Total binomial decomposition (TBD)

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Setup

- Let k be a field. For computations we use $k = \mathbb{Q}$.
- $k[p] := k[p_1, \ldots, p_n]$ the polynomial ring in n indeterminates
- For each $u \in \mathbb{N}^n$ there is a monomial $p^u = \prod_{i=j}^n p_j^{u_j}$.
- For $u, v \in \mathbb{N}^n, \lambda \in k$ there is a binomial $p^u - \lambda p^v$.

Definition

A binomial ideal $I \subseteq k[p_1, \ldots, p_n]$ is an ideal that can be generated by binomials.

Binomial ideals

- Monomial ideals have boring varieties
- Binomial ideals: tractable and flexible
- For many purposes a trinomial ideal is a general ideal.

Binomial prime ideals can be characterized. Up to scaling p_j they are:

Definition

Let $A \in \mathbb{Z}^{d \times n}$. The toric ideal for A is the prime ideal

$$I_A := \langle p^u - p^v : u, v \in \mathbb{N}^n, u - v \in \ker A \rangle$$

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Primary ideals can be characterized too, but depends on char(k).

Monomial maps

Let $k[t^{\pm}] = k[t_1^{\pm}, \ldots, t_d^{\pm}]$. Consider the k-algebra homomorphism

$$\phi_A : k[p] \to k[t^{\pm}], \qquad p_j \mapsto t^{A_j} = t_1^{A_{1j}} \cdots t_d^{A_{dj}}$$

where A_j is the j-th column of A.

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- Claim $I_A = \ker \phi_A$.
  - $\subseteq$: $p^u \mapsto$??
  - $\supseteq$: Exercise 1

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- Claim $I_A = \ker \phi_A$.
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  - $\supseteq$: Exercise 1
- This proves that I_A is prime
- The toric variety $V(I_A)$ has a monomial parametrization.

Toric ideals in application: Log-linear models

- One discrete random variable with values in $[n]$.
- A distribution is an element of the probability simplex

$$\Delta_{n-1} = \{p \in \mathbb{R}^n : p_j \geq 0, \sum_j p_j = 1\}.$$

- A model is a subset $M \subseteq \Delta_{n-1}$.

Log-linear models

A log-linear model is specified by linear constraints on logs of p_j

$$\log p = M\theta, \qquad \theta \in \mathbb{R}^d.$$

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Let's write $M = A^T$ and assume $A \in \mathbb{Z}^{d\times n}$. Then

$$\log p_j = \theta A_j$$

where A_j is the j-th column of A.

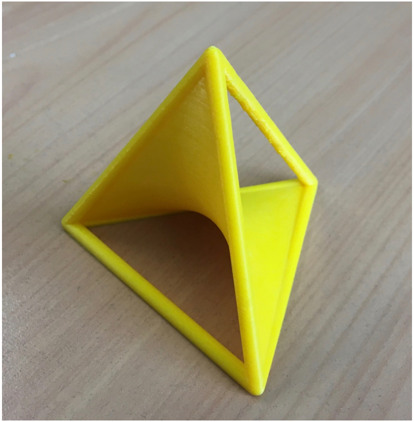
The log-linear constraint encodes a monomial parametrization:

$$\begin{aligned} \log p_j = \theta A_j &\Leftrightarrow \\ p_j = e^{\theta A_j} &\Leftrightarrow \\ p_j = t^{A_j} & \end{aligned}$$

if we put $t_j = e^{\theta_j}$ and let $t_j > 0, j = 1, \ldots, d$ be the parameters.

Observation

Each log-linear model is the intersection of a toric variety with Δ_{n-1}.



The independence model $= \mathbb{P}^1 \times \mathbb{P}^1$

Some consequences

- Testing if a given distribution is in the model is checking binomial equations.
- Nearest point methods, Kullback–Leibler geometry
- Binomial equations can have meaning in terms of (conditional) independence $\rightarrow$ Graphical models.
- The boundary of a log-linear model looks like the boundary of the polytope $\mathrm{conv}\{A_i, i = 1, \ldots, n\}$ $\rightarrow$ Existence of the MLE.

Computational problems

Given A, how to find a finite generating set of I_A?

- Let $B \subseteq \ker_{\mathbb{Z}} A$ be a lattice basis.
- Decompose $b = b^+ - b^-$ with

$$b_i^{\pm} = \max\{\pm b_i, 0\}$$

- Then

$$\left\langle p^{b^+} - p^{b^-} \right\rangle \subseteq I_A.$$

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  Equality does not hold, but

$$\left\langle p^{b^+} - p^{b^-} \right\rangle : \left(\prod_j p_j \right)^{\infty} = I_A$$

Generators of toric ideals

- The most efficient computational way to find them is 4ti2 (FourTiTwo package in Macaulay2).
- The exponents appearing in a finite generating set are sometimes called a Markov basis $\rightarrow$ Database
- Exercise: Given a toric ideal, how to find A?

Some combinatorial commutative algebra

An abstract reason why binomial ideals are good are monoid gradings.

- Define a $\mathbb{Z}^d$-valued grading on $k[p]$ via $\deg p_j = A_j$.

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- Define a $\mathbb{Z}^d$-valued grading on $k[p]$ via $\deg p_j = A_j$.
- I_A is homogeneous
- The Hilbert function of $k[p]/I_A$ takes values only 0 and 1.
  - 1 for all $b \in \mathbb{N}A = \{Au : u \in \mathbb{N}^n\}$ the monoid generated by A
  - 0 for all other $b \in \mathbb{Z}^d \setminus \mathbb{N}A$

Let Q be a commutative Noetherian monoid.

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Monoid Algebras

The monoid algebra over Q is the k-vector space

$$k[Q] := \bigoplus_{q \in Q} k\{x^q\} \qquad \text{with} \qquad x^q x^u := x^{q+u}.$$

A binomial ideal is an ideal generated by binomials

$$x^q - \lambda x^u, \quad q, u \in Q, \lambda \in k.$$

Examples

- $k[\mathbb{N}^n] = k[p_1, \ldots, p_n]$
- $k[\mathbb{N}A] = k[p_1, \ldots, p_n]/I_A$

This generalizes to

Eisenbud–Sturmfels

An ideal $I \subseteq k[p]$ is binomial if and only if $k[p]/I$ is finely graded by a commutative Noetherian monoid.

Combinatorial commutative algebra

This leads to a very nice theory of binomial ideals based on the separation of combinatorics (the monoid) and arithmetics (the coefficients)

Not every ideal is prime or toric!

- Every ideal $I \subseteq k[p_1, \ldots, p_n]$ is a finite intersection of primary ideals
$$I = \bigcap_i Q_i, \qquad \sqrt{Q_i} = P_i \text{ is prime}$$
(Q is primary, if in $k[p]/Q$ every element is regular or nilpotent.)
- If k is algebraically closed, every binomial ideal is an intersection of primary binomial ideals (Eisenbud/Sturmfels).
- Independent of k, decompositions of congruences point the way!
$\rightarrow$ mesoprimary decomposition

Combinatorial versions of binomial ideals

A congruence on Q is an equivalence relation $\sim$ such that

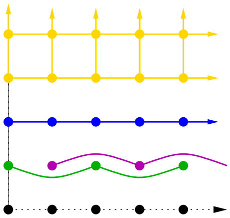
$$a \sim b \Rightarrow a + q \sim b + q \quad \forall q \in Q$$

- Congruences are the kernels of monoid homomorphisms
- Quotients $\overline{Q} := Q/\sim$ are monoids again.

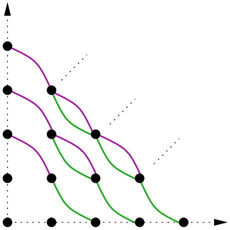
Congruences from binomial ideals

Each binomial ideal $I \subseteq k[Q]$ induces a congruence $\sim_I$ on Q:

$$a \sim_I b \Leftrightarrow \exists \lambda \neq 0 : x^a - \lambda x^b \in I$$



$\langle y^3, y^2(x-1), y(x^2-1)\rangle$



$\langle x^2 - xy, xy - y^2\rangle$

Decompositions of binomial ideals in action

Consider distributions of 3 binary random variables:

$$(p_{000}, p_{001}, \ldots, p_{111}).$$

Assume we want to study the following conditional independencies:

$$\mathcal{C} = \{\, X_1 \perp\!\!\!\perp X_2 \,|X_3 \,,\, X_1 \perp\!\!\!\perp X_3 \,|X_2 \,\}$$

As you will see, this leads to binomial conditions:

$$\begin{vmatrix} p_{000} & p_{010} \\ p_{100} & p_{110} \end{vmatrix} = 0, \quad \begin{vmatrix} p_{001} & p_{011} \\ p_{101} & p_{111} \end{vmatrix} = 0 \qquad X_1 \perp\!\!\!\perp X_2 \,|X_3$$

$$\begin{vmatrix} p_{000} & p_{001} \\ p_{100} & p_{101} \end{vmatrix} = 0, \quad \begin{vmatrix} p_{010} & p_{011} \\ p_{110} & p_{111} \end{vmatrix} = 0 \qquad X_1 \perp\!\!\!\perp X_3 \,|X_2$$

The prime decomposition of the corresponding ideal $I_{\mathcal{C}}$ is

$$I_{\mathcal{C}} = \left\langle \operatorname{rk}\begin{pmatrix} p_{000} & p_{001} & p_{010} & p_{011} \\ p_{100} & p_{101} & p_{110} & p_{111} \end{pmatrix} = 1 \right\rangle$$

$$\cap \langle p_{000}, p_{100}, p_{011}, p_{111} \rangle$$

$$\cap \langle p_{001}, p_{010}, p_{101}, p_{110} \rangle$$

- The model (inside Δ_7) consists of three (toric) components
    - An independence model $(d = 4)$ $X_1 \perp\!\!\!\perp \{X_2, X_3\}$. $\operatorname{conv} A_i \cong \Delta_1 \times \Delta_1$ is a prism over a 3d-simplex.
    - 2 copies of Δ_3 embedded in faces of Δ_7.

Theorem

If for the distribution of 3 binary random variables both $X_1 \perp\!\!\!\perp X_2 \,|X_3$ and $X_1 \perp\!\!\!\perp X_3 \,|X_2$ hold, then either

- $X_1 \perp\!\!\!\perp \{X_2, X_3\}$ ("the intersection axiom holds"), or
- $p_{000} = p_{100} = p_{011} = p_{111} = 0$ ("$X_2 = 1 - X_3$"), or
- $p_{001} = p_{010} = p_{101} = p_{110} = 0$ ("$X_2 = X_3$").