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The 4-sample theorem on planar graphs

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The famous *4-color theorem* from graph theory says that the vertices of any planar graph can be colored with four colors, so that no adjacent vertices have the same color. The *4-sample theorem* from algebraic statistics says that the maximum likelihood estimator for a Gaussian graphical model of a planar graph exists with probability one, if one has at least four samples. This number of necessary samples, the *maximum likelihood threshold*, is a graph invariant from algebraic statistics and connected not only to parameter estimation, but also to matrix completion, rigidity theory, and matroid theory.

1 The 4-sample theorem from algebraic statistics

Statistics and algebra look back on a long joint history, maybe starting with Pearson's algebraic analysis of the distribution of crabs in the bay of Naples [2]. In the 21st century, algebraic statistics is both an exciting branch of statistics [16] and a vibrant community that continuously uncovers new connections between data science and algebraic, geometric and discrete structures in mathematics. Here we want to tell one such story, namely how the theory of estimation for multivariate normal distributions, through topics like matrix completion and rigidity theory, is connected to basic invariants of graphs. In this snapshot we are mostly intereted in planar graphs, that is, graphs that can be drawn in the plane so that no two edges cross. The (very convincing) name of the following theorem was suggested by Steffen Lauritzen during the 2022 Oberwolfach Workshop *Algebraic Structures in Statistical Methodology.*

Theorem 1.1 (4-sample theorem, [11, Corollary 3.11])**.** Let G be a planar graph. If there are at least four samples from a distribution in the Gaussian graphical model of G, the maximum likelihood estimator exists almost surely.

The number of vertices of the graph G corresponds to the number of Gaussian random variables (or *covariates*). One exciting consequence of the theorem is that the number of required samples does not depend on the number of covariates. This is important in biological applications and machine learning, which both feature a very large number of variables and very few samples.

2 Gaussian graphical models

Consider a random vector $X = (X_1, X_2, \dots, X_m)$ with a multivariate normal distribution. This means that the probability that X takes values in a subset of $\mathbb{R}^m$ is determined by a *mean* parameter $\mu \in \mathbb{R}^m$ and a symmetric positive definite (PD) *covariance matrix* $\Sigma \in \mathrm{PD}_m$. To simplify matters, we can assume here that each of our variables is centered, so that $\mu = 0$ in what follows and the distribution is completely determined by Σ.

We receive n samples of X and wish to make estimation about the distribution of X. Here we should think of m as being large compared to the sample size n.

Such an estimation is most often based on model assumptions. A very extensively used class of models are *Gaussian graphical models.* Here we use undirected simple graphs G on the vertex set $\{1, 2, \dots, m\}$ and each vertex corresponds to one component of X. Intuitively, an edge (or by extension, connectivity) in G should represent interaction or dependence of the corresponding covariates. The Gaussian graphical model associated to G is the set of all multivariate normal distributions whose covariance matrices lie in the set

$$\mathcal{M}(G) = \left\{ \Sigma \in \mathrm{PD}_m : \Sigma^{-1}_{ij} = 0 \text{ for } ij \notin E(G) \right\}.$$

In other words, we say that a covariance matrix belongs to the model if its inverse has a zero in the entry (i, j) whenever there is no edge between i and j in G. [1] For example, consider $G = C_4$ to be the 4-cycle below:

[1] This condition is natural because it is equivalent to the statement that X_i is *conditionally independent* of X_j given the rest of the components of the Gaussian vector X.

$$
\begin{tikzcd}
1 \arrow[r, dash] \arrow[d, dash] & 2 \arrow[d, dash] \\
4 \arrow[r, dash] & 3
\end{tikzcd}
$$

Then

$$
\mathcal{M}(C_4) = \left\{ \Sigma \in \mathrm{PD}_4 : \Sigma^{-1} = \begin{pmatrix} * & * & 0 & * \\ * & * & * & 0 \\ 0 & * & * & * \\ * & 0 & * & * \end{pmatrix} \right\}.
$$

We can describe this model by conditions on the entries of Σ itself, namely by the two equations:

$$
\begin{aligned}
\sigma_{13}\sigma_{24}^2 + \sigma_{14}\sigma_{22}\sigma_{34} + \sigma_{12}\sigma_{23}\sigma_{44} - \sigma_{14}\sigma_{23}\sigma_{24} - \sigma_{12}\sigma_{24}\sigma_{34} - \sigma_{13}\sigma_{22}\sigma_{44} = 0 \\
\sigma_{13}^2\sigma_{24} + \sigma_{12}\sigma_{14}\sigma_{33} + \sigma_{11}\sigma_{23}\sigma_{34} - \sigma_{13}\sigma_{14}\sigma_{23} - \sigma_{11}\sigma_{24}\sigma_{33} - \sigma_{12}\sigma_{13}\sigma_{34} = 0
\end{aligned}
$$

These nice cubic polynomials are 3×3-minors obtained from the adjugate matrix of Σ. The appearance of polynomials as defining equations of statistical models is a mantra in algebraic statistics.

3 Estimating the graph from data

In practical applications, the graph G is often unknown. The estimation would then proceed in two steps. First, a graph G is estimated (potentially together with an initial estimate of Σ). Then maximum likelihood estimation[2] for the graphical model $\mathcal{M}(G)$ is based on that graph. A common method for the first step is the *graphical LASSO* [8] which works with the penalized likelihood function for the inverse covariance matrix $K = \Sigma^{-1}$:

$$
\log \det(K) - \mathrm{tr}(SK) - \beta \|K\|_1.
$$

The term $\|K\|_1$ measures (twice) the size of entries corresponding to the potential edges of G. The maximizer of this function over all matrices $K \in \mathrm{PD}_m$ is found numerically. Solving this optimization problem comes with its own set of practical problems which we do not consider here. The penalization parameter β is picked empirically based on the common principle “let’s see what works”. The larger β is, the more expensive having an edge is, so a large β results in a sparse graph. Once an optimal K is found, one can in principle invert that K and use it as an estimate for Σ, but because of the penalty term, this is not the

[2] We will not go into the details of maximum likelihood estimation here. It is arguably the most common estimation method in parametric statistics and also featured in MFO Snapshot No 1/2018 by Anna Seigal [14].

maximum likelihood estimate. It does make sense, though, to use the graph G whose edges are those ij such that $K_{ij} \neq 0$ for the estimated K, and then perform maximum likelihood estimation in $\mathcal{M}(G)$. However, the question arises whether the *maximum likelihood estimate* (MLE) even exists.

A concrete example of this approach is in [18]. The authors consider a climate network grid with 2562 nodes (variables) and they have 756 samples, which are real vectors of length 2562. They want to estimate both the graph structure and the parameters of the corresponding Gaussian graphical model. They employ the graphical LASSO, and they find that the MLE doees exist. The results in this snapshot explain why and how the existence of the MLE is connected to the structure of the graph.

As always in mathematics, it is useful to first give a name to the thing one wants to study. Algebraic statisticians have coined the term *maximum likelihood threshold (MLT)* for the number of samples that is necessary to have an MLE with probability one. See Definition 4.1. Interestingly, this number is independent of the concrete data (up to events of probability zero). An even more interesting fact is, that this number only depends on certain graph theoretic invariants and thus becomes independent of the concrete number of covariates, as long as the graph structure does not change too much. Practical examples to keep in mind are the various meshes and grids that are used for discretization in numerical simulations and spatial measurements. Here one models interaction between neighbors and not over longer distances. The graph structure that is independent of the number of vertices is that locally, the graph always looks the same. For example, in a square grid every vertex has exactly four neighbors.

Classical results in statistics did not consider the graph structure. For example, it has long been known that if the number of samples exceeds the number of covariates, then the MLE exists with probability one. This goes back to the theory of exponential families of Barndorff-Nielsen and Dempster. The input for inference algorithms is the *empirical covariance matrix* S, computed from the vector valued observations. This matrix need not be positive definite (like an actual covariance matrix). In fact, if the number of samples is less than the number of covariates, it is always rank deficient because then S is a sum of n rank-one matrices.

Theorem 3.1 ([6, Theorem 2.1])**.** The MLE exists with probability one in $\mathcal{M}(G)$ if and only if the empirical covariance matrix S restricted to the diagonal entries and the entries corresponding to edges of G has a PD-completion.

Here the *PD-completion* is a positive definite matrix that has the same entries like S on the diagonal and in those positions whose index pair (i, j) corresponds to an edge in the graph G. If the number of samples exceeds the number of variables, the sample covariance matrix itself is PD and thus a PD-completion with probability one.

For many modern applications, e.g. in biology, the number of variables n is *very large* and gathering samples is *very expensive*. It is therefore natural to ask for MLE existence results that are independent of n. That such bounds exist and that they are connected to graph theory became clear already in the 1990s in [6], but only recently, through the connection to and renewed interest in matrix completion, several breakthroughs have been possible. In particular the matrix completion problem in Theorem 3.1 has been connected to rigidity theory of graphs in the work of Bernstein, Gross, Sullivant and others [4, 5, 11].

Example 3.2. When data has a spatial interpretation, grids are very natural as they arise from discretization of a two-dimensional space where due to some physical model the interaction of variables is restricted to locations that are close in distance. As it turns out, for any graphical model of a rectangular grid, four samples suffice for the MLE to exist with probability one, no matter the size of the grid.

To illustrate the PD-completion, consider the small 2×3 grid below. The six vertices mean that we deal with a 6×6-completion problem.

$$\begin{tikzcd}
1 \arrow[r, dash] \arrow[d, dash] & 2 \arrow[r, dash] \arrow[d, dash] & 3 \arrow[d, dash] \\
4 \arrow[r, dash] & 5 \arrow[r, dash] & 6
\end{tikzcd}$$

Consider the following partial symmetric matrices:

$$\begin{pmatrix}
6 & 1 & & -2 & & \\
1 & 4 & 2 & & 3 & \\
 & 2 & 2 & & & 3 \\
-2 & & & 5 & 1 & \\
 & 3 & & 1 & 5 & -5 \\
 & & 3 & & -5 & 10
\end{pmatrix}
\qquad
\begin{pmatrix}
6 & 1 & & -2 & & \\
1 & 4 & 2 & & 3 & \\
 & 2 & 2 & & & 3 \\
-2 & & & 5 & 1 & \\
 & 3 & & 1 & 5 & -5 \\
 & & 3 & & -5 & 5
\end{pmatrix}$$

The entries that are left out correspond exactly to the non-edges of the grid. The completion in Theorem 3.1 means filling in these entries so that the resulting matrix is positive definite. Whether this is possible can depend on the exact matrix. In fact, the matrix on the right is *not* PD-completable because its last 2×2 minor in the bottom right is $5 \cdot 5 - (-5) \cdot (-5) = 0$. By contrast, the matrix on the left has a PD-completion (can the reader find one?). In such a small example, the MLE could be computed by solving the likelihood equations. For larger matrices one uses approximation algorithms like iterative proportional scaling [13, 15]. The key insight is that *generically*, we will always be in the situation on the left, once the sample covariance matrix has been computed from enough samples. The sporadic cases like the one on the right happen with probability zero and arise for example if by chance all samples would be exactly equal. Whether almost all sample covariance matrices can be completed does only depend on G and the number of samples n.

4 The maximum likelihood threshold

As explained above, the maximum likelihood threshold of a graph is the least number of samples required so that the maximum likelihood estimate in the Gaussian graphical model exists with probability one.

Let $\mathrm{Sym}(m, n)$ be the set of symmetric $m \times m$-matrices of rank at most n. These matrices arise as sample covariance matrices for n observations.

Definition 4.1. The *maximum likelihood threshold* $\mathrm{mlt}(G)$ of a graph G is the smallest n such that for almost all $\Sigma_0 \in \mathrm{Sym}(m, n)$ there exists a $\Sigma \in \mathrm{PD}_m$ that *completes* Σ_0 in the sense that

$$\Sigma_{ij} = (\Sigma_0)_{ij} \qquad \text{for all } ij \in E(G) \text{ or } i = j. \tag{1}$$

Definition 4.1 is attractive because it defines a *graph invariant* – $\mathrm{mlt}(G)$ is a specific number that we want to know for each graph G. There is no general method known to compute $\mathrm{mlt}(G)$ given G. So far the community has focused on providing combinatorial bounds.

From Theorem 3.1 it is clear that $\mathrm{mlt}(G)$ is bounded by the number of vertices of G and this bound is achieved for the complete graph: $\mathrm{mlt}(K_n) = n$, but for applications such as the ones outlined above, it is desirable to bound $\mathrm{mlt}(G)$ *independent of the number of vertices*, or in terms of graph invariants.

Such results existed before the new developments that we report on here. For example, it was known that, if G is a chordal graph (one with no induced cycles of length ≥ 4), then the completion exists if and only if all submatrices of Σ_0 corresponding to maximal cliques of G are positive definite [10]. The algebraic statistics community got interested in this problem maybe in 2008, when Steffen Lauritzen posted the benchmark problem of understanding the maximum likelihood threshold for the 3×3-grid (which is obviously not chordal). See [17].

Improved combinatorial bounds have been achieved by transforming the problem again, this time to a geometric problem! The question of determining $\mathrm{mlt}(G)$ can be formulated as a question about geometric structures made of rigid bars connected at freely rotating joints. This is *rigidity theory*. We come back to it in Section 6 after talking about planar graphs which are crucial for the 4-sample theorem (Theorem 1.1).

5 Planar graphs

The first reduction in the proof of Theorem 1.1 arises from considering only *maximal planar graphs*. These are planar graphs, such that adding any further edge makes them non-planar. To every planar graph, one can add edges until it is a maximal planar graph. It can be checked that the number of edges of a maximal planar graph with m vertices is $3m - 6$. If G is maximal planar, then all regions arising when drawing the graph have exactly three sides. This also applies to the unbounded outside region. Note that this does not imply that the graph is chordal. The chordal maximal planar graphs are exactly the so-called *Apollonian networks*. Additionally, any maximal planar graph is 3-*connected*, meaning that it stays connected after removing 3 or fewer vertices. An interesting maximal planar graph is the Goldner–Harary graph in Figure 1.

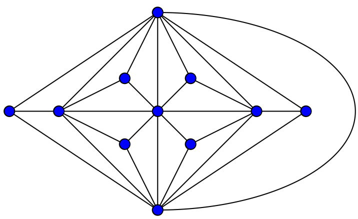


Figure 1: The Goldner–Harary graph is a (chordal) maximal planar graph on 11 vertices and with $27 = 3 \cdot 11 - 6$ edges. It was discovered in the search of small simplicial polyhedron with no Hamiltonian cycles [12, Section 17.1] and [9].

To prove the 4-sample theorem, we can assume that G is maximal planar because, according to Definition 4.1, adding edges to G increases the number of constraints and therefore $\mathrm{mlt}(G)$ can only go up.

6 Graphs and frameworks

Our goal below is to reduce Theorem 1.1 to another break-through theorem of two algebraic statisticians: Elizabeth Gross and Seth Sullivant. Their result, Theorem 6.2 below, is about *frameworks*, i.e. embeddings of the vertices (and thus the entire graph) in affine space, where one can then argue about angles and lengths.

Definition 6.1. A *framework* in $\mathbb{R}^d$ is a pair (G, p) where G is a graph with m vertices and p is a collection of m points $p_1, \ldots, p_m \in \mathbb{R}^d$. Two frameworks

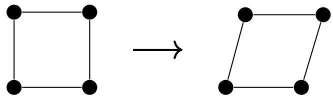


Figure 2: Two equivalent frameworks of 4 points in $\mathbb{R}^2$ that are not congruent.

(G, p) and (G, q) for the same graph are *equivalent* if, for each edge $ij \in E(G)$, the distance between points i and j agrees, i.e. $\|p_i - p_j\| = \|q_i - q_j\|$.

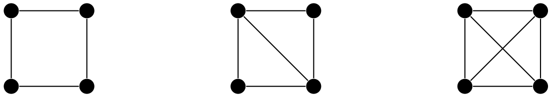
Equivalence is a somewhat weaker notion than that of *congruence*. Two frameworks are *congruent* if there exists an isometry of Euclidean space mapping one onto the other. To formulate rigidity of frameworks, one considers continuous changes to the points $p = (p_1, \ldots, p_m) \in \mathbb{R}^{md}$ so that all frameworks along the continuous deformation are equivalent. A framework is *rigid* if any two equivalent frameworks arising from such a continuous deformation are congruent. For example, a triangle is rigid but a square is not, as seen in Figure 2.

Let us also consider the following complementary property. A framework is *independent* if for any choice of an edge and any sufficiently small $\varepsilon > 0$, there exists a framework with the same graph but such that the chosen edge has its length modified by ε while all other lengths stay the same.

These two notions are very much analogous to sets of vectors being independent or spanning in linear algebra (or, more abstractly, in *matroid theory*). A framework is *isostatic* if it is both rigid and independent (think: a basis). This is consistent with the intuition that a framework is more rigid if it has more edges and more independent if it has fewer edges. If a framework is isostatic, removing any edge from it makes it non-rigid and adding any edge makes it dependent.

While it is conceivable that the rigidity of a framework for a given graph could depend on the concrete framework chosen, this is not the case. One can consider the space of all frameworks in fixed dimension for a given graph, and in principle there could be complicated regions of rigid frameworks and non-rigid frameworks. Fortunately, it has been known since the 1970s [3] that for a fixed graph, either almost all d-dimensional frameworks with that graph are rigid, or almost all are not rigid. This means that we can treat rigidity of a framework as a property of its graph.

Independence of frameworks is not directly a graph property, though. For every graph G there does exist an independent framework with that graph, e.g. by choosing a framework in $\mathbb{R}^n$ where n is the number of edges of G. Generally, one wants to minimize the dimension and the result depends on the graph. A graph G is *d-independent* if that d is the minimal dimension for which an independent framework with graph G exists. For example, the square is 2-independent because it can be embedded in the plane as an independent framework, albeit not rigid. Any edge can be made a little shorter or longer, while keeping the combinatorics and the other edge lengths (just the angles would change). [3] The diamond graph with one added edge is still 2-independent, but the complete graph on the right is not. The diamond graph is isostatic – rigid and 2-independent.



We can now restate [11, Theorem 1.2] from Gross and Sullivant as follows.

Theorem 6.2. If a graph G is $(n-1)$-independent, then $\mathrm{mlt}(G) \le n$.

Therefore, if we show that any (maximal) planar graph can be realized by an independent framework in 3-space, we are able to conclude the 4-sample theorem. This is what we aim for in the next section.

7 Proof of the 4-sample theorem

Let G be a maximal planar graph. The celebrated Steinitz-Theorem from 1916 says that the graphs of 3-dimensional polytopes are precisely the finite 3-connected planar graphs. Since G is 3-connected, there exists a 3-dimensional polyhedron whose graph is G. Of course, we now view the vertices of this polyhedron as a framework in $\mathbb{R}^3$, but is it rigid?

At this point, we employ a theorem of Cauchy which originated in Euclid's Elements and has a proof from THE BOOK [1, Chapter 14] (at least after Steinitz, Schoenberg, and Aleksandrov ironed out all the issues in Cauchy's proof of the main lemma). That theorem says that if two 3-dimensional convex polytopes have the same graphs and under that correspondence of graphs, all facets are pairwise congruent (as 2-dimensional convex polygons), then the 3-dimensional polytopes are congruent. In particular the framework is rigid. [4]

There is an experiment illustrating this. In this experiment one builds a graph of a 3-dimensional polytope from pieces of maccheroni (or other rigid tubes) and connects the edges in a flexible way, e.g. by running a thread through all edges. A cube built like this will just fall flat, but a tetrahedron will be rigid. Dehn has shown in 1916 that *simplicial* polytopes are infinitesimally

[3] Of course, one also needs to check that the square cannot be embedded as an independent framework in $\mathbb{R}$.

[4] In the world of non-convex polyhedra there also exist *flexible* polyhedra which have an interesting history too.

rigid [7], which implies the result of the experiment. This differs from Cauchy's rigidity because here the 2-dimensional faces themselves can be deformed, while in Cauchy's theorem they are rigid.

Back in the proof, since maximal planar graphs subdivide the plane into triangles, our polytope with graph G is a simplicial polytope – all of its faces are triangles. By the SSS-Theorem [5], each face is rigid. Hence Cauchy's theorem can be applied.

We have produced a rigid framework from the 3-polytope from the maximal planar graph G. In $\mathbb{R}^3$ the minimal number of edges of a rigid framework turns out to be $3m - 6$. By this minimality, our framework is isostatic and hence G is 3-independent. Using Theorem 6.2 we have achieved $\mathrm{mlt}(G) \leq 4$. $\square$

8 Conclusion, Questions, Outlook

Graphical models associated to planar graphs are very important in spatial statistics. The 4-sample-theorem shows that a small constant number of samples suffices to consistently do estimation in these models.

In some applications it might still be too much to ask for the MLT to exist almost surely, and a positive probability of existence would suffice. This is captured by the *weak maximum likelihood threshold*. For example, the weak MLT of any square-grid graph such as the one in Example 3.2 is 2 while the MLT is 3.

The bound in Theorem 1.1 is sharp, and there exist examples of planar graphs for all values of the MLT. A graph with no edges, corresponding to the model of total independence, satisfies $\mathrm{mlt} = 1$. Any tree T has $\mathrm{mlt}(T) = 2$, the four cycle C_4 has $\mathrm{mlt}(C_4) = 3$ and finally K_4 satisfies $\mathrm{mlt}(K_4) = 4$.

As always, the mathematical story continues. Matroid theory is a crucial tool to express the independence that surfaced in the proof, and is widely recognized as the right language to talk about rigidity and the MLT as a graph invariant. This connection is actively being developed. See [4] for recent bounds on $\mathrm{mlt}(G)$ in terms of rigidity theoretic properties of G.

Algebraic statistics also contributes back to graph theory. The new graph invariant $\mathrm{mlt}(G)$ can be studied in terms of common constructions from graph theory, such as glueing, subgraphs, minors, etc. The MLT is minimal on the empty graph, maximal on the complete graph and monotonous on the edge set, meaning that if H, G are both graphs on the same vertex set and the edge set of H is contained in that of G, then $\mathrm{mlt}(H) \leq \mathrm{mlt}(G)$. It is not known, however, whether the property $\mathrm{mlt}(G) \leq n$ has a characterization by forbidden minors.

[5] The Side-Side-Side theorem states that two triangles with equal corresponding side lengths must be congruent.

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