

The binomial ideal of the intersection axiom for conditional probabilities

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Abstract The binomial ideal associated with the intersection axiom of conditional probability is shown to be radical and is expressed as an intersection of toric prime ideals. This solves a problem in algebraic statistics posed by Cartwright and Engström.

Keywords Conditional independence · Intersection axiom

Conditional independence constraints are a family of natural constraints on probability distributions, describing situations in which two random variables are independently distributed given knowledge of a third. Statistical models built around considerations of conditional independence, in particular *graphical models* in which the constraints are encoded in a graph on the random variables, enjoy wide applicability in determining relationships among random variables in statistics and in dealing with uncertainty in artificial intelligence.

One can take a purely combinatorial perspective on the study of conditional independence, as does Studený [10], conceiving of it as a relation on triples of subsets of a set of observables which must satisfy certain axioms. A number of elementary implications among conditional independence statements are recognized as axioms. Among these are the *semi-graphoid axioms*, which are implications of conditional independence statements lacking further hypotheses, and hence are purely combinatorial statements. The *intersection axiom* is also often added to the collection, but unlike the semi-graphoid axioms it is not uniformly true; it is our subject here.

Formally, a conditional independence model \mathcal{M} is a set of probability distributions characterized by satisfying several conditional independence constraints. We

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will work in the discrete setting, where a probability distribution p is a multi-way table of probabilities, and we follow the notational conventions in [1].

Consider the discrete conditional independence model \mathcal{M} given by

$$\{X_1 \perp\!\!\!\perp X_2 \mid X_3, X_1 \perp\!\!\!\perp X_3 \mid X_2\}$$

where X_i is a random variable taking values in the set $[r_i] = \{1, \dots, r_i\}$. Throughout we assume $r_1 \geq 2$. Let p_{ijk} be the unknown probability $P(X_1 = i, X_2 = j, X_3 = k)$ in a distribution from the model \mathcal{M} . The set of distributions in the model \mathcal{M} is the variety whose defining ideal $I_{\mathcal{M}} \subseteq S = \mathbb{C}[p_{ijk}]$ is

$$I_{\mathcal{M}} = (p_{ijk}p_{i'j'k} - p_{ij'k}p_{i'jk}: i, i' \in [r_1], j, j' \in [r_2], k \in [r_3]) \\ + (p_{ijk}p_{i'jk'} - p_{ij'k'}p_{i'jk}: i, i' \in [r_1], j \in [r_2], k, k' \in [r_3]).$$

The intersection axiom is the implication whose premises are the statements of \mathcal{M} and whose conclusion is $X_1 \perp\!\!\!\perp (X_2, X_3)$. To be true, this implication requires the further hypothesis that the distribution p is in the interior of the probability simplex, i.e. that no individual probability p_{ijk} is zero. It is thus a natural question to ask what can be inferred about distributions p which may lie on the boundary of the probability simplex. In algebraic terms, we are asking for the (set-theoretic) components of the variety $V(I_{\mathcal{M}})$.

A problem posed by Dustin Cartwright and Alexander Engström appears in Sect. 6.6.3 of [1], giving a conjectural description of the associated primes of $I_{\mathcal{M}}$ in terms of certain subgraphs of a complete bipartite graph. Our main theorem resolves this conjecture in the positive, and gives stronger information, namely the primary decomposition of $I_{\mathcal{M}}$.

In the course of this project the author computed primary decompositions of $I_{\mathcal{M}}$ for various values of r_1, r_2 , and r_3 with the computer algebra system Singular [4, 5]. Thomas Kahle has recently written dedicated Macaulay2 code [3] for binomial primary decompositions [7], in which the same computations may be carried out.

A broad generalization of this paper’s results to the class of *binomial edge ideals* of graphs has been obtained by Herzog, Hibi, Hreinsdóttir, Kahle, and Rauh [6]. The $r = 2$ case of $I_{\mathcal{M}}$ is treated, with a different term order, in their Sect. 4.

Let $K_{p,q}$ be the complete bipartite graph with bipartitioned vertex set $[p] \sqcup [q]$. Given a subgraph G of K_{r_2,r_3} with edge set $\text{Edges}(G)$, the prime P_G to which it corresponds is defined to be

$$P_G = P_G^{(0)} + P_G^{(1)}$$

where

$$P_G^{(0)} = (p_{ijk}: i \in [r_1], (j, k) \notin \text{Edges}(G)), \\ P_G^{(1)} = (p_{ijk}p_{i'j'k'} - p_{ij'k'}p_{i'jk}: i, i' \in [r_1]; \text{ and} \\ j, j' \in [r_2], k, k' \in [r_3] \text{ are in the same connected component of } G).$$

Note that j need not be distinct from j' , nor k from k' . We will also want to refer to the individual summands $P_C^{(1)}$ of $P_G^{(1)}$, where $P_C^{(1)}$ includes only the generators $\{p_{ijk}: (j, k) \in C\}$ arising from edges in the connected component C of G . Then

$$P_G = P_G^{(0)} + \sum_C P_C^{(1)}, \tag{1}$$

where C runs over connected components of G .

We say that a subgraph G of K_{r_2, r_3} is *admissible* if G has vertex set $[r_2] \sqcup [r_3]$ and all connected components of G are isomorphic to some complete bipartite graph $K_{p, q}$ with $p, q \geq 1$.

Let $<_{dp}$ be the revlex term order on S over the lexicographic variable order on subscripts, with earlier subscripts more significant. Thus under $<_{dp}$, we have $P_{111} <_{dp} P_{112} <_{dp} P_{211}$.

Theorem 1 *The primary decomposition*

$$I_{\mathcal{M}} = \bigcap_G P_G \tag{2}$$

holds and is an irredundant decomposition, where the union is over admissible graphs G on $[r_2] \sqcup [r_3]$. We also have

$$\text{in}_{<_{dp}} I_{\mathcal{M}} = \bigcap_G \text{in}_{<_{dp}} P_G.$$

Each $\text{in}_{<_{dp}} P_G$ is squarefree, so $\text{in}_{<_{dp}} I_{\mathcal{M}}$ and hence $I_{\mathcal{M}}$ are radical ideals.

In particular, the value of r_1 is irrelevant to the combinatorial nature of the primary decomposition.

Corollary 2 (Conjecture, Cartwright–Engström) *The set of minimal primes of the ideal $I_{\mathcal{M}}$ is*

$$\{P_G: G \text{ an admissible graph on } [r_2] \sqcup [r_3]\}.$$

Remark 3 This corollary amounts to the set-theoretic identity

$$V(I_{\mathcal{M}}) = \bigcup_{G \text{ admissible}} V(P_G).$$

Points (p_{ijk}) on the variety $V(P_G)$ are characterized by the conditions that $p_{ijk} = 0$ for $(j, k) \notin \text{Edges}(G)$, and that for any two edges (j, k) and (j', k') in the same connected component of G , the vectors $(p_{.jk})$ and $(p_{.j'k'})$ in \mathbb{C}^{r_1} are proportional.

The core ideas of a proof of Corollary 2 are present in [1, Sect. 6.6.4]. That discussion focuses on the prime $P_{K_{r_2, r_3}}$, corresponding to the locus where the conclusion of the intersection axiom is valid, but it extends without great difficulty to any P_G .

It is noted in [1, §6.6] that the number $\eta(p, q)$ of admissible graphs G on $[p] \sqcup [q]$ is given by the generating function

$$\exp((e^x - 1)(e^y - 1)) = \sum_{p, q \geq 0} \eta(p, q) \frac{x^p y^q}{p!q!}, \tag{3}$$

which in that reference is said to follow from manipulations of Stirling numbers. This equation (3) can also be obtained as a direct consequence of a bivariate form of the exponential formula for exponential generating functions [9, §5.1], using the observation that

$$(e^x - 1)(e^y - 1) = \sum_{p, q \geq 1} \frac{x^p y^q}{p!q!}$$

is the exponential generating function for complete bipartite graphs with $p, q \geq 1$, and these are the possible connected components of admissible graphs.

We now review some standard facts on binomial and toric ideals [2]. Let I be a binomial ideal in $\mathbb{C}[x_1, \dots, x_n]$, generated by binomials of the form $x^v - x^w$ with $v, w \in \mathbb{N}^n$. There is a lattice $L_I \subseteq \mathbb{Z}^n$ such that the localization $I_{x_1 \dots x_n} \subseteq \mathbb{C}[x_1^{\pm 1}, \dots, x_n^{\pm 1}]$ has the form $(x^v - 1 : v \in L_I)$, provided that this localization is a proper ideal, i.e. I contains no monomial. If $\phi_I : \mathbb{Z}^n \rightarrow \mathbb{Z}^m$ is a \mathbb{Z} -linear map whose kernel contains L_I , then ϕ_I provides a multigrading with respect to which I is homogeneous. (If $\ker \phi_I = L_I$ exactly then ϕ_I is said to compute the *minimal sufficient statistics* for the statistical model associated to I .)

The condition that a multivariate Laurent polynomial $f \in \mathbb{C}[x_1^{\pm 1}, \dots, x_n^{\pm 1}]$ lies in $I_{x_1 \dots x_n}$ can be expressed in terms of a graph Γ' , whose vertices are \mathbb{Z}^n and whose edge set is $\{(v, w) : x^v - x^w \text{ is a Laurent monomial multiple of a generator of } I\}$; in the statistical context these edges are known as *moves*. To wit, f is in $I_{x_1 \dots x_n}$ if and only if, for each connected component C of Γ' , the sum of the coefficients on all monomials x^v with $v \in C$ is zero. In particular $I_{x_1 \dots x_n}$ is determined by the partition of \mathbb{Z}^n into connected components of Γ' . Note that this partition refines the partition of \mathbb{Z}^n into fibers of ϕ_I , for any map ϕ_I as in the last paragraph. If we are concerned with membership in I rather than $I_{x_1 \dots x_n}$, analogues of everything in this paragraph are true if we substitute \mathbb{N}^n for \mathbb{Z}^n and use ordinary monomials rather than Laurent monomials in defining the edges. We will denote the resulting graph on \mathbb{N}^n by $\Gamma(I)$, and its induced subgraph on a subset $F \subseteq \mathbb{N}^n$ by $\Gamma_F(I)$.

Any prime binomial ideal I is equal to the toric ideal I_A of a lattice point configuration A , where I_A is the kernel of the monomial map whose monomials are the points of A . Sturmfels shows in [8] that the radicals of the monomial initial ideals of I_A are exactly the Stanley–Reisner ideals of regular triangulations of A . The Stanley–Reisner ideal I_Δ of a simplicial complex Δ on a vertex set T is the monomial ideal of $\mathbb{C}[x_t : t \in T]$ generated by the products of variables $x_{t_1} \cdots x_{t_k}$ for which $\{t_1, \dots, t_k\}$ is not a face of Δ . Primary decompositions of Stanley–Reisner ideals are easily described: I_Δ is the intersection of the ideals $(x_t : t \notin F)$ over all facets F of Δ .

Sturmfels treats explicitly the 2×2 determinantal ideal of an $r \times s$ matrix, which is the toric ideal I_A for A the set of vertices of the product $\Delta_{r-1} \times \Delta_{s-1}$ of two simplices.

Theorem 4 (Sturmfels [8]) *Let I be the ideal of 2×2 minors of an $r \times s$ matrix of indeterminates $Y = (y_{ij})$. For any term order \prec , $\text{in}_\prec I$ is a squarefree monomial ideal.*

Remark 5 If \prec is the revlex term order on the y_{ij} , set up analogously to \prec_{dp} , then Δ has a pleasant description [8]: it is the *staircase triangulation*. The facets of Δ are the sets π of entries of the matrix Y which form maximal (“staircase”) paths through Y starting at the upper left corner, taking steps right and down, and terminating at the lower right corner. Note that staircase paths are maximal subsets of indeterminates not including both $y_{ij'}$ and $y_{i'j}$ for any $i < i'$ and $j < j'$. Thus the associated primes of $\text{in}_\prec I$ are generated by minimal sets of variables y_{ij} which include at least one of $y_{ij'}$ and $y_{i'j}$ whenever $i < i'$ and $j < j'$.

The significance of the ideals $P_C^{(1)}$ of connected components comes from the following fact.

Fact 6 If G is an admissible graph, then (1) expresses P_G as a sum of primes in disjoint sets of variables.

Indeed, $P_G^{(0)}$ is the irrelevant ideal in the p_{ijk} with $(j, k) \notin \text{Edges}(G)$, and for each connected component C of G with s left and t right vertices, $P_C^{(1)}$ is the 2×2 determinantal ideal of the $r_1 \times st$ matrix of indeterminates (p_{ijk}) where the row indices are $i \in [r_1]$ and the column indices $(j, k) \in \text{Edges } C$. The irrelevant ideal can mostly be ignored, and so this fact reduces many of our considerations to handling 2×2 determinantal ideals. (Note that the hypothesis that G be admissible is needed, since otherwise $P_G^{(1)}$ includes variables corresponding to nonedges of G . We could amend the definition of P_G to salvage Fact 6, but we would lose the also important fact that the summands are determinantal.)

For a first immediate application, by Theorem 4 the $\text{in}_{\prec_{\text{dp}}} P_G$ are squarefree monomial ideals, implying the radicality claim of Theorem 1.

For a second, we recover the primary decomposition of $\text{in}_\prec P_G$ for an arbitrary admissible graph G . Let the connected components of G be C_1, \dots, C_l . Fact 6 implies that $\text{in}_\prec P_G = \text{in}_\prec P_G^{(0)} + \sum_i \text{in}_\prec P_{C_i}^{(1)}$. It then also gives us that if $\text{in}_\prec P_{C_i}^{(1)} = \bigcap_j Q_{C_i, j}$ are primary decompositions of the $\text{in}_\prec P_{C_i}^{(1)}$, then

$$\text{in}_\prec P_G = \bigcap_{\mathbf{j}} \left(P_G^{(0)} + \sum_{i=1}^l \text{in}_\prec Q_{C_i, j_i} \right)$$

is a primary decomposition of P_G , where $\mathbf{j} = (j_1, \dots, j_l)$ ranges over the Cartesian product of the index sets in $\bigcap_j Q_{C, j}$.

Lemma 7 *Let G and G' be subgraphs of K_{r_2, r_3} . Then $P_{G'} \subseteq P_G$ if and only if $\text{Edges}(G) \subseteq \text{Edges}(G')$ and every connected component of G' is a union of connected components C_1, \dots, C_l of G such that at most one C_i contains more than one vertex.*

In particular, for any subgraph G of $K_{r_2r_3}$ there exists an admissible graph G' such that $P_{G'} \subseteq P_G$. Such a G' can be constructed from G as follows: add to G one new edge incident to each of its isolated vertices, and then complete each connected component of the new graph to a bipartite complete graph.

Proof First suppose the consequence fails. Then either

- (1) G contains an edge not in G' , or
- (2) some connected component of G is not contained in a single connected component of G' , or
- (3) a connected component of G' contains two connected components of G both larger than one vertex.

In case (1), let (j, k) be an edge of G not in G' . Then $p_{1jk} \in P_{G'}$, but $p_{1jk} \notin P_G$, since Remark 3 describes points in $V(P_G)$ with $p_{1jk} \neq 0$. Case (2) implies case (1). And in case (3), let (j, k) and (j', k') be edges of G in different connected components there but in the same connected component of G' . Then $p_{1jk}p_{2j'k'} - p_{1j'k'}p_{2jk}$ is in $P_{G'}$ but not P_G , again using Remark 3.

Suppose instead the consequence holds. The generators of $P_{G'}^{(0)}$ are in P_G , since nonedges of G' are nonedges of G . The generators of $P_{G'}^{(1)}$ are also in P_G . For every pair of edges $(j, k), (j', k')$ in a connected component of G' , either all their endpoints are in the same component of G or one of their endpoints is isolated: in the former case $p_{ijk}p_{i'j'k'} - p_{i'jk}p_{ij'k'}$ is in $P_G^{(1)}$, in the latter case in $P_G^{(0)}$. □

Proof of Theorem 1 We first check that the right side of (2) is an irredundant primary decomposition. Let G be an admissible graph. Since P_G is a sum of primes in disjoint variables by Fact 6, it is prime. Irredundance of (2) is the assertion that for G and G' distinct admissible graphs, P_G is not contained in $P_{G'}$. This follows directly from the definition of admissibility and Lemma 7.

So we must prove the intersection statement (2). Let $<$ be $<_{dp}$, and write $I = I_{\mathcal{M}}$. It is apparent that

$$I \subseteq P_G \tag{4}$$

for each G (without using admissibility). Indeed, given a generator f of I , without loss of generality of the form $f = p_{ijk}p_{i'j'k} - p_{ij'k}p_{i'jk}$, either both edges (j, k) and (j', k) lie in $\text{Edges}(G)$, in which case f is a generator of $P_G^{(1)}$, or one of these edges is not in $\text{Edges}(G)$, in which case $f \in P_G^{(0)}$. Therefore the containments

$$\text{in}_{<} I \subseteq \text{in}_{<} \bigcap_G P_G \subseteq \bigcap_G \text{in}_{<} P_G$$

hold, the intersections still being over admissible G . It now suffices to show an equality of Hilbert functions

$$H(S/\text{in}_{<} I) = H\left(S/\bigcap_G \text{in}_{<} P_G\right), \tag{5}$$

forcing these containments to be equalities.

The lattice L_I associated to our I is generated by all vectors of the form $e_{ijk} + e_{i'j'k} - e_{ij'k} - e_{i'jk}$ and $e_{ijk} + e_{i'jk'} - e_{ijk'} - e_{i'jk}$. The map $\phi = \phi_I : \mathbb{Z}^{r_1 r_2 r_3} \rightarrow \mathbb{Z}^{r_1+r_2+r_3}$ sending (u_{ijk}) to

$$\left(\sum_{(j,k)} u_{1jk}, \dots, \sum_{(j,k)} u_{r_1jk}, \sum_i u_{i11}, \dots, \sum_i u_{ir_2r_3} \right)$$

has kernel containing L_I . Therefore we obtain a $\mathbb{Z}^{r_1+r_2+r_3}$ -valued multigrading on S , $\text{deg}_\phi p_{ijk} = (e_i, e_{jk})$, in which I is homogeneous. The deg_ϕ multigrading refines the standard grading. We will prove that (5) holds in this stronger context of ϕ -graded Hilbert functions.

Let $d \in \mathbb{Z}^{r_1+r_2+r_3}$ be the multidegree of some monomial, and write its components as d_i for $i \in [r_1]$ and d_{jk} for $(j, k) \in [r_2] \times [r_3]$. Let $G(d)$ be the bipartite graph with vertex set $[r_2] \sqcup [r_3]$ and edge set $\{(j, k) : d_{jk} \neq 0\}$. We now prove the following two claims:

Claim 1 $I_d = (P_{G(d)})_d$.

Claim 2 $(\bigcap_{G \text{ admissible}} \text{in}_{<} P_G)_d = (\text{in}_{<} P_{G(d)})_d$.

These claims imply

$$\begin{aligned} H(\text{in}_{<} I)(d) &= H(I)(d) = H(P_{G(d)})(d) = H(\text{in}_{<} P_{G(d)})(d) \\ &= H\left(\bigcap_G \text{in}_{<} P_G\right)(d). \end{aligned}$$

Thence we conclude that (5) holds, proving Theorem 1.

Proof of Claim 1 Observe first that no polynomial homogeneous of multidegree d can be divisible by any p_{ijk} with $(j, k) \notin \text{Edges}(G(d))$. Accordingly we have $(P_{G(d)})_d = (P_{G(d)}^{(1)})_d$, and we will work with $P_{G(d)}^{(1)}$.

Since I and $P_{G(d)}^{(1)}$ are binomial ideals generated by differences of monomials, it will suffice to show that the two graphs $\Gamma_F(I)$ and $\Gamma_F(P_{G(d)}^{(1)})$ of moves on the fiber $F = \phi^{-1}(d)$ have the same partition into connected components. It is clear that $\Gamma_F(I)$ is a subgraph of $\Gamma_F(P_{G(d)}^{(1)})$, since containment (4) implies $I_d \subseteq (P_{G(d)})_d = (P_{G(d)}^{(1)})_d$.

So given an edge of $\Gamma_F(P_{G(d)}^{(1)})$, say with endpoints $u, u' \in F$, we must show that this edge is contained in a connected component of $\Gamma_F(I)$, i.e. that $p^u - p^{u'} \in I$. We have $u = u' + e_{i_0 j_0 k_0} + e_{i_\ell j_\ell k_\ell} - e_{i_0 j_\ell k_\ell} - e_{i_\ell j_0 k_0}$ for some $i_0, i_\ell \in [r_1]$ and some two edges $(j_0, k_0), (j_\ell, k_\ell)$ of $G(d)$ in the same component. Let $(j_m, k_m)_{m=0, \dots, \ell}$ be the edges of a path in $G(d)$ between these, so that for each $0 \leq m < \ell$ either $j_m = j_{m+1}$ or $k_m = k_{m+1}$. Assume the (j_m, k_m) are pairwise distinct. For each $1 \leq m \leq \ell - 1$, let i_m be such that $p_{i_m j_m k_m}$ divides $p^{u'}$. Such an i_m must exist because $d_{j_m k_m}$ is positive. Then

$$\begin{aligned}
 & (P_{i_0 j_0 k_0} P_{i_\ell j_\ell k_\ell} - P_{i_0 j_\ell k_\ell} P_{i_\ell j_0 k_0}) P_{i_1 j_1 k_1} \cdots P_{i_{\ell-1} j_{\ell-1} k_{\ell-1}} \\
 &= \sum_{m=0}^{\ell-1} P_{i_1 j_0 k_0} \cdots P_{i_m j_{m-1} k_{m-1}} g_{i_{m+1} j_{m+1} k_{m+1}}^{i_0 j_m k_m} P_{i_{m+2} j_{m+2} k_{m+2}} \cdots P_{i_\ell j_\ell k_\ell} \\
 &\quad - \sum_{m=0}^{\ell-2} P_{i_1 j_0 k_0} \cdots P_{i_m j_{m-1} k_{m-1}} g_{i_{m+1} j_{m+1} k_{m+1}}^{i_\ell j_m k_m} \\
 &\quad \times P_{i_{m+2} j_{m+2} k_{m+2}} \cdots P_{i_{\ell-1} j_{\ell-1} k_{\ell-1}} P_{i_0 j_\ell k_\ell}
 \end{aligned}$$

is in I , where to save space $g_{i'j'k'}^{i''j''k''}$ denotes the generator $p_{i'jk'} p_{i''j''k''} - p_{i''j''k''} p_{i'jk'}$ of I . The binomial $p^u - p^{u'}$ is a monomial multiple of this binomial, so $p^u - p^{u'} \in I$.

Proof of Claim 2 There is an admissible graph G' such that $P_{G'} \subseteq P_{G(d)}$, by Lemma 7. Then $\text{in}_< P_{G'} \subseteq \text{in}_< P_{G(d)}$, which implies $\bigcap_{G \text{ admissible}} \text{in}_< P_G \subseteq \text{in}_< P_{G(d)}$, one of the containments of the claim.

For the other containment, suppose p^u is a monomial of multidegree d belonging to $\text{in}_< P_{G(d)}$. By Remark 5, p^u is divisible by some $p_{i'j'k'} p_{i''j''k''}$ for $i < i'$ in $[r_1]$ and $(j, k), (j', k')$ two edges lying in the same connected component of $G(d)$ with $(j, k) < (j', k')$ lexicographically. Now let G be any admissible graph. If $G(d)$ is not a subset of G , then p^u is divisible by some indeterminate $p_{i'j''k''}$ with $(j'', k'') \notin E(G)$, so $p^u \in \text{in}_< P_G$. Otherwise $G(d) \subseteq G$, in which case the edges (j, k) and (j', k') lie in the same component of G , so $p_{i'j'k'} p_{i''j''k''} \in \text{in}_< P_G$, implying $p^u \in \text{in}_< P_G$. Therefore $\text{in}_< P_{G(d)} \subseteq \bigcap_{G \text{ admissible}} \text{in}_< P_G$. \square

Observe finally that Claim 1 alone would suffice for the radicality in Theorem 1, supposing we already knew the P_G to be the associated primes. For radicality it suffices that I contain the intersection of its minimal primes, and this follows using Claim 1 one multidegree at a time, since the multidegree d part of this intersection is contained in $(P_{G(d)})_d$.

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