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.

Conditional independence contraints 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 recognised 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 characterised by satisfying several conditional independence constraints. We 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 $[r_i] = \{1, \ldots, r_i\}$. Throughout we assume $r_1 \ge 2$. 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

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

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The intersection axiom is the axiom whose premises are the statements of \mathcal{M} and whose conclusion is $X_1 \perp (X_2, X_3)$. 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 a primary decomposition of $I_{\mathcal{M}}$.

Our Proposition 1 resolves a problem posed by Dustin Cartwright and Alexander Engström in [1, p. 152]. The problem concerned the primary decomposition of $I_{\mathcal{M}}$; they conjectured a description in terms of subgraphs of a complete bipartite graph, which we show here to be correct.

In the course of this project the author carried out computations of primary decompositions for the ideal \mathcal{M}_I 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 generalisation 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].

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

Given a subgraph G with edge set $\operatorname{Edges}(G)$, the prime P_G to which it corresponds is defined to be

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

where

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

Note that j and j', and k and k', need not be distinct. That is, for (p_{ijk}) on the variety $V(P_G)$, $p_{ijk} = 0$ for $(j,k) \notin \text{Edges}(G)$, and any pair of vectors $p_{\cdot jk}$ and $p_{\cdot j'k'}$ are proportional for (j,k) and (j',k') two edges in Edges(G) in the same connected component of G. Later 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.

Proposition 1. The set of minimal primes of the ideal $I_{\mathcal{M}}$ is

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

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

Proposition 1 was the original conjecture of Cartwright and Engström. It is a purely set-theoretic assertion, and is equivalent to the fact that

(2)
$$V(I_{\mathcal{M}}) = \bigcup_{G} V(P_G)$$

as sets, where the union is over admissible graphs G. The ideas of a proof of Proposition 1 were anticipated in part 4 of the problem stated in [1, §6.6] which was framed for the prime corresponding to the subgraph G, the case where the conclusion of the intersection axiom is valid; they extend without great difficulty to the general case.

We will prove a stronger ideal-theoretic result. Let \prec_{dp} be the revlex term order on S over the lexicographic variable order on subscripts, with earlier subscripts more significant: thus under \prec_{dp} , we have $p_{111} \prec_{dp} p_{112} \prec_{dp} p_{211}$.

Theorem 2. The primary decomposition

(3)
$$I_{\mathcal{M}} = \bigcap_{G} P_{G}$$

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

$$\operatorname{in}_{\prec_{\mathrm{dp}}} I_{\mathcal{M}} = \operatorname{in}_{\prec_{\mathrm{dp}}} \bigcap_{G} P_{G} = \bigcap_{G} \operatorname{in}_{\prec_{\mathrm{dp}}} P_{G}.$$

Furthermore, each primary component $\operatorname{in}_{\prec_{dp}} P_G$ is squarefree, so $\operatorname{in}_{\prec_{dp}} I_{\mathcal{M}}$ and hence $I_{\mathcal{M}}$ are radical ideals.

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

(4)
$$\exp((e^x - 1)(e^y - 1)) = \sum_{p,q \ge 0} \eta(p,q) \frac{x^p y^q}{p! q!}.$$

which in that reference is said to follow from manipulations of Stirling numbers. This equation (4) 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

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

is the exponential generating function for complete bipartite graphs with $p, q \ge 1$, 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 $\mathbb{C}[x_1, \ldots, x_n]$, generated by binomials of the form $x^v - x^w$ with $v, w \in \mathbb{N}^n$. There is a lattice $L_I \subseteq Z^n$ such that the localisation $I_{x_1 \cdots x_n} \subseteq \mathbb{C}[x_1^{\pm 1}, \ldots, x_n^{\pm 1}]$ has the form $(x^v - 1 : v \in L_I)$, provided that this localisation is a proper ideal, i.e. I contains no monomial. If $\phi_I : \mathbb{Z}^n \to \mathbb{Z}^m$ is a \mathbb{Z} -linear map whose kernel is L_I , then ϕ_I provides a multigrading with respect to which I is homogeneous. In statistical terms ϕ_I computes the minimal sufficient statistics for the statistical model associated to I.

Given a multivariate Laurent polynomial $f \in \mathbb{C}[x_1^{\pm 1}, \ldots, x_n^{\pm 1}]$, f lies in $I_{x_1 \cdots x_n}$ if and only if, for each fiber F of ϕ_I , the sum of the coefficients on all monomials x^v with $v \in F$ is zero. With respect to $\mathbb{C}[x_1, \ldots, x_n]$ a modified statement holds, as follows. For each fiber F, consider the graph $\Gamma_F(I)$ whose vertices are the set of vectors in F with all entries nonnegative, and whose edge set is $\{(v, w) : x^v - x^w \text{ is}$ a monomial multiple of a generator of $I\}$. In the statistical context these edges are known as *moves*. Then f lies in $I \subseteq \mathbb{C}[x_1, \ldots, x_n]$ if and only if, for each connected component C of each $\Gamma_F(I)$, the sum of the coefficients on all monomials x^v with $v \in C$ is zero. In particular I is determined by this set of connected components.

Viewing $I \subseteq \mathbb{C}[x_1^{\pm 1}, \ldots, x_n^{\pm 1}]$ as the ideal of the toric subvariety of $(\mathbb{C}^*)^n$ associated to the lattice polytope A, Sturmfels in [8] shows that the radicals of the monomial initial ideals of I are exactly the Stanley-Reisner ideals of regular triangulations of A. The Stanley-Reisner ideal I_{Δ} of a simplicial complex Δ on a set Tis the monomial ideal of $\mathbb{C}[x_t : t \in T]$ generated as a vector space by the products of variables $x_{t_1} \cdots x_{t_k}$ for which $\{t_1, \ldots, t_k\}$ does not contain a face of Δ . Every squarefree monomial ideal is the Stanley-Reisner ideal of some simplicial complex, and 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 also treats explicitly the ideal I of 2×2 minors of an $r \times s$ matrix $Y = (y_{ij})$, of which $P_K := P_{K_{r_2r_3}}$ is a particular case. In this case the polytope A is the product of two simplices, $\Delta_{r-1} \times \Delta_{s-1}$.

Theorem 3 ([8]). Let I be the ideal of 2×2 minors of an $r \times s$ matrix of indeterminates. For any term order \prec , in \downarrow I is a squarefree monomial ideal.

This immediately yields the radicality claim of Theorem 2: the in P_G are squarefree monomial ideals, so their associated primes are generated by subsets of the variables $\{p_{ijk}\}$.

We repeat from [8] one especially describable example of an initial ideal of this ideal I, namely $in_{\prec dp} I$, corresponding to the case that Δ is the so-called staircase triangulation. Then the vertices of the simplices of Δ correspond to those sets π of entries of the matrix Y which form ("staircase") paths through Y starting at the upper-left corner, taking only steps right and down, and terminating at the lower left corner. Hence to each such π corresponds one primary component $Q_{G,\pi}$, generated by all (r-1)(s-1) indeterminates not lying on π . Note that staircase paths are maximal subsets of indeterminates not including both $x_{ij'}$ and $x_{i'j}$ for any i < i' and j < j'.

This framework suffices to understand the primary decomposition of $\operatorname{in}_{\prec} P_G$ for an arbitrary admissible graph G. Let the connected components of G be C_1, \ldots, C_l , so that, from (1), $\operatorname{in}_{\prec} P_G$ is the sum of the ideal $\operatorname{in}_{\prec} P_G^{(0)} = P_G^{(0)}$ and the various ideals $\operatorname{in}_{\prec} P_{C_i}^{(1)}$, and moreover these summands use disjoint sets of variables. Suppose that $\operatorname{in}_{\prec} P_{C_i}^{(1)} = \bigcap_j Q_{C_i,j}$ are primary decompositions of the $\operatorname{in}_{\prec} P_{C_i}^{(1)}$. Then it follows that we have the primary decomposition

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

where $\mathbf{j} = (j_1, \ldots, j_l)$ ranges over the Cartesian product of the index sets in $\bigcap_j Q_{C,j}$.

Proof of Theorem 2. We begin by proving that the right side of (3) is an irredundant primary decomposition. Let G be an admissible graph. For each connected component $C \subseteq G$ and fixed i, $P_C^{(1)}$ are the determinantal ideal of 2×2 minors of the matrix with r_1 rows and columns indexed by $\operatorname{Edges}(C)$, whose i, (j, k) entry is p_{ijk} . Being a determinantal ideal, $P_C^{(1)}$ is prime. The ideal $P_G^{(0)}$ is also prime, as it is generated by a collection of variables. Now P_G is the sum of the prime ideals $P_G^{(0)}$ and $P_C^{(1)}$ for each C, and the generators of these primes involve pairwise disjoint subsets of the unknowns p_{ijk} . It follows that P_G itself is prime.

Irredundance is the assertion that for G and G' distinct admissible graphs, P_G is not contained in $P_{G'}$. As above, we will think of the 3-tensor (p_{ijk}) as a size $r_2 \times r_3$ table whose entries are vectors $(p_{\cdot jk})$ of length r_1 . Then if $(p_{ijk}) \in V(P_G)$, all nonzero vectors in each subtable determined by a connected component of G are proportional, while vectors outside of any subtable must be the zero vector. There is an open dense subset $U_G \subseteq V(P_G)$ such that for $(p_{ijk}) \in U_G$, no vector $p_{\cdot jk}$ associated to a connected component of G is zero, and no two associated to distinct components are dependent.

Now, G may differ from G' in two fashions. If G contains an edge (j, k) that G' doesn't, the vector $(p_{\cdot jk})$ is zero on $V(P_{G'})$ but is nonzero on U_G : hence $V(P_G) \not\subseteq V(P_{G'})$. If not, $G \subseteq G'$, but two edges (j,k), (j',k') in different components of G must be in the same component of G', in which case the vectors $(p_{\cdot jk})$ and $(p_{\cdot j'k'})$ are linearly dependent for $(p_{ijk}) \in V(P_{G'})$ but linearly independent on U_G : hence also $V(P_G) \not\subseteq V(P_{G'})$. This proves irredundance.

Now we turn to proving (3). Let \prec be \prec_{dp} . Write $I = I_{\mathcal{M}}$. It is apparent that $I \subseteq P_G$ for each G. Indeed, given a generator f of I, without loss of generality $f = p_{ijk}p_{i'j'k} - p_{ij'k}p_{i'jk}$, either both edges (j,k) and (j',k) lie in Edges(G), in which case f is a generator of $P_G^{(1)}$, or one of these edges is not in Edges(G), in which case $f \in P_G^{(0)}$. Therefore the containments

$$\mathrm{in}_{\prec}I\subseteq\mathrm{in}_{\prec}\bigcap_{G}P_{G}\subseteq\bigcap_{G}\mathrm{in}_{\prec}P_{G}$$

hold. It now suffices to show an equality of Hilbert functions

(5)
$$H(S/\operatorname{in}_{\prec} I) = H(S/\bigcap_{G} \operatorname{in}_{\prec} P_{G}).$$

In the present case, the lattice L_I associated to I is generated by all vectors of the forms $e_{ijk} + e_{i'j'k} - e_{ij'k} - e_{i'jk}$ and $e_{ijk} + e_{i'jk'} - e_{ijk'} - e_{i'jk}$. The map $\phi_I : \mathbb{Z}^{r_1 r_2 r_3} \to \mathbb{Z}^{r_1 + r_2 r_3}$ 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 L_I and thus induces the multigrading on S by minimal sufficient statistics, with respect to which I is homogeneous. In fact the analogue of (5) using Hilbert functions in the multigrading ϕ is also true, and it is this we will prove.

Let $d \in \mathbb{Z}^{r_1+r_2r_3}$ 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 $[r_2] \amalg [r_3]$ 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. $(\bigcap_G \operatorname{in}_{\prec} P_G)_d = (\operatorname{in}_{\prec} P_{G(d)})_d$.

These claims, and the fact that an ideal and its initial ideal have the same Hilbert function, imply

$$H(\text{in}_{\prec} I)(d) = H(I)(d) = H(P_{G(d)})(d) = H(\text{in}_{\prec} P_{G(d)})(d) = H(\bigcap_{G} \text{in}_{\prec} P_{G})(d),$$

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We conclude that (5) holds, proving Theorem 2.

Proof of Claim 1. Observe first that no polynomial homogeneous of multidegree dcan be divisible by any p_{ijk} with $(j,k) \notin \text{Edges}(G(d))$. Accordingly we have $(P_{G(d)})_d = (P_{G(d)}^{(1)})_d$, in the notation of (1), and we will work with $P_{G(d)}^{(1)}$ hereafter. 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 $F = \phi_I^{-1}(d)$ have the same partition into connected components. The refinement in one direction is clear: $\Gamma_F(I)$ is a subgraph of $\Gamma_F(P_{G(d)}^{(1)})$, since $I_d \subseteq (P_{G(d)})_d =$ $(P_{G(d)}^{(1)})_d$, and indeed each generator of I of multidegree at most d is a monomial multiple of a generator of $P_{G(d)}^{(1)}$.

So given an edge of $\Gamma_F(P_{G(d)}^{(1)})$, we must show that this edge is contained in a connected component of $\Gamma_F(I)$. Let $u, u' \in F$ be the endpoints of an edge of $\Gamma_F(P_{G(d)}^{(1)})$. Then $u = u' + e_{ijk} + e_{i'j'k'} - e_{ij'k'} - e_{i'jk}$ for some $i, i' \in [r_1]$ and (j,k), (j',k') edges of G(d) in the same component. By connectedness, there is a path of edges $e_0 = (j',k'), e_1, \ldots, e_l = (j,k)$ of G(d) such that e_i and e_{i+1} share a vertex for each i. Corresponding to this path there exists a sequence of moves $(M_m)_{m=0,\ldots,l-1}$ in I, say $M_m = p^{u_m} - p^{u_{m+1}}$, where $u_0 = u', u_l = u$, and where M_m is a monomial multiple of

$p_{i,e_m}p_{i_m,e_{m+1}} - p_{i_m,e_m}p_{i,e_{m+1}}$

for some $i_m \in [r_1]$. So u and u' are in a single connected component of $\Gamma_F(I)$. *Proof of Claim 2.* Again, one containment is straightforward, namely $\operatorname{in}_{\prec} P_{G(d)} \subseteq \bigcap_G \operatorname{in}_{\prec} P_G$. There is an admissible graph G such that $P_G \subseteq P_{G(d)}$. Such a G can be constructed per the discussion of irredundance, if we take p to be a generic point of $V(P_{G(d)})$. Then $\operatorname{in}_{\prec} P_G \subseteq \operatorname{in}_{\prec} P_{G(d)}$ and this latter initial ideal is one of the ideals being intersected in $\bigcap_G \in_{\prec} P_G$.

For the other containment, let C be any connected bipartite graph on vertex set $[r_2] \amalg [r_3]$, such that $d_{jk} = 0$ for $(j, k) \notin E(C)$. By the Stanley-Reisner description of the initial ideal for \prec_{dp} , a monomial $p^u \in S$ of degree d lies in $in_{\prec} P_C = in_{\prec} P_{K_{r_2r_3}}$ if and only if p^u is divisible by $p_{ij'k'}p_{i'jk}$ for some i < i' and (j,k) < (j',k') lexicographically.

So if p^u is a monomial of multidegree d lying in $\operatorname{in}_{\prec_{dp}} P_{G(d)}$, it's divisible by some $p_{ij'k'}p_{i'jk}$ with i < i' in $[r_1]$ and (j,k) < (j',k') two edges lying in the same connected component of G(d); it cannot occur that instead p^u is divisible by some indeterminate $p_{ij''k''}$ for (j'',k'') not an edge of G(d), since p_u has multidegree d. Now let G be any admissible graph. If G(d) is not a subset of G, then p^u is divisible by some indeterminate $p_{ij''k''}$ with $(j'',k'') \notin E(G)$, so $p^u \in \operatorname{in}_{\prec} P_G$. Otherwise $G(d) \subseteq G$. In this case the edges (j,k) and (j',k') lie in the same component of G, and so $p_{ij'k'}p_{i'jk} \mid p^u$ implies $p^u \in \operatorname{in}_{\prec} P_G$ again. Therefore $\operatorname{in}_{\prec} P_{G(d)} \supseteq \bigcap_G \operatorname{in}_{\prec} P_G$.

We close with the remark that we can describe explicitly which components of (3) contain a given point of $V(I_{\mathcal{M}})$. Let $p = (p_{ijk}) \in \mathbb{C}^{r_1 r_2 r_3}$, and define G(p)to be the bipartite graph on $[r_2] \amalg [r_3]$ with edge set $\{(j,k) : p_{ijk} \neq 0 \text{ for some } i\}$. Then the components $V(P_G)$ containing (p_{ijk}) are exactly those for which G can be

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obtained from G(p) by adding edges which don't unite two connected components of the latter containing respective edges (j, k) and (j', k') such that $p_{\cdot jk}$ and $p_{\cdot j'k'}$ are not proportional. If $p \in U_{G(p)}$, then these components are exactly those for which G adds only edges which don't unite two connected components of G(p), neither of which is an isolated vertex.

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