding hierarchical model is a log-linear model with the following matrix

Definition

Let $\mathcal{A}_{\mathcal{C},\mathbf{d}}$ be the matrix defined as follows:

- Columns are indexed by elements of $\bigoplus_{i=1}^{n}[d_i]$
- Rows are indexed by $\bigoplus_{F \in \text{facet}(\mathcal{C})} \bigoplus_{j \in F}[d_j]$
- Entry in row $(F, (j_1, \ldots, j_k))$ and column $(i_1, \ldots, i_n)$ is 1 if $i|_F = (j_1, \ldots, j_k)$
- All other entries are 0

Example

- Let $n = 3$ with $d_1 = 3, d_2 = 2, d_3 = 2$
- Let $\mathcal{C}$ be the complex 

- Then $\mathcal{A}_{\mathcal{C},\mathbf{d}}$ is the following matrix:

	111	112	121	122	211	212	221	222	311	312	321	322
$\{1\},1$	1	1	1	1	0	0	0	0	0	0	0	0
$\{1\},2$	0	0	0	0	1	1	1	1	0	0	0	0
$\{1\},3$	0	0	0	0	0	0	0	0	1	1	1	1
$\{2,3\},11$	1	0	0	0	1	0	0	0	1	0	0	0
$\{2,3\},12$	0	1	0	0	0	1	0	0	0	1	0	0
$\{2,3\},21$	0	0	1	0	0	0	1	0	0	0	1	0
$\{2,3\},22$	0	0	0	1	0	0	0	1	0	0	0	1

Unimodularity

Definition (Unimodularity)

Assume $A \in \mathbb{Z}^{d \times n}$ has full row rank. We say that A is **unimodular** if all $d \times d$ submatrices have determinant $0, 1$, or -1.

Example

The matrix $\mathcal{A}$ is unimodular, whereas $\mathcal{B}$ is not

$$\mathcal{A} = \begin{pmatrix} -1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \mathcal{B} = \begin{pmatrix} 1 & 1 & -1 \\ 0 & 1 & 1 \end{pmatrix}$$

Applications include:

- Integer programming over fibers $\mathcal{F}_{A,b}$
- Disclosure limitation
- Computing Markov basis and universal Gröbner basis of $\mathcal{I}_{\mathcal{A}}$

Unimodularity

Question

When is $\mathcal{A}_{\mathcal{C},\mathbf{d}}$ unimodular?

Observation

If $\mathcal{A}_{\mathcal{C},\mathbf{d}}$ is unimodular, then so is $\mathcal{A}_{\mathcal{C}} := \mathcal{A}_{\mathcal{C},(2,\dots,2)}$.

- Terminology abuse "$\mathcal{C}$ is unimodular" means "$\mathcal{A}_{\mathcal{C}}$ is unimodular"

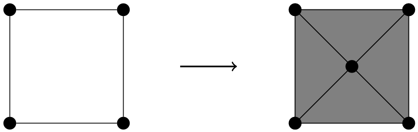
We have a complete classification of unimodular $\mathcal{C}$

Unimodularity-Preserving Operations

Definition (Adding a cone vertex)

If $\mathcal{C}$ is a simplicial complex on $[n]$, define cone($\mathcal{C}$) to be the complex on $[n+1]$ with facets

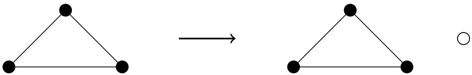
$$\text{facet}(\text{cone}(\mathcal{C})) = \{F \cup \{n+1\} : F \in \text{facet}(\mathcal{C})\}.$$



Unimodularity-Preserving Operations

Definition (Adding a ghost vertex)

If $\mathcal{C}$ is a simplicial complex on $[n]$, define $G(\mathcal{C})$ to be the simplicial complex on $[n+1]$ that has exactly the same faces as $\mathcal{C}$.

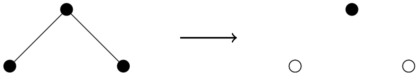


Unimodularity-Preserving Operations

Definition (Alexander Duality)

If $\mathcal{C}$ is a simplicial complex on $[n]$, then the *Alexander dual* complex $\mathcal{C}^*$ is the simplicial complex on $[n]$ with facets

$$\text{facet}(\mathcal{C}^*) = \{[n] \setminus S : S \text{ is a minimal non-face of } \mathcal{C}\}.$$



Unimodularity: Constructive Classification

Definition

We say that a simplicial complex $\mathcal{C}$ is *nuclear* if it satisfies one of the following:

1. $\mathcal{C} = \Delta_k$ for some $k \geq -2$ (i.e. a simplex)
2. $\mathcal{C} = \Delta_m \sqcup \Delta_n$ (i.e. a disjoint union of simplices)
3. $\mathcal{C} = \text{cone}(\mathcal{D})$ where $\mathcal{D}$ is nuclear
4. $\mathcal{C} = G(\mathcal{D})$ where $\mathcal{D}$ is nuclear
5. $\mathcal{C}$ is the Alexander dual of a nuclear complex.

Theorem (B.-Sullivant 2015)

The matrix $\mathcal{A}_{\mathcal{C}}$ is unimodular if and only if $\mathcal{C}$ is nuclear.

Simplicial Complex Minors

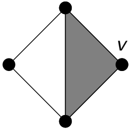
Definition (Deletion and Link)

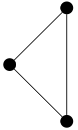
Let $\mathcal{C}$ be a simplicial complex on $[n]$. Let $v \in [n]$ be a vertex of $\mathcal{C}$. Then $\mathcal{C} \setminus v$ denotes the induced simplicial complex on $[n] \setminus \{v\}$, and $\text{link}_v(\mathcal{C})$ denotes the simplicial complex on $[n] \setminus \{v\}$ with facets

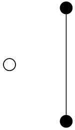
$$\text{facet}(\text{link}_v(\mathcal{C})) = \{F \setminus \{v\} : F \text{ is a facet of } \mathcal{C} \text{ with } v \in F\}.$$

Definition (Simplicial Complex Minor)

We say that $\mathcal{D}$ is a minor of $\mathcal{C}$ if $\mathcal{D}$ can be obtained from $\mathcal{C}$ via a series of deletion and link operations.

$\mathcal{C} =$ 

$\mathcal{C} \setminus v =$ 

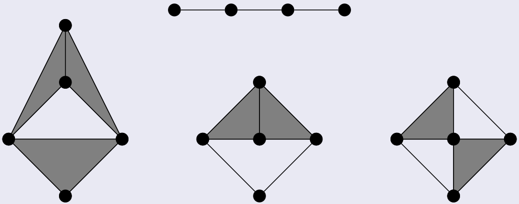
$\text{link}_v\mathcal{C} =$ 

Unimodularity: Excluded Minor Classification

Theorem (B.-Sullivant 2015)

The matrix $\mathcal{A}_{\mathcal{C}}$ is unimodular if and only if $\mathcal{C}$ has no simplicial complex minors isomorphic to any of the following

- $\partial\Delta_k \sqcup \{v\}$, *the disjoint union of the boundary of a simplex and an isolated vertex*
- O_6, *the boundary complex of an octahedron, or its Alexander dual* O_6^*
- *The four simplicial complexes shown below*



Sketch of Proof

- $\mathcal{C}$ nuclear $\implies$ $\mathcal{C}$ unimodular
  - Simplices are unimodular
  - A disjoint union of two simplices is unimodular
  - Adding cone and ghost vertices and taking duals preserves unimodularity
- $\mathcal{C}$ unimodular $\implies$ $\mathcal{C}$ avoids forbidden minors
  - The forbidden minors are not unimodular
  - Taking minors preserves unimodularity
- $\mathcal{C}$ avoids forbidden minors $\implies$ $\mathcal{C}$ nuclear
  - If $\mathcal{C}$ avoids the forbidden minors but has a 4-cycle, then it must be an iterated cone over the 4-cycle. This is nuclear.
  - So focus on 4-cycle-free complexes. Then the 1-skeleton is either a complete graph, or two complete graphs glued along a clique.
  - Complex induction argument based on the link of a vertex of $\mathcal{C}$.

Next Steps - Unimodularity

Question

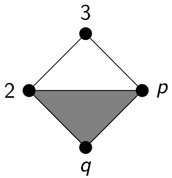
Given a simplicial complex $\mathcal{C}$ on $[n]$ and an integer vector $\mathbf{d} = (d_1, \ldots, d_n)$ with $d_i \geq 2$, is $\mathcal{A}_{\mathcal{C},\mathbf{d}}$ unimodular?

Corollary (B.-Sullivant 2015)

If $\mathcal{A}_{\mathcal{C},\mathbf{d}}$ is unimodular, then $\mathcal{C}$ is nuclear.

Question

Let $\mathcal{C}$ and $\mathbf{d}$ be specified by the figure below. For which values of p and q is $\mathcal{A}_{\mathcal{C},\mathbf{d}}$ unimodular?



Normality

Let $A \in \mathbb{N}^{d \times n}$. We define:

- $\mathbb{N}A := \{Ax : x \in \mathbb{N}^n\}$ (Semigroup generated by columns of A)
- $\mathbb{Z}A := \{Ax : x \in \mathbb{Z}^n\}$ (Lattice generated by columns of A)
- $\mathbb{R}_{\geq 0}A := \{Ax : x \in \mathbb{R}, x \geq 0\}$ (Cone generated by columns of A)

Definition (Normality)

We say that A is *normal* if

$$\mathbb{N}A = \mathbb{R}_{\geq 0}A \cap \mathbb{Z}A.$$

If A is not normal and

$$h \in \mathbb{R}_{\geq 0}A \cap \mathbb{Z}A \setminus \mathbb{N}A$$

the we say that h is a *hole* of $\mathbb{N}A$.

Normality: Non-example

The following matrix is *not* normal

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

because $\begin{pmatrix} 1 \\ 2 \end{pmatrix}$ is a hole. Note:

$$\begin{pmatrix} 1 \\ 2 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 & 3 \end{pmatrix} \begin{pmatrix} -1 \\ 2 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} 1 \\ 2 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 & 3 \end{pmatrix} \begin{pmatrix} 0 \\ 1/2 \\ 1/2 \end{pmatrix}$$

so $\begin{pmatrix} 1 \\ 2 \end{pmatrix} \in \mathbb{R}_{\geq 0}A \cap \mathbb{Z}A$. However, $\begin{pmatrix} 1 \\ 2 \end{pmatrix} \notin \mathbb{N}A$.

Normality

Question

When is $\mathcal{A}_{\mathcal{C},\mathbf{d}}$ normal?

Observation

If $\mathcal{A}_{\mathcal{C},\mathbf{d}}$ is normal, then so is $\mathcal{A}_{\mathcal{C}} := \mathcal{A}_{\mathcal{C},(2,\ldots,2)}$.

- Terminology abuse "$\mathcal{C}$ is normal" means "$\mathcal{A}_{\mathcal{C}}$ is normal"

Applications include:

- Integer table feasibility problem
- Toric fiber products for constructing Markov bases work best with normal $\mathcal{A}_{\mathcal{C},\mathbf{d}}$ (Rauh-Sullivant 2014)
- Sequential importance sampling works best with normal $\mathcal{A}_{\mathcal{C},\mathbf{d}}$

We have some partial results towards classification of normal $\mathcal{C}$

Known Classification Results - Normality

Theorem (Sullivant 2010)

If $\mathcal{C}$ is a graph, then $\mathcal{A}_\mathcal{C}$ is normal if and only if $\mathcal{C}$ is free of K_4-minors.

Theorem (Bruns, Hemmecke, Hibi, Ichim, Ohsugi, Köppe, Söger 2007-2011)

Let $\mathcal{C}$ be a complex whose facets are all $m-1$ element subsets of $[m]$. Then $\mathcal{A}_{\mathcal{C},\mathbf{d}}$ is normal in precisely the following situations up to symmetry:

1. *At most two of the d_v are greater than two*
2. $m = 3$ *and* $\mathbf{d} = (3, 3, a)$ *for any* $a \in \mathbb{N}$
3. $m = 3$ *and* $\mathbf{d} = (3, 4, 4), (3, 4, 5)$ *or* $(3, 5, 5)$.

Theorem (Rauh-Sullivant 2014)

Let $\mathcal{C}$ be the four-cycle graph. Then $\mathcal{A}_{\mathcal{C},\mathbf{d}}$ is normal if $\mathbf{d} = (2, a, 2, b)$ *or* $\mathbf{d} = (2, a, 3, b)$ *with* $a, b, \in \mathbb{N}$.

Corollary of Unimodular Classification

Definition

Let $\mathcal{C}$ be a simplicial complex on $[n]$. We say a facet of $\mathcal{C}$ that has $n-1$ vertices is called a *big facet*.

Proposition

If $\mathcal{C}$ is a complex with a big facet, then $\mathcal{C}$ is normal if and only if unimodular.

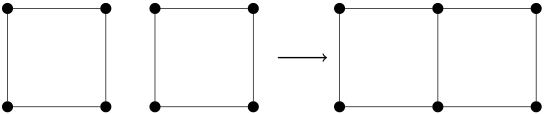
So our classification result on unimodular $\mathcal{C}$ immediately gives a classification of the normal $\mathcal{C}$ when $\mathcal{C}$ has a big facet.

Normality Preserving Operations

Theorem (Sullivant 2010)

Normality of $\mathcal{A}_{\mathcal{C},\mathbf{d}}$ is preserved under the following operations on the simplicial complex

1. *Deleting vertices*
2. *Contracting edges*
3. *Gluing two simplicial complexes along a common face*
4. *Adding or removing a cone or ghost vertex.*



Theorem (B.-Sullivant 2015)

Normality of $\mathcal{A}_{\mathcal{C},\mathbf{d}}$ is preserved when taking links of vertices of $\mathcal{C}$.

Minimally Non-Normal Simplicial Complexes

Question

Which simplicial complexes are minimally non-normal with respect to the operations of deleting vertices, contracting edges, gluing two complexes along a facet, removing cone and ghost vertices, and taking links of vertices?

Computational method:

- All simplicial complexes on 3 or fewer vertices are normal
- Choose two normal simplicial complexes $\mathcal{C}, \mathcal{D}$ on $n-1$ vertices. Create simplicial complex $\mathcal{C}'$ on n vertices by attaching a new vertex v to $\mathcal{C}$ such that $\text{link}_v(\mathcal{C}') = \mathcal{D}$
- See if (non)normality of $\mathcal{C}'$ can be certified by reducing to a smaller complex via our normality-preserving operations
- If not, check normality of $\mathcal{C}'$ using Normaliz. If non-normal, then minimally non-normal

Minimally Non-Normal Simplicial Complexes

We were able to use the computational method to determine normality on all complexes on up to 6 vertices

So far, we know that the set of minimally non-normal simplicial complexes consists of:

- 20 sporadic complexes, obtained by computational method
- Two infinite families, obtained by theoretical means

Next Steps

- Develop new procedures for constructing normal $\mathcal{C}$
- Develop methods for constructing holes of $\mathbb{N}\mathcal{A}_{\mathcal{C}}$
- Classify normal complexes within certain families (e.g., surfaces)

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