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PROOF OF A CONJECTURE OF STURMFELS, TIMME AND ZWIERNIK

LAURENT MANIVEL

ABSTRACT. We prove a conjecture of Sturmfels, Timme and Zwiernik on the ML-degrees of linear covariance models in algebraic statistics. As in our previous works on linear concentration models, the proof ultimately relies on the computation of certain intersection numbers on the varieties of complete quadrics.

1. INTRODUCTION

In algebraic statistics, there is a notion of maximum likelihood estimation whose complexity is governed by a fundamental invariant called maximum likelihood degree or *ML-degree* (see e.g. [St21, SU10, HS14] for an introduction). This degree depends very much on the statistical model; here we consider the so-called linear covariance models, whose ML-degree defines a rather mysterious invariant of a space of symmetric matrices. These models are very different from the linear concentration models considered in [MMMSV20], for which we obtained quite explicit polynomial formulas for the generic ML-degrees, proving conjectures of Sturmfels-Uhler and Nie-Ranestad-Sturmfels. In this note we use closely related techniques to compute, in small dimension, the generic ML-degree of a linear covariance model. This degree can be defined very explicitly as follows [STZ20, Proposition 3.1].

Let us denote by \mathbb{S}_n the vector space of complex symmetric matrices of size n . It is endowed with the standard scalar product $\langle A, B \rangle = \text{Tr}(AB)$.

Definition 1. *Consider a subspace $\mathcal{L} \subset \mathbb{S}_n$, of dimension m . The ML-degree of \mathcal{L} is the number of solutions, for S a generic symmetric matrix, of the following system of linear and quadratic equations in K and Σ :*

$$(1) \quad \Sigma \in \mathcal{L}, \quad K\Sigma = I_n, \quad KSK - K \in \mathcal{L}^\perp.$$

We will compute the ML-degree ML_m for \mathcal{L} generic of dimension m up to four.

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Theorem 2. *For $m \leq 4$, the ML-degree ML_m of a generic linear concentration model of dimension m is:*

$$\begin{aligned} (2) \quad ML_2 &= 2n - 3, \\ (3) \quad ML_3 &= 3n^2 - 9n + 7, \\ (4) \quad ML_4 &= \frac{11}{3}n^3 - 18n^2 + \frac{85}{3}n - 15. \end{aligned}$$

Statement (1) was proved in [CMR20]. Statements (2) and (3) were conjectured in [STZ20, Conjecture 4.2].

As in [MMMSV20] we will reduce the problem of computing ML_m to a computation on the space of complete quadrics. There are two main difficulties. First, one has to understand the contributions of the exceptional divisors, dominating the loci of symmetric matrices of a given rank; up to dimension $m = 4$, only corank one and two need to be taken into account, which strongly simplifies the problem. Second, we need to make an intersection product in a situation which is not quite generic, and we need to be cautious about the transversality conditions that are required to make the computation meaningful. Let us start with a brief reminder on complete quadrics.

2. COMPLETE QUADRICS

The space of complete quadrics CQ_n is a compactification of the space of invertible symmetric matrices (up to scalar) $\mathbb{P}(\mathbb{S}_n)^\circ \subset \mathbb{P}(\mathbb{S}_n)$, or equivalently, of smooth quadrics in \mathbb{P}^{n-1} , which is well-suited for enumerative geometry. Denote by $D_i \subset \mathbb{P}(\mathbb{S}_n)$ the degeneracy locus consisting of matrices of rank at most i , an irreducible variety whose singular locus is D_{i-1} . Note that by mapping a rank i matrix to its image, we get a morphism from $D_i - D_{i-1}$ to the Grassmannian $Gr(i, n)$, which is an open subset of the vector bundle $S^2\mathcal{U}$ for \mathcal{U} the tautological vector bundle of rank i . We will also denote by \mathcal{Q} the tautological quotient bundle of rank $n - i$ on $Gr(i, n)$.

Definition 3. *The space of complete quadrics CQ_n is the successive blow-up of $\mathbb{P}(\mathbb{S}_n)$ along the degeneracy loci:*

$$CQ_n = Bl_{\tilde{D}_{n-2}} \cdots Bl_{\tilde{D}_2} Bl_{D_1} \mathbb{P}(\mathbb{S}_n),$$

where \tilde{D}_i is the (smooth) proper transform of D_i by the previous blow-ups.

See [MMMSV20] and references therein for more details and other equivalent definitions. We will denote by $N = \binom{n+1}{2} - 1$ the dimension of CQ_n and of $\mathbb{P}(\mathbb{S}_n)$.

Note that by construction, CQ_n admits a natural basis (over \mathbb{Q}) of divisors E_1, \dots, E_{n-1} consisting of the strict transforms of the exceptional divisors of the successive blow-ups, plus E_{n-1} which is the proper transform of the determinant hypersurface of singular matrices. These divisors are smooth

and meet transversally in the variety of complete quadrics. They give to CQ_n a kind of Russian doll structure since one can show that

$$E_i \simeq CQ_i(\mathcal{U}) \times_{G(i,n)} CQ_{n-i}(\mathcal{Q}^\vee).$$

One of the most useful properties of C_n is that it factorizes the inversion morphism ι for symmetric matrices: there is a commutative diagram

$$\begin{array}{ccc} & CQ_n & \\ p \swarrow & & \searrow q \\ \mathbb{P}(\mathbb{S}_n) & \xrightarrow{\iota} & \mathbb{P}(\mathbb{S}_n), \end{array}$$

where p is the cascade of blow-ups that defines CQ_n , while q is obtained by contracting the exceptional divisors in reverse order, first E_2 to D_{n-2} , and so on up to E_{n-1} contracting to D_1 (note that the comatrix of a matrix of corank one is a rank one matrix). In particular p and q identify to $\mathbb{P}(\mathbb{S}_n)^\circ$ the complement CQ_n° of the union of the exceptional divisors in CQ_n . Of course this diagram is compatible with the relative product structure of each of the exceptional divisors E_i , that admit a natural contraction map to

$$F_i \simeq \mathbb{P}(S^2\mathcal{U}) \times_{G(i,n)} \mathbb{P}(S^2\mathcal{Q}^\vee).$$

Finally, we will need to know that the pull-backs H_1 and H_{n-1} of the hyperplane divisors on $\mathbb{P}(\mathbb{S}_n)$ by p and q are given in terms of the exceptional divisors by the formulas

$$nH_1 = (n-1)E_1 + (n-2)E_2 + \cdots + E_{n-1},$$

$$nH_{n-1} = E_1 + 2E_2 + \cdots + (n-1)E_{n-1}.$$

In fact they are part of an alternative \mathbb{Q} -basis $(H_1, H_2, \dots, H_{n-1})$ of the Picard group of CQ_n , where H_k is obtained by pulling-back the hyperplane divisor by the morphism defined by the $k \times k$ minors of the generic matrix (or the $(n-k) \times (n-k)$ minors of the inverse matrix).

Now we will try to reduce the computation of the generic ML-degree to an enumerative problem on the variety of complete quadrics.

3. DEGENERACY LOCUS INTERPRETATION

Recall that our main goal is to count the number of solutions of the system of equations (1). We can replace K by KS and Σ by $S^{-1}\Sigma$, and get rid of S by noticing that $\mathcal{L}^\perp S = (S^{-1}\mathcal{L})^\perp$. So our problem is equivalent to counting the number of solutions, for \mathcal{L} generic, of the system

$$(5) \quad \Sigma \in \mathcal{L}, \quad K\Sigma = I_n, \quad K^2 - K \in \mathcal{L}^\perp.$$

After homogeneizing, the last condition simply means that we want $[K] \in \mathbb{P}(\mathbb{S}_n)^\circ$ to be such that K^2 is proportional to K modulo $\mathcal{M} := \mathcal{L}^\perp$. This makes sense on CQ_n and we would be tempted to try to count the number of points $Q \in CQ_n$ verifying the previous conditions for $[K] = p(Q)$ and $[\Sigma] =$

$q(Q)$. The proportionality condition may be interpreted as a degeneracy condition for the morphism between vector bundles on CQ_n given by

$$\phi_{\mathcal{M}} : \mathcal{O}_{CQ_n}(-L_1) \oplus \mathcal{O}_{CQ_n}(-2L_1) \xrightarrow{(K, K^2)} \mathcal{O}_{CQ_n} \otimes \mathbb{S}_n / \mathcal{M}.$$

Let $D(\phi_{\mathcal{M}})$ denote the degeneracy locus in CQ_n , where this morphism is not injective. By definition

$$ML_m = \# \left(D(\phi_{\mathcal{M}}) \cap q^{-1}\mathbb{P}(\mathcal{L})^\circ \right),$$

where the exponent means that we restrict to invertible matrices in \mathcal{L} .

Recall that the expected codimension of the degeneracy locus of a morphism between vector bundles is the difference between their ranks plus one. Here this gives $m - 2 + 1 = m - 1$, which is the dimension of $\mathbb{P}(\mathcal{L})$. So we expect, if everything goes fine, a finite number of intersection points. Moreover these points should be smooth points, which means that the intersection of $D(\phi_{\mathcal{M}})$ and $q^{-1}\mathbb{P}(\mathcal{L})$ should be transverse at every such point. This would necessarily be the case, by general arguments, if we could replace $\mathbb{P}(\mathcal{L})$ by some $\mathbb{P}(\mathcal{L}')$ (of the same dimension) that could be chosen generically. But here \mathcal{L} is directly involved in the definition of $\phi_{\mathcal{M}}$, so we have to be careful. We prove the following statement.

Lemma 4. *For \mathcal{L} generic, the intersection of $D(\phi_{\mathcal{M}})$ with $q^{-1}\mathbb{P}(\mathcal{L})^\circ$ is everywhere transverse.*

Proof. By the general irreducibility argument, it suffices to exhibit one transverse intersection point, for some \mathcal{L} . We will suppose that the identity matrix I_n belongs to \mathcal{L} and that our intersection point is given by $K_0 = I_n$. Then $K = I_n + J$ is tangent to the locus where K^2 is proportional to K modulo \mathcal{L}^\perp iff J belong to \mathcal{L}^\perp . Since the inverse of K is $I_n - J$ at first order, the transversality condition will be verified as soon as $\mathcal{L} \cap \mathcal{L}^\perp = 0$. This means that the standard scalar product on \mathbb{S}_n must remain non degenerate when we restrict it to \mathcal{L} , which is clearly the case in general. \square

Note that this immediately implies that the intersection of $D(\phi_{\mathcal{M}})$ with CQ_n° has the expected codimension. Indeed, if its dimension was bigger than expected, it would have to intersect in $\mathbb{P}(\mathbb{S}_n)$ any linear space of dimension $m-1$ along a positive dimensional subvariety, and the transversality property could not hold.

This being established, if we could prove that $D(\phi_{\mathcal{M}})$ and $q^{-1}\mathbb{P}(\mathcal{L})$ intersect only in $CQ_n^\circ \simeq \mathbb{P}(\mathbb{S}_n)^\circ$, we would conclude that ML_m can be computed from the intersection theory of CQ_n . Indeed, if $D(\phi_{\mathcal{M}})$ is of the expected codimension $m - 1$, its fundamental class in the Chow ring of CQ_n is given by the Thom-Porteous formula [Fu98, Chapter 14]:

$$[D(\phi_{\mathcal{M}})] = c_{m-1}(\mathcal{O}_{CQ_n} \otimes \mathbb{S}_n / \mathcal{M} - (\mathcal{O}_{CQ_n}(-H_1) \oplus \mathcal{O}_{CQ_n}(-2H_1))).$$

Here we need to recall that the Chern class of a formal difference $E - F$ between two vector bundles E and F is simply $c(E - F) = c(E)/c(F)$, the

quotient of their full Chern classes. Since $c(E)$ and $c(F)$ are graded series starting with one in degree zero, this quotient can be expanded formally and $c_k(E - F)$ is the term of degree k . In our setting E is trivial, so we simply get the inverse of the Chern class of F , which is the Segre class of F^\vee . We would therefore deduce that the ML-degree coincides with

$$ML_m^{(0)} = \int_{CQ_n} [D(\phi_{\mathcal{M}})] H_{n-1}^{N-m+1} = \int_{CQ_n} s_{m-1}(H_1, 2H_1) H_{n-1}^{N-m+1}.$$

We will soon see that this identity is utterly wrong – but can be corrected. Of course the problems come from the exceptional divisors.

4. FIRST EXCEPTIONAL DIVISOR

When a matrix K has rank one, K^2 is always proportional to K . Thus $D(\phi_{\mathcal{M}})$ always contains E_1 , which is certainly not of the expected codimension! More precisely $K^2 = \text{trace}(K)K$, so if we replace K^2 by $K^2 - \text{tr}(K)K$ in $\phi_{\mathcal{M}}$, the second component factorizes through $\mathcal{O}(-2H_1 + E_1)$, which turns out to be $\mathcal{O}_{CQ_n}(-H_2)$ (see [MMMSV20]): indeed, 2×2 minors span the linear system of quadrics vanishing on rank one matrices. Hence a morphism

$$\phi'_{\mathcal{M}} : \mathcal{O}_{CQ_n}(-H_1) \oplus \mathcal{O}_{CQ_n}(-H_2) \longrightarrow \mathcal{O}_{CQ_n} \otimes \mathbb{S}_n / \mathcal{M},$$

which coincides with $\phi_{\mathcal{M}}$ outside E_1 .

Lemma 5. *For \mathcal{L} generic, $D(\phi'_{\mathcal{M}}) \cap q^{-1}\mathbb{P}(\mathcal{L})$ does not meet E_1 .*

Proof. We make a local computation on E_1 , over the rank one matrix $K = e_1^2$, where e_1 is the first vector in the canonical basis of \mathbb{C}^n . In other words, the entries of K are $K_{ij} = \delta_{i1}\delta_{j1}$. Locally around $[K]$ in $\mathbb{P}(\mathbb{S}_n)$ we get local coordinates by restricting to matrices X with $X_{11} = 1$, and D_1 is cut out by the local equations $X_{ij} = X_{1i}X_{1j}$, for $i, j \geq 2$. We can therefore describe the blowup along D_1 locally around $[K]$ as the set of pairs $(X, [Y])$ with $Y = (Y_{ij})_{i,j \geq 2} \in \mathbb{S}_{n-1}$ a nonzero symmetric matrix such that $X_{ij} - X_{1i}X_{1j} = tY_{ij}$ for all i, j , for some scalar t . A straightforward computation then shows that

$$X^2 - \text{tr}(X)X = t \begin{pmatrix} -\text{tr}(Y) & 0 \\ 0 & Y \end{pmatrix} + \mathcal{O}(t^2).$$

Since $(t = 0)$ is the equation of the exceptional divisor E_1 on the blowup, the fact that t factorizes confirms that the morphism can be extended from $\mathcal{O}(-2H_1)$ to $\mathcal{O}(-2H_1 + E_1)$, which amounts precisely to dividing the above expression by t . Then letting $t = 0$, we get the morphism $\phi'_{\mathcal{M}}$ restricted to E_1 , and we see that its image at $([K], [Y])$ is the pencil $\langle K, Y \rangle$ of matrices generated by K and Y (the latter being considered as a matrix in \mathbb{S}_n by letting $Y_{1i} = 0$ for all i).

So our claim amounts to saying that for \mathcal{L} general there is no pair of non zero matrices $(K, Y) \in D_1 \times D_{n-1}$, with $KY = 0$, such that $Y \in \mathcal{L}$ and $\langle K, Y \rangle \cap \mathcal{L}^\perp \neq \emptyset$. In order to prove this, it is enough to check that the set S of triples $([K], [Y], \mathcal{L})$ verifying the previous conditions has dimension smaller

than $m(N+1-m)$: since this number is the dimension of the Grassmannian G of m -dimensional subspaces of \mathbb{S}_n , the image of the projection of S to G will have to be a proper subset of G , proving the claim.

In order to estimate the dimension of S , we will of course project it to F_2 , whose dimension is $N-1$. So we fix $([K], [Y])$ and we ask \mathcal{L}^\perp to be contained in Y^\perp and to meet $\langle K, Y \rangle$ non trivially.

There are two cases. If $\langle K, Y \rangle \cap Y^\perp$ is a line D , we need $D \subset \mathcal{L}^\perp \subset Y^\perp$, so that \mathcal{L} belongs to a Grassmannian of dimension $(m-1)(N-m)$. Adding the parameters for $([K], [Y])$, we get $(m-1)(N-m) + (N-1) = m(N+1-m) - 1 = \dim(G) - 1$, as required. If $\langle K, Y \rangle \subset Y^\perp$, then \mathcal{L}^\perp has to belong to the Grassmannian of dimension $N+1-m$ subspaces of Y^\perp , which has dimension $(m-1)(N+1-m)$, and meet a plane non trivially, which is a codimension $m-2$ condition. Adding at most $N-2$ parameters for $([K], [Y])$, since they are not generic in F_2 , we get a total of $(m-1)(N+1-m) - (m-2) + (N-2) = m(N+1-m) - 1 = \dim(G) - 1$, as required again. \square

Applying the Thom-Porteous formula as above, we would get the refined expectation that the ML-degree should coincide with

$$ML_m^{(1)} = \int_{CQ_n} s_{m-1}(H_1, H_2) H_{n-1}^{N-m+1}.$$

This will be true for $m \leq 3$, but not for $m \geq 4$, because the next exceptional divisors also needs to be taken into account.

5. SECOND EXCEPTIONAL DIVISOR

Suppose $X = a^2 + b^2$ has rank two, so that a and b are independent vectors. To compose symmetric matrices we use the standard quadratic form q on \mathbb{C}^n , in which terms we get

$$X^2 = q(a)a^2 + q(b)b^2 + 2q(a, b)ab.$$

So X^2 is proportional to X iff $q(a) = q(b)$ and $q(a, b) = 0$. If the restriction of q to the plane $U = \langle a, b \rangle$ is non degenerate, this exactly means that X is (up to scalars) the restriction to U of the dual quadratic form.

Now if we cut out E_2 with $q^{-1}\mathbb{P}(\mathcal{L})$, we get pairs of matrices $([X], [Y]) \in D_2 \times D_{n-2}$ with $[Y] \in \mathcal{L}$. For \mathcal{L} general of dimension $m \leq 3$, the intersection is therefore empty since $\mathbb{P}(\mathcal{L}) \cap D_{n-2} = \emptyset$. For $m = 4$, $\mathbb{P}(\mathcal{L}) \cap D_{n-2}$ is a collection of δ_n smooth points, where $\delta_n = \binom{n+1}{3}$ is the degree of D_{n-2} . Moreover, for each of these points, by the generality assumption the matrix Y has rank exactly $n-2$, and the quadratic form q is non degenerate on its kernel; so $[X]$ is uniquely determined.

We now have enough information to prove our main result.

6. PROOF OF THE THEOREM

Let us summarize our discussion. We have seen that the ML-degree counts the number of points in a finite intersection inside the open subset CQ_n^0 of the variety of complete quadrics. Globally over CQ_n , we have expressed this intersection as that of the degeneracy locus $D(\phi'_{\mathcal{M}})$ with the pre-image $q^{-1}\mathbb{P}(\mathcal{L})$ of a linear space. If this intersection is finite, then we can compute its degree as an intersection number in the variety of complete quadrics, between the class of $D(\phi'_{\mathcal{M}})$ in the Chow ring, and the class of $q^{-1}\mathbb{P}(\mathcal{L})$. On the one hand, if $D(\phi'_{\mathcal{M}})$ has the expected dimension, then its class is given by the Thom-Porteous formula, which yields a Segre class $s_{m-1}(H_1, H_2)$. On the other hand, the class of $q^{-1}\mathbb{P}(\mathcal{L})$ is simply a power of the pull-back by q of the hyperplane class. So the relevant intersection number on CQ_n can be computed. But we have to be careful about the intersection points that may belong to the exceptional divisors, which should not be counted in the ML-degree. This yields a relation

$$\int_{CQ_n} s_{m-1}(H_1, H_2) H_{n-1}^{N-m+1} = ML_m + \Delta_m^{(1)} + \cdots + \Delta_m^{(n-1)},$$

where $\Delta_m^{(i)}$ is the contribution of E_i to our intersection problem. We have seen that $\Delta_m^{(1)} = 0$. We claim that for dimensional reasons,

$$\Delta_m^{(i)} = 0 \quad \text{for} \quad m \leq \binom{i+1}{2}.$$

Indeed, $\mathbb{P}(\mathcal{L})$ is a generic linear subspace of dimension $m-1$ in $\mathbb{P}(\mathbb{S}_n)$, so it does not meet the degeneracy locus D_{n-i} , when $m-1$ is smaller than the codimension $\binom{i+1}{2}$ of the latter. Since $D_{n-i} = q(E_i)$, this implies our claim.

m = 2. By the previous claims the exceptional divisors do not contribute to our intersection number, and we directly get that

$$ML_2 = \int_{CQ_n} (H_1 + H_2) H_{n-1}^{N-1} = (n-1) + (n-2) = 2n-3.$$

Indeed, H_{n-1}^{N-1} is represented by a projective line of matrices, and H_1 (resp. H_2) by a linear relation between the maximal (resp. submaximal) minors of these matrices, which of course have degree $n-1$ (resp. $n-2$).

m = 3. Here again the exceptional divisors do not contribute, hence

$$ML_3 = \int_{CQ_n} s_2(H_1, H_2) H_2^{N-2} = \int_{CQ_n} (H_1^2 + H_1 H_2 + H_2^2) H_{n-1}^{N-2}.$$

By the previous interpretation this yields the expected result:

$$ML_3 = (n-1)^2 + (n-1)(n-2) + (n-2)^2 = 3n^2 - 9n + 7.$$

m = 4. Here E_2 has to be taken into account, and we have

$$ML_4 = \int_{CQ_n} s_3(H_1, H_2) H_{n-1}^{N-3} - \Delta_4^{(2)}.$$

In order to compute these numbers we argue as follows. As before H_{n-1}^{N-3} is represented by a generic \mathbb{P}^3 of symmetric matrices, and its intersection with $H_1^a H_2^{3-a}$ is represented by a complete intersection of a hypersurfaces of degree $n-1$ and $3-a$ hypersurfaces of degree $n-2$. By Bertini these hypersurfaces intersect in general transversely outside the base loci of the corresponding linear systems, which we can avoid since the base locus of H_2 has codimension six; with a caveat when $a=3$, in which case we only have H_1 whose base locus has only codimension three and cannot be avoided, and then we need to subtract the degree δ_n of the variety of corank two matrices (see [SU10, section 2.2]). This yields

$$\int_{CQ_n} H_2^3 H_{n-1}^{N-3} = (n-2)^3, \quad \int_{CQ_n} H_1 H_2^2 H_{n-1}^{N-3} = (n-1)(n-2)^2,$$

$$\int_{CQ_n} H_1^2 H_2 H_{n-1}^{N-3} = (n-1)^2(n-2), \quad \int_{CQ_n} H_1^3 H_{n-1}^{N-3} = (n-1)^3 - \delta_n.$$

Finally, we have seen in the previous section that

$$\Delta_4^{(2)} = \delta_n = \binom{n+1}{3}.$$

Putting all this together we finally conclude that

$$ML_4 = (n-2)^3 + (n-1)(n-2)^2 + (n-1)^2(n-2) + (n-1)^3 - 2 \binom{n+1}{3},$$

which is exactly the conjectured formula.

7. SOME QUESTIONS

How could we go beyond the results of this note?

- (1) For $m \geq 5$ our degeneracy locus always contains the $\mathcal{C}_2 \subset E_2$, whose codimension (three) is smaller than the expected codimension $m-1$. This is a serious problem in order to compute ML_m from intersection theory on complete quadrics. Excess intersection theory deals with this sort of situations and might allow to overcome the problem, at least up to $m=6$, after which E_3 will also enter the show.

More directly, one could try to blow-up CQ_n along \mathcal{C}_2 and try to define a new morphism $\phi'_{\mathcal{M}}$ on the blow-up, whose degeneracy locus could hopefully be of the correct codimension.

- (2) By the same argument as for E_2 , each exceptional divisor E_s contains a component \mathcal{C}_s of the degeneracy locus, of codimension $\binom{s+1}{2} - 1$. Moreover this component should contribute for $m > \binom{s+1}{2}$. Is there a simple formal argument to prove that this contribution is polynomial in n ?
- (3) More generally, is there any formal reason to expect that, like for generic linear concentration models, the ML-degrees of generic linear covariance models should be polynomial in n ? This would again be

a very remarkable phenomenon, but our concrete evidence for that is still rather limited.

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