OPEN PROBLEMS IN ALGEBRAIC STATISTICS

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Abstract. Algebraic statistics is concerned with the study of probabilistic models and techniques for statistical inference using methods from algebra and geometry. This article presents a list of open mathematical problems in this emerging field, with main emphasis on graphical models with hidden variables, maximum likelihood estimation, and multivariate Gaussian distributions. These are notes from a lecture presented at the IMA in Minneapolis during the 2006/07 program on Applications of Algebraic Geometry.

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1. Introduction. This article is based on a lecture given in March 2007 at the workshop on Statistics, Biology and Dynamics held at the Institute for Mathematics and its Applications (IMA) in Minneapolis as part of the 2006/07 program on Applications of Algebraic Geometry. In four sections we present mathematical problems whose solutions would likely become important contributions to the emerging interactions between algebraic geometry and computational statistics. Each of the four sections starts out with a “specific problem” which plays the role of representing the broader research agenda. The latter is summarized in a “general problem”.

Algebraic statistics is concerned with the study of probabilistic models and techniques for statistical inference using methods from algebra and geometry. The term was coined in the book of Pistone, Riccomagno and Wynn [25] and subsequently developed for biological applications in [24]. Readers from statistics will enjoy the introduction and review recently given by Drton and Sullivant [8], while readers from algebra will find various points of entry cited in our discussion and listed among our references.

2. Graphical Models with Hidden Variables. Our first question concerns three-dimensional contingency tables \((p_{ijk})\) whose indices \(i, j, k\) range over a set of four elements, such as the set \(\{A, C, G, T\}\) of DNA bases.

Specific Problem: Consider the variety of \(4 \times 4 \times 4\)-tables of tensor rank at most \(4\). There are certain known polynomials of degree at most nine which vanish on this variety. Do they suffice to cut out the variety? This particular open problem appears in [24] Conjecture 3.24], and it here serves as a placeholder for the following broader direction of inquiry.

General Problem: Study the geometry and commutative algebra of graphical models with hidden random variables. Construct these varieties by gluing familiar secant varieties, and by applying representation theory.

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We are interested in statistical models for discrete data which can be represented by polynomial constraints. As is customary in algebraic geometry, we consider varieties over the field of complex numbers, with the tacit understanding that statisticians mostly care about points whose coordinates are real and non-negative. The model referred to in the Specific Problem lives in the 64-dimensional space \( \mathbb{C}^4 \otimes \mathbb{C}^4 \otimes \mathbb{C}^4 \) of \( 4 \times 4 \times 4 \)-tables \((p_{ijk})\), where \( i, j, k \in \{A, C, G, T\}\). It has the parametric representation
\[
p_{ijk} = \rho_{ki} \cdot \sigma_{kj} \cdot \theta_{kk} + \rho_{ci} \cdot \sigma_{cj} \cdot \theta_{ck} + \rho_{gi} \cdot \sigma_{gj} \cdot \theta_{gk} + \rho_{ti} \cdot \sigma_{tj} \cdot \theta_{tk}.
\]

Our problem is to compute the homogeneous prime ideal \( I \) of all polynomials which vanish on this model. The desired ideal \( I \) lives in the polynomial ring \( \mathbb{Q}[p_{AAA}, p_{AAC}, p_{AAT}, \ldots, p_{TTG}, p_{TTT}] \) with 64 unknowns. In principle, one can compute generators of \( I \) by applying Gröbner bases methods to the parametrization (2.1). However, our problem has 64 probabilities and 48 parameters, and it is simply too big for the kind of computations which were performed in [24, §3.2] using the software package Singular [13].

Given that Gröbner basis methods appear to be too slow for any problem size which is actually relevant for real data, skeptics may wonder why a statistician should bother learning the language of ideals and varieties. One possible response to the practitioner’s legitimate question “Why (pure) mathematics?” is offered by the following quote due to Henri Poincaré:

“Mathematics is the Art of Giving the Same Name to Different Things”.

Indeed, our prime ideal \( I \) gives the same name to the following things:
- the set of \( 4 \times 4 \times 4 \)-tables of tensor rank \( \leq 4 \),
- the mixture of four models for three independent random variables,
- the naive Bayes model with four classes,
- the conditional independence model \([X_1 \independent X_2 \independent X_3 | Y]\),
- the fourth secant variety of the Segre variety \( \mathbb{P}^3 \times \mathbb{P}^3 \times \mathbb{P}^3 \),
- the general Markov model for the phylogenetic tree \( K_{1,3} \),
- superposition of four pure states in a quantum system [4, 14].

These different terms have been used in the literature for the geometric object represented by (2.1). The concise language of commutative algebra and algebraic geometry can be an effective channel of communication for the different communities of statisticians, computer scientists, physicists, engineers and biologists, all of whom have encountered formulas like (2.1).

The generators of lowest degree in our ideal \( I \) have degree five, and the known generators of highest degree have degree nine. The analysis of Landsberg and Manivel in [20, Proposition 6.3] on \( 3 \times 3 \times 4 \)-tables of tensor rank four implies the existence of additional ideal generators of degree six in \( I \). This analysis had been overlooked by the authors of [24] when they formulated their Conjecture 3.24. Readers of [24, Chapter 3] are herewith kindly asked to replace “of degree 5 and 9” by “of degree at most 9”.

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In what follows we present the known minimal generators of degree five and nine in our prime ideal $I$, and we postpone a more detailed discussion of the Landsberg-Manivel sextics in [20, Proposition 6.3] to a future study.

Consider any $3 \times 4 \times 4$-subtable $(p_{ijk})$ and let $A, B, C$ be the $4 \times 4$-slices gotten by fixing $i$. To be precise, the entry of the $4 \times 4$-matrix $A$ in row $j$ and column $k$ equals $p_{Ajk}$, the entry of $B$ in row $j$ and column $k$ equals $p_{Cjk}$, and the entry of $C$ in row $j$ and column $k$ equals $p_{Gjk}$. We can check that the following identity of $4 \times 4$-matrices holds for all tables in our model, provided the matrix $B$ is invertible:

$$A \cdot B^{-1} \cdot C = C \cdot B^{-1} \cdot A$$

After clearing the denominator $\det(B)$, we can write this identity as

$$A \cdot \adj(B) \cdot C - C \cdot \adj(B) \cdot A = 0, \quad (2.2)$$

where $\adj(B) = \det(B) \cdot B^{-1}$ is the adjoint matrix of $B$. The matrix entries on the left hand side give 16 quintic polynomials which lie in our prime ideal $I$. Each matrix entry is a polynomial with 180 terms which involve only 30 of the 64 unknowns. For example, the upper left entry looks like this:

$$p_{AAC}p_{CPP}\cdot p_{CTT}p_{GAA}p_{AAC}p_{CCG}\cdot p_{CGA}p_{CTT}p_{GAA}p_{AAC}\cdot p_{CCP}\cdot p_{CGA}p_{CTT}p_{GAA} - \cdots$$

We note that there are no non-zero polynomials of degree $\leq 4$ in the ideal $I$. This follows from general results on secant varieties [5, 17].

An explicit linear algebra computation reveals that all polynomials of degree five in $I$ are gotten from the above construction by relabeling and considering all subtables of format $3 \times 4 \times 4$, format $4 \times 3 \times 4$ and format $4 \times 4 \times 3$, and by applying the natural action of the group $GL(\mathbb{C}^4) \times GL(\mathbb{C}^4) \times GL(\mathbb{C}^4)$ on $4 \times 4 \times 4$-tables. This action leaves the ideal $I$ fixed. We identify the representation of this group on the space of quintics in $I$.

**Proposition 2.1.** The space of quintic polynomials in the prime ideal $I$ of (2.1) has dimension 1728. As a $GL(\mathbb{C}^4)^3$-module, it is isomorphic to

$$S_{311}(\mathbb{C}^4) \otimes S_{2111}(\mathbb{C}^4) \otimes S_{2111}(\mathbb{C}^4)$$

$$\oplus S_{2111}(\mathbb{C}^4) \otimes S_{311}(\mathbb{C}^4) \otimes S_{2111}(\mathbb{C}^4)$$

$$\oplus S_{2111}(\mathbb{C}^4) \otimes S_{2111}(\mathbb{C}^4) \otimes S_{311}(\mathbb{C}^4).$$

Here $S_\lambda(\mathbb{C}^4)$ denotes the Schur modules which are the irreducible representations of $GL(\mathbb{C}^4)$. We refer to [10] for the relevant basics on representation theory of the general linear group, and to [17, 18, 19] for more detailed information about the specific modules under consideration here.
The known invariants of degree nine are also obtained by a similar construction. Consider any $3 \times 3 \times 3$-subtable $(p_{ijk})$ and denote the three slices of that table by $A$, $B$ and $C$. We now consider the $3 \times 3$-determinant

$$
\text{det}(A \cdot B^{-1} \cdot C - C \cdot B^{-1} \cdot A).
$$

The denominator of the rational function (2.3) is $\text{det}(B)^2$ and not $\text{det}(B)^3$ as one might think on first glance. The numerator of (2.3) is a homogeneous polynomial of degree nine with 9216 terms which remains invariant under permuting $A$, $B$ and $C$. This homogeneous polynomial of degree nine lies in the ideal $I$ and is known as the Strassen invariant.

**Proposition 2.2.** The $\GL(C^4)^3$-submodule of the degree 9 component $I_9$ generated by the Strassen invariant is not contained in the ideal $(I_5)$ generated by the quintics in Proposition 2.1. This module has vector space dimension 8000 and it is isomorphic to the representation

$$
S_{333}(C^4) \otimes S_{333}(C^4) \otimes S_{333}(C^4).
$$

The first appearance of the Strassen invariant in algebraic statistics was [11, Proposition 22]. A conceptual study of the matrix construction $AB^{-1}C - CB^{-1}A$ was undertaken by Landsberg and Manivel in [18].

The Specific Problem at the beginning of this section plays a pivotal role also in algebraic phylogenetics [1, 2, 3]. Our model (2.1) is known there as the general Markov model on a tree with three leaves branching off directly from the root. Allman and Rhodes [2, §6] showed that phylogenetic invariants which cut out the general Markov model on any larger binary rooted tree can be constructed from the generators of our ideal $I$ by a gluing process. The invariants of degree five and nine arising from (2.2) and (2.3) are therefore basic building blocks for phylogenetic invariants on arbitrary trees whose nodes are labeled with the four letters $A$, $C$, $G$ and $T$.

In her lecture at the same IMA conference in March 2007, Elizabeth Allman [1] offered an extremely attractive prize for the resolution of the Specific Problem. She offered to personally catch and smoke wild salmon from the Copper River, located in her “backyard” in Alaska, and ship it to anyone who will determine a minimal generating set of the prime ideal $I$.

In Propositions 2.1 and 2.2, we emphasized the language of representation theory in characterizing the defining equations of graphical statistical models. This methodology is a main focus in the forthcoming book by J.M. Landsberg and Jason Morton, which advocates the idea of using Schur modules $S_{\lambda}(C^n)$ in the description of such models. Morton’s key insight is that this naturally generalizes conditional independence, the current language of choice for characterizing graphical models. Conditional independence statements can be interpreted as a convenient shorthand for large systems of quadratic equations; see [12, §4.1] or [27, Proposition 8.1].
In the absence of hidden random variables, the quadratic equations expressed implicitly by conditional independence are sufficient to characterize graphical models. This is the content of the Hammersley-Clifford Theorem (see e.g. [12, Theorem 4.1] or [24, Theorems 1.30 and 1.33]). However, when some of the random variables in a graphical model are hidden then the situation becomes much more complicated. We believe that representation theory of the general linear group can greatly enhance the conditional independence calculus which is so widely used by graphical models experts. The representation-theoretic notation was here illustrated for a tiny graphical model, having three observed random variables and one hidden random variable, all four having the same state space \{A, C, G, T\}.

3. Maximum Likelihood Estimation. In this section we discuss topics concerning the algebraic approach to maximum likelihood estimation [24, §3.3]. The following open problem was published in [10, Problem 13].

Specific Problem: Find a geometric characterization of those projective varieties whose maximum likelihood degree (ML degree) is equal to one.

This question and others raised in [6, 10] are just the tip of an iceberg:

General Problem: Study the geometry of maximum likelihood estimation for algebraic statistical models.

Here algebraic statistical models are regarded as projective varieties. A model has ML degree one if and only if its maximum likelihood estimator is a rational function of the data. Models which have this property tend to be very nice. For instance, in the special context of undirected graphical models (Markov random fields), the property of having ML degree one is equivalent to the statement that the graph is decomposable [12, Theorem 4.4]. For toric varieties, our question was featured in [27, Problem 8.23].

It is hoped that the ML degree is related to convergence properties of numerical algorithms used by statisticians, such as iterative proportional scaling or the EM algorithm, but no systematic study in this direction has yet been undertaken. In general, we wish to learn how statistical features of a model relate to geometric properties of the corresponding variety.

Here are the relevant definitions for our problems. We fix the complex projective space \(\mathbb{P}^n\) with coordinates \((p_0 : p_1 : \cdots : p_n)\). The coordinate \(p_i\) represents the probability of the \(i\)th event. The \(n\)-dimensional probability simplex is identified with the set \(\mathbb{P}^n_{\geq 0}\) of points in \(\mathbb{P}^n\) which have non-negative real coordinates. The data comes in the form of a non-negative integer vector \((u_0, u_1, \ldots, u_n) \in \mathbb{N}^{n+1}\). Here \(u_i\) is the number of times the \(i\)th event was observed. The corresponding likelihood function is defined as

\[
L(p_0, p_1, \ldots, p_n) = \frac{p_0^{u_0} \cdot p_1^{u_1} \cdot p_2^{u_2} \cdots p_n^{u_n}}{(p_0 + p_1 + \cdots + p_n)^{u_0 + u_1 + \cdots + u_n}}. \tag{3.1}
\]

Statistical computations are typically done in affine \(n\)-space specified by \(p_0 + p_1 + \cdots + p_n = 1\), where the denominator of \(L\) can be ignored. However,
the denominator is needed in order for $L$ to be a well-defined rational function on $\mathbb{P}^n$. The unique critical point of the likelihood function $L$ is at $(u_0 : u_1 : \cdots : u_n)$, and this point is the global maximum of $L$ over $\mathbb{P}^n_{\geq 0}$.

By a critical point we mean any point at which the gradient of $L$ vanishes.

An algebraic statistical model is represented by a subvariety $M$ of the projective space $\mathbb{P}^n$. The model itself is the intersection of $M$ with the probability simplex $\mathbb{P}^n_{\geq 0}$. The ML degree of the variety $M$ is the number of complex critical points of the restriction of the likelihood function $L$ to $M$. Here we disregard singular points of $M$, we only count critical points that are not poles or zeros of $L$, and $u_0, u_1, \ldots, u_n$ are assumed to be generic.

If $M$ is smooth and the divisor on $M$ defined by $L$ has normal crossings then there is a geometric characterization of the ML degree, derived in the paper [6] with Catanese, Hosten and Khetan. The assumptions of smoothness and normal crossing are very restrictive and almost never satisfied for models of statistical interest. In general, to understand the ML degree will require invoking some resolution of singularities and its algebraic underpinnings.

We illustrate the computation of the ML degree for the case when $M$ is a plane curve. Here $n = 2$ and $M$ is the zero set of a homogeneous polynomial $F(p_0, p_1, p_2)$. Using Lagrange multipliers or [16, Proposition 2], we derive that the condition for $(p_0 : p_1 : p_2)$ to be a critical point of the restriction of $L$ to $M$ is equivalent to the system of two equations

$$F(p_0, p_1, p_2) = \det \begin{pmatrix} u_0 & p_0 & p_0 \cdot \partial F / \partial p_0 \\ u_1 & p_1 & p_1 \cdot \partial F / \partial p_1 \\ u_2 & p_2 & p_2 \cdot \partial F / \partial p_2 \end{pmatrix} = 0.$$ 

For a general polynomial $F$ of degree $d$, these equations will have $d(d+1)$ solutions, by Bézout’s Theorem. Moreover, all of these solutions satisfy

$$p_0 \cdot p_1 \cdots p_n \cdot (p_0 + p_1 + \cdots + p_n) \neq 0,$$

and we conclude that the ML degree of a general plane curve of degree $d$ is equal to $d(d+1)$. However, that number can drop considerably for special curves. For instance, while the ML degree of a general plane quadric equals six, the special quadric \{\(p_1^2 = \lambda p_0 p_2\)\} has ML degree two for $\lambda \neq 4$, and it has ML degree one for $\lambda = 4$. Thus, returning to the Special Problem, our first example of a variety of ML degree one is the plane curve defined by

$$F = \det \begin{pmatrix} 2p_0 \\ p_1 \\ 2p_2 \end{pmatrix}.$$ 

Biologists know this as the Hardy-Weinberg curve, with the parametrization

$$p_0 = \theta^2, \quad p_1 = 2\theta(1-\theta), \quad p_2 = (1-\theta)^2.$$ 

The unique critical point of the likelihood function $L$ on this curve equals

$$((2u_0 + u_1)^2 : 2(2u_0 + u_1)(u_1 + 2u_2) : (u_1 + 2u_2)^2).$$
Determinantal varieties arise naturally in statistics. They are the models $\mathcal{M}$ that are specified by imposing rank conditions on a matrix of unknowns. A first example is the model (3.4) for two i.i.d. binary random variables. For a second example we consider the general $3 \times 3$-matrix

$$
P = \begin{pmatrix}
p_{00} & p_{01} & p_{02} \\
p_{10} & p_{11} & p_{12} \\
p_{20} & p_{21} & p_{22}
\end{pmatrix}
$$

(3.5)

which represents two ternary random variables. The independence model for these two random variables is the variety of rank one matrices. This model also has ML degree one, i.e., the maximum likelihood estimator is a rational function in the data. It is given by the $3 \times 3$-matrix whose entry in row $i$ and column $j$ equals $(u_{i0} + u_{i1} + u_{i2}) \cdot (u_{0j} + u_{1j} + u_{2j})$.

By contrast, consider the mixture model based on two ternary random variables. It consists of all matrices $P$ of rank at most two. Thus this model is the hypersurface defined by the cubic polynomial $F = \det(P)$. Explicit computation shows that the ML degree of this hypersurface is ten. In general, it remains an open problem to find a formula, in terms of $m, n$ and $r$, for the ML degree of the variety of $m \times n$-matrices of rank $\leq r$.

The first interesting case arises when $m = n = 4$ and $r = 2$. At present we are unable to solve the likelihood equations for this case symbolically. The following concrete biology example was proposed in [24, Example 1.16]:

“Our data are two aligned DNA sequences ... 

ATCACAAACATTGGGATGCTGTCATTGCAAGCGGT
ATGAGTCTTAAACGCTGGCCATGTCCTTAGACAGCG

.. test the hypothesis that these two sequences were generated by DiaNA using one biased coin and four tetrahedral dice....”

Here the model $\mathcal{M}$ consists of all (positive) $4 \times 4$-matrices $(p_{ij})$ of rank at most two. In the given alignment, each match occurs four times and each mismatch occurs two times. Hence the likelihood function (3.1) equals

$$
L = \left( \prod_{i} p_{ii} \right)^4 \cdot \left( \prod_{i \neq j} p_{ij} \right)^2 \cdot \left( \sum_{i,j} p_{ij} \right)^{-40}.
$$

Based on experiments with the EM algorithm, we conjectured that the matrix $(\hat{p}_{ij}) = \frac{1}{40} \begin{pmatrix}
3 & 3 & 2 & 2 \\
2 & 2 & 3 & 3 \\
2 & 3 & 3 & 3
\end{pmatrix}$ is a global maximum of the likelihood function $L$. In the Nachdiplomsverlesung (postgraduate course) which I held at ETH Zürich in the summer of 2005, I offered a cash prize of 100 Swiss Francs for the resolution of this very specific conjecture, and this prize remains unclaimed and is still available at this time (August 2007).
The state of the art on this 100 Swiss Francs Conjecture is the work of Hersh which originated in March 2007 at the IMA. She proved a range of constraints on the maximum likelihood estimates of determinantal models, especially when the data $u_{ij}$ have symmetry. A discussion of these ideas appears in Hersh’s paper with Fienberg, Rinaldo and Zhou [9]. That paper gives an exposition of MLE for determinantal models aimed at statisticians.

4. Gaussian Conditional Independence Models. The early literature on algebraic statistics, including the book [24], dealt primarily with discrete random variables (binary, ternary, …). The set-up was as described in the previous two sections. We now shift gears and consider multivariate Gaussian distributions. For continuous random variables, we must work in the space of model parameters in order to apply algebraic geometry. The following concrete problem concerns Gaussian distributions on $\mathbb{R}^5$.

**Specific Problem:** Which sets of almost-principal minors can be zero for a positive definite symmetric $5 \times 5$-matrix?

The general question behind this asks for characterization of all conditional independence models which can be realized by Gaussians on $\mathbb{R}^n$.

**General Problem:** Study the geometry of conditional independence models for multivariate Gaussian random variables.

The state of the art on these problems appears in the work of František Matuš and his collaborators. In particular, Matuš’ recent paper with Luňiška [20] on representation of gaussoids solves our Specific Problem for symmetric $4 \times 4$-matrices. Sullivant’s construction in [28] complements that work. For more information see also the article by Šímeček [26].

Let us begin, however, with some basic definitions. Our aim is to discuss these problems in a self-contained manner. A multivariate Gaussian distribution on $\mathbb{R}^n$ with mean zero is specified by its covariance matrix $\Sigma = (\sigma_{ij})$. The $n \times n$-matrix $\Sigma$ is symmetric and it is positive definite, which means that all its $2^n$ principal minors are positive real numbers.

An almost-principal minor of $\Sigma$ is a subdeterminant which has row indices $\{i\} \cup K$ and column indices $\{j\} \cup K$ for some $K \subset \{1, \ldots, n\}$ and $i, j \in \{1, \ldots, n\} \setminus K$. We denote this subdeterminant by $[i \perp j \mid K]$. For example, if $n = 5$, $i = 2$, $j = 4$ and $K = \{1, 5\}$ then the corresponding almost-principal minor of the symmetric $5 \times 5$-matrix $\Sigma$ equals

$$[2 \perp 4 \mid \{1, 5\}] = \det \begin{pmatrix} \sigma_{24} & \sigma_{12} & \sigma_{25} \\ \sigma_{14} & \sigma_{11} & \sigma_{15} \\ \sigma_{45} & \sigma_{15} & \sigma_{55} \end{pmatrix}$$

Our notation for almost-principal minors is justified by their intimate connection to conditional independence, expressed in the following lemma. We note that the almost-principal minors are referred to as partial covariance (or, if renormalized, partial correlations) in the statistics literature.
Lemma 4.1. The subdeterminant \([i \perp j | K]\) is zero for a positive definite symmetric \(n \times n\)-matrix \(\Sigma\) if and only if, for the Gaussian random variable \(X\) on \(\mathbb{R}^n\) with covariance matrix \(\Sigma\), the random variable \(X_i\) is independent of the random variable \(X_j\) given the joint variable \(X_K\).

Proof. See [7, Equation(5)], [22, Section 1], or [28, Proposition 2.1].

Let \(\mathcal{P}_n\) denote the \((n^2 + 1)/2\)-dimensional cone of positive definite symmetric \(n \times n\)-matrices. Note that this cone is open. A Gaussian conditional independence model, or GCI model for short, is any semi-algebraic subset of the cone \(\mathcal{P}_n\) which can be defined by polynomial equations of the form

\[
\begin{bmatrix}
  i \perp j \\
  \uparrow \downarrow \\
  K
\end{bmatrix} = 0.
\]

(4.1)

In algebraic geometry, we simplify matters by studying the complex algebraic varieties defined by equations of the form (4.1). Of course, what we are particularly interested in is the real locus of such a complexified GCI model, and how it intersects the positive definite cone \(\mathcal{P}_n\) and its closure.

As an illustration of algebraic reasoning for Gaussian conditional independence models, we examine an example taken from [28]. Let \(n = 5\) and consider the GCI model given by the five quadratic polynomials

\[
\begin{align*}
[1 \perp 2 & \mid \{3\}] = \sigma_{12} \sigma_{33} - \sigma_{13} \sigma_{23} \\
[2 \perp 3 & \mid \{4\}] = \sigma_{23} \sigma_{44} - \sigma_{24} \sigma_{34} \\
[3 \perp 4 & \mid \{5\}] = \sigma_{34} \sigma_{55} - \sigma_{35} \sigma_{45} \\
[4 \perp 5 & \mid \{1\}] = \sigma_{45} \sigma_{11} - \sigma_{41} \sigma_{55} \\
[5 \perp 1 & \mid \{2\}] = \sigma_{15} \sigma_{22} - \sigma_{25} \sigma_{12}
\end{align*}
\]

This variety is a complete intersection (it has dimension ten) in the 15-dimensional space of symmetric \(5 \times 5\)-matrices. Primary decomposition reveals that it is the union of precisely two irreducible components, namely,

- the linear space \(\{\sigma_{12} = \sigma_{23} = \sigma_{34} = \sigma_{45} = \sigma_{15} = 0\}\), and
- the toric variety defined by the five quadrics plus the extra equation

\[
\sigma_{11} \sigma_{22} \sigma_{33} \sigma_{44} \sigma_{55} = \sigma_{13} \sigma_{14} \sigma_{24} \sigma_{25} \sigma_{35}.
\]

(4.2)

All matrices in the open cone \(\mathcal{P}_5\) satisfy the inequalities \(\sigma_{ii} > 0\) and

\[
\sigma_{11} \sigma_{33} > \sigma_{13}^2, \quad \sigma_{22} \sigma_{44} > \sigma_{24}^2, \quad \sigma_{33} \sigma_{55} > \sigma_{35}^2, \quad \sigma_{44} \sigma_{11} > \sigma_{14}^2, \quad \sigma_{55} \sigma_{22} > \sigma_{25}^2.
\]

Multiplying the left hand sides and right hand sides respectively, we find

\[
\sigma_{11}^2 \sigma_{22}^2 \sigma_{33}^2 \sigma_{44}^2 \sigma_{55}^2 > \sigma_{13}^2 \sigma_{14}^2 \sigma_{24}^2 \sigma_{25}^2 \sigma_{35}^2.
\]

This is a contradiction to the equation (4.2), and we conclude that the intersection of our GCI model with \(\mathcal{P}_5\) is contained in the linear space \(\{\sigma_{12} = \sigma_{23} = \sigma_{34} = \sigma_{45} = \sigma_{15} = 0\}\). The vanishing of the off-diagonal entry \(\sigma_{ij}\) means that \(X_i\) is independent of \(X_j\), or, in symbols, \([i \perp j]\). Our algebraic computation thus implies the following axiom for GCI models.
Corollary 4.1. Suppose the conditional independence statements \([1 \perp 2 \mid \{3\}], [2 \perp 3 \mid \{4\}], [3 \perp 4 \mid \{5\}], [4 \perp 5 \mid \{1\}], [5 \perp 1 \mid \{2\}]\) hold for some multivariate Gaussian distribution. Then also the following five statements must hold: \([1 \perp 2], [2 \perp 3], [3 \perp 4], [4 \perp 5], [5 \perp 1]\).

Let us now return to the question “which almost-principal minors can simultaneously vanish for a positive definite symmetric \(n \times n\)-matrix?” Corollary 4.1 gives a necessary condition for \(n = 5\). We next discuss the answer to our question for \(n \leq 4\). For \(n = 3\), the necessary and sufficient conditions are given (up to relabeling) by the following four axioms:

- \((a)\) \([1 \perp 2]\) and \([1 \perp 3 \mid \{2\}]\) implies \([1 \perp 3]\) and \([1 \perp 2 \mid \{3\}]\),
- \((b)\) \([1 \perp 2 \mid \{3\}]\) and \([1 \perp 3 \mid \{2\}]\) implies \([1 \perp 2]\) and \([1 \perp 3]\),
- \((c)\) \([1 \perp 2]\) and \([1 \perp 3 \mid \{2\}]\) implies \([1 \perp 2 \mid \{3\}]\),
- \((d)\) \([1 \perp 2 \mid \{3\}]\) implies \([1 \perp 3]\) or \([2 \perp 3]\).

The necessity of these axioms can be checked by simple calculations involving almost-principal minors of positive definite symmetric \(3 \times 3\)-matrices:

- \((a)\) \(\sigma_{12} = \sigma_{13}\sigma_{22} - \sigma_{12}\sigma_{23} = 0\) implies \(\sigma_{13} = \sigma_{12}\sigma_{33} - \sigma_{13}\sigma_{23} = 0\),
- \((b)\) \(\sigma_{12}\sigma_{33} - \sigma_{13}\sigma_{23} = \sigma_{13}\sigma_{22} - \sigma_{12}\sigma_{23} = 0\) implies \(\sigma_{12} = \sigma_{13} = 0\),
- \((c)\) \(\sigma_{12} = \sigma_{13} = 0\) implies \(\sigma_{12}\sigma_{33} - \sigma_{13}\sigma_{23} = \sigma_{13}\sigma_{22} - \sigma_{12}\sigma_{23} = 0\),
- \((d)\) \(\sigma_{12} = \sigma_{12}\sigma_{33} - \sigma_{13}\sigma_{23} = 0\) implies \(\sigma_{13} = 0\) or \(\sigma_{23} = 0\).

The sufficiency of these axioms was noted in \([22, \text{Example } 1]\).

For arbitrary \(n \geq 3\), a collection of almost-principal minors is called a **gaussoid** if it satisfies the axioms \((a)-(d)\), after relabeling and applying Schur complements. For instance, axiom \((a)\) is then written as follows: \([i \perp j \mid L]\) and \([i \perp k \mid \{j\} \cup L]\) implies \([i \perp k \mid L]\) and \([i \perp j \mid \{k\} \cup L]\).

This axiom is known as the **semigraphoid axiom**. See \([23]\) for a discussion.

A gaussoid is **representable** if it is the set of vanishing almost-principal minors of some matrix in \(\text{PD}_n\). For \(n = 3\) every gaussoid is representable by \([22, \text{Example } 1]\). For \(n = 4\), a complete classification of the representable gaussoids was given in \([20]\). We are here asking for the extension to \(n = 5\).

We now introduce a conceptual framework for our General Problem. For each subset \(S\) of \(\{1, 2, \ldots, n\}\) we introduce one unknown \(H_S\), and we define the **submodular cone** to be the solution set in \(\mathbb{R}^2^n\) of the system of linear inequalities

\[
H_{S \cup K} + H_{S \cup K} \leq H_{S \cup K} + H_K, \tag{4.3}
\]

where \(K\) is any subset of \(\{1, \ldots, n\}\) and \(i, j \in \{1, \ldots, n\} \setminus K\). We denote this cone by \(\text{SubMod}_n \subset \mathbb{R}^2^n\). Note that \(\text{SubMod}_n\) is a polyhedral cone living in a high-dimensional space while \(\text{PD}_n\) is a non-polyhedral cone in a low-dimensional space. Between these two cones we have the **entropy map**

\[
H : \text{PD}_n \to \text{SubMod}_n,
\]

which is given by the logarithms of all \(2^n\) principal minors of a positive definite matrix \(\Sigma = (\sigma_{ij})\). Namely, the coordinates of the entropy map are

\[
H(\Sigma)_I = -\log \det(\Sigma I),
\]
where $I$ is any subset of $\{1, \ldots, n\}$ and $\Sigma_I$ the corresponding principal minor. Note that the entropy map is well-defined because of the inequality

$$\det(\Sigma_{\{i\} \cup K}) \cdot \det(\Sigma_{\{j\} \cup K}) \geq \det(\Sigma_{\{i,j\} \cup K}) \cdot \det(\Sigma_K). \quad (4.4)$$

A matrix $\Sigma \in \mathbb{P}D_n$ satisfies (4.1) if and only if equality holds in (4.4) if and only if equality holds in (4.3). This implies the following result.

**Proposition 4.1.** The Gaussian conditional independence models are those subsets of the positive definite cone $\mathbb{P}D_n$ that arise as inverse images of the faces of the submodular cone $\text{SubMod}_n$ under the entropy map $H$.

The importance of the submodular cone for probabilistic inference with discrete random variables was highlighted in [23]. Here we are concerned with Gaussian random variables, and it is the geometry of the entropy map which we must study. We can thus paraphrase our problem as follows.

**General Problem:** Characterize the image of the entropy map $H$ and how it intersects the various faces of $\text{SubMod}_n$. Study the fibers of this map.

One approach to this problem is to work with the algebraic equations satisfied by the principal minors of a symmetric matrix. A characterization of these relations in terms of hyperdeterminants was proposed in [15]. What we are interested in here is the logarithmic image (or amoeba) of the positive part of the hyperdeterminantal variety of [15]. A reasonable first approximation to this amoeba is the tropicalization of that variety. More precisely, we seek to compute the positive tropical variety [24, §3.4] parametrically represented by the principal minors of a symmetric $n \times n$-matrix.

5. **Bonus Problem on Rational Points.** Section 4 dealt with conditional independence (CI) models for Gaussians. Our bonus problem concerns CI models for discrete random variables, thus returning to the setting of Section 2. Consider $n$ discrete random variables $X_1, X_2, \ldots, X_n$ with $d_1, d_2, \ldots, d_n$ states. Any collection of CI statements $X_i \perp \perp X_j | X_K$ specifies a determinantal variety in the space of tables

$$\mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2} \otimes \cdots \otimes \mathbb{C}^{d_n}. \quad (5.1)$$

We call such a variety a CI variety. It is the zero set of a large collection of $2 \times 2$-determinants. These constraints are well-known and listed explicitly in [12 §4.1] or [27, Proposition 8.1]. The corresponding strict CI variety is the set of tables for which the given CI statements hold but all other CI statements do not hold. Thus a strict CI variety is a constructible subset of which is Zariski open in a CI variety. The corresponding strict CI model is the intersection of the strict CI variety with the positive orthant. It consists of all positive $d_1 \times d_2 \times \cdots \times d_n$-tables that lie in a common equivalence class, where two tables are equivalent if precisely the same CI statements $X_i \perp \perp X_j | X_K$ are valid (resp. not valid) for both tables.

**Bonus Problem:** Does every strict CI model have a $\mathbb{Q}$-rational point?
This charming problem was proposed by F. Matúš in [21, page 275]. It suggests that algebraic statistics has something to offer also for arithmetic geometers. One conceivable solution to the Bonus Problem might say that CI models with no rational points exist but that rational points always appear when the number of states grows large, that is, for \( d_1, d_2, \ldots, d_n \gg 0 \). But that is pure speculation. At present we know next to nothing.

6. Brief Conclusion. This article offered a whirlwind introduction to the emerging field of algebraic statistics, by discussing a few of its numerous open problems. Aside from the Bonus Problem above, we had listed three Specific Problems whose solution might be particularly rewarding:

- Consider the variety of 4×4×4-tables of tensor rank at most 4. Do the known polynomial invariants of degree at most nine suffice to define this variety? Set-theoretically? Ideal-theoretically?
- Characterize all projective varieties whose maximum likelihood degree is equal to one.
- Which sets of almost-principal minors can be simultaneously zero for a positive definite symmetric 5×5-matrix?

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