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Algebraic Identifiability of Gaussian  
Mixtures

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# Algebraic Identifiability of Gaussian Mixtures

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## Abstract

We prove that all moment varieties of univariate Gaussian mixtures have the expected dimension. Our approach rests on intersection theory and Terracini's classification of defective surfaces. The analogous identifiability result is shown to be false for mixtures of Gaussians in dimension three and higher. Their moments up to third order define projective varieties that are defective. Our geometric study suggests an extension of the Alexander-Hirschowitz Theorem for Veronese varieties to the Gaussian setting.

## 1 Introduction

The Gaussian moment variety  $\mathcal{G}_{n,d}$  is a subvariety of  $\mathbb{P}^N$ , where  $N = \binom{n+d}{d} - 1$ . Following [2], its points are the vectors of all moments of order  $\leq d$  of an  $n$ -dimensional Gaussian distribution, parametrized birationally by the entries of the mean vector  $\mu = (\mu_1, \dots, \mu_n)$  and the covariance matrix  $\Sigma = (\sigma_{ij})$ . The variety  $\mathcal{G}_{n,d}$  is rational of dimension  $n(n+3)/2$  for  $d \geq 2$ . Its  $k$ th secant variety  $\text{Sec}_k(\mathcal{G}_{n,d})$  is the Zariski closure in  $\mathbb{P}^N$  of the set of vectors of moments of order  $\leq d$  of any probability distribution on  $\mathbb{R}^n$  that is the mixture of  $k$  Gaussians, for  $k \geq 2$ . Our aim is to determine the dimension of the secant variety  $\text{Sec}_k(\mathcal{G}_{n,d})$ .

That dimension is always bounded above by the number of parameters, so we have

$$\dim(\text{Sec}_k(\mathcal{G}_{n,d})) \leq \min \{ N, kn(n+3)/2 + k - 1 \}. \quad (1)$$

The right hand side is the *expected dimension*. If equality holds in (1) then  $\text{Sec}_k(\mathcal{G}_{n,d})$  is *nondefective*. If this holds, and  $N \geq \frac{1}{2}kn(n+3) + k - 1$ , then the Gaussian mixtures are algebraically identifiable from their  $N$  moments of order  $\leq d$ . Here *algebraically identifiable* means that the map from the model parameters to the moments is finite-to-one, so the parameters can be recovered by solving a zero-dimensional system of polynomial equations.

In this article we prove the following result that contrasts the cases  $n = 1$  and  $n \geq 3$ .

**Theorem 1.** *Equality holds in (1) for  $n = 1$  and all values of  $d$  and  $k$ . Hence all moment varieties of mixtures of univariate Gaussians are algebraically identifiable. The same is false for  $n \geq 3$ ,  $d = 3$  and  $k = 2$ : here the right hand side of (1) exceeds the left hand side by two.*

Defective Veronese varieties are classified by the celebrated *Alexander-Hirschowitz Theorem* [4]. This is relevant for our discussion because each Veronese variety is naturally contained in a corresponding Gaussian moment variety. The latter is a noisy version of

the former, since the Veronese variety consists of the points on  $\mathcal{G}_{n,d}$  where the covariance matrix is zero. We refer to the discussion in [2, Sec. 6]. Theorem 1 proves the first part of Conjecture 15 in [2], and it disproves the “natural conjecture” stated after Problem 17 in [2].

Our result for  $d = 3$  is a Gaussian analogue to the infinite family ( $d = 2$ ) in the Alexander-Hirschowitz classification [4] of defective Veronese varieties. Many further defective cases for  $d = 4$  are exhibited in Table 2 and Conjecture 20. Extensive computer experiments (up to  $d = 24$ ) suggest that moment varieties are never defective for bivariate Gaussians ( $n = 2$ ).

**Conjecture 2.** *Equality holds in (1) for  $n = 2$  and all values of  $d$  and  $k$ . In particular, all moment varieties of mixtures of bivariate Gaussians are algebraically identifiable.*

Our presentation is organized as follows. In Section 2 we focus on the case  $n = 1$ . We review basics on the Gaussian moment surfaces  $\mathcal{G}_{1,d}$ , and what is known classically on defectivity of surfaces. Based on this, we then prove the first part of Theorem 1. In Section 3 study our problem for  $n \geq 2$ . We begin with the parametric representation of  $\text{Sec}_k(\mathcal{G}_{n,d})$ , we next establish the second part of Theorem 1, and thereafter we study the defect and we examine higher moments. Section 4 discusses what little we know about the degree and equations of the varieties  $\text{Sec}_k(\mathcal{G}_{n,d})$ . Both Sections 3 and 4 feature many open problems.

## 2 One-dimensional Gaussians

The moments  $m_0, m_1, m_2, \dots, m_d$  of a Gaussian distribution on the real line are polynomial expressions in the mean  $\mu$  and the covariance  $\sigma^2$ . These expressions will be reviewed in Remark 5. They give a parametric representation of the Gaussian moment surface  $\mathcal{G}_{1,d}$  in  $\mathbb{P}^d$ . The following implicit representation of that surface was derived in [2, Proposition 2].

**Proposition 3.** *Let  $d \geq 3$ . The homogeneous prime ideal of the Gaussian moment surface  $\mathcal{G}_{1,d}$  is minimally generated by  $\binom{d}{3}$  cubics. These are the  $3 \times 3$ -minors of the  $3 \times d$ -matrix*

$$G_d = \begin{pmatrix} 0 & m_0 & 2m_1 & 3m_2 & 4m_3 & \cdots & (d-1)m_{d-2} \\ m_0 & m_1 & m_2 & m_3 & m_4 & \cdots & m_{d-1} \\ m_1 & m_2 & m_3 & m_4 & m_5 & \cdots & m_d \end{pmatrix}.$$

*The  $3 \times 3$ -minors of the matrix  $G_d$  form a Gröbner basis for the prime ideal of  $\mathcal{G}_{1,d}$  with respect to the reverse lexicographic term order. This implies that  $\mathcal{G}_{1,d}$  has degree  $\binom{d}{2}$  in  $\mathbb{P}^d$ .*

Our first new result concerns the singular locus on the Gaussian moment surface.

**Lemma 4.** *The singular locus of the surface  $\mathcal{G}_{1,d}$  is the line defined by  $\langle m_0, m_1, \dots, m_{d-2} \rangle$ .*

*Proof.* Let  $\mathcal{L}$  be the line defined by  $\langle m_0, m_1, \dots, m_{d-2} \rangle$  and  $\mathcal{S} = \text{Sing}(\mathcal{G}_{1,d})$ . We claim  $\mathcal{L} = \mathcal{S}$ .

We first show that  $\mathcal{S} \subseteq \mathcal{L}$ . Consider the affine open chart  $\{m_0 = 1\}$  of  $\mathcal{G}_{1,d}$ . On that chart, the coordinates  $m_i$  are polynomial functions in the earlier unknowns  $m_0, \dots, m_{i-1}$ . Indeed, the  $3 \times 3$ -minor of  $G_d$  with column indices 1, 2 and  $i$  has the form  $m_i - h(m_0, \dots, m_{i-1})$ . Hence  $\mathcal{G}_{1,d} \cap \{m_0 = 1\} \simeq \mathbb{A}^2$ , and therefore  $\mathcal{S} \subset \{m_0 = 0\}$ . Next suppose  $m_0 = 0$ . The

leftmost  $3 \times 3$ -minor of  $G_d$  implies  $m_1 = 0$ . Now, the minor with columns 2, 3, 4 implies that  $m_2 = 0$ , the minor with columns 3, 4, 5 implies that  $m_3 = 0$ , etc. From the rightmost minor we conclude  $m_{d-2} = 0$ . This shows that  $\mathcal{G}_{1,d} \cap \{m_0 = 0\} = \mathcal{L}$ , and we conclude  $\mathcal{S} \subseteq \mathcal{L}$ .

For the reverse inclusion  $\mathcal{L} \subseteq \mathcal{S}$ , we consider the Jacobian matrix of the cubics that define  $\mathcal{G}_{1,d}$ . That matrix has  $d+1$  rows and  $\binom{d}{3}$  columns. We claim that it has rank  $\leq d-3$  on  $\mathcal{L}$ . To see this, note that the term  $m_i m_{d-1}^2$  appears in the minor of  $G_d$  with columns  $i, d-1, d$  for  $i = 2, \dots, d-2$ , and that all other occurrences of  $m_{d-1}$  or  $m_d$  in any of the  $3 \times 3$ -minors of  $G_d$  is linear. Therefore the Jacobian matrix restricted to  $\mathcal{L}$  has only  $d-3$  non-zero entries, and so its rank is at most  $d-3$ . This is less than  $d-2 = \text{codim}(\mathcal{G}_{1,d})$ . We conclude that all points on the line  $\mathcal{L}$  are singular points in the Gaussian moment surface  $\mathcal{G}_{1,d}$ .  $\square$

The  $3 \times d$ -matrix  $G_d$  has entries that are linear forms in  $d+1$  unknowns  $m_0, \dots, m_d$ . That matrix may be interpreted as a 3-dimensional tensor of format  $3 \times d \times (d+1)$ . That tensor can be turned into a  $d \times (d+1)$  matrix whose entries are linear forms in three unknowns  $x, y, z$ . The result is what we call the *Hilbert-Burch matrix* of our surface  $\mathcal{G}_{1,d}$ . It equals

$$B_d = \begin{pmatrix} y & z & 0 & 0 & \cdots & 0 \\ x & y & z & 0 & \cdots & 0 \\ 0 & 2x & y & z & \cdots & 0 \\ 0 & 0 & 3x & y & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & (d-1)x & y & z \end{pmatrix}. \quad (2)$$

This tridiagonal matrix has  $x, 2x, \dots, (d-1)x$  as subdiagonal,  $y$  throughout the diagonal, and  $z$  along the superdiagonal. Let  $\phi: \mathbb{P}^2 \dashrightarrow \mathbb{P}^d$  be the map defined by the maximal minors of  $B_d$ . The base locus of the map  $\phi$  is the point  $(1:0:0)$ , and its image is the surface  $\mathcal{G}_{1,d}$ .

**Remark 5.** The parametrization  $\phi$  is birational. It coincides with the familiar affine parametrization, as in (9), of the Gaussian moments in terms of mean and variance if we set

$$x = -\sigma^2, \quad y = \mu \quad \text{and} \quad z = 1. \quad (3)$$

We now come to our main question, namely whether there exist  $d$  and  $k$  such that  $\mathcal{G}_{1,d}$  is  $k$ -defective in  $\mathbb{P}^d$ . Theorem 1 asserts that this is not the case. Equivalently, the dimension of  $\text{Sec}_k(\mathcal{G}_{1,d})$  is always equal to the minimum of  $d$  and  $3k-1$ , which is the upper bound in (1).

Curves can never be defective, but surfaces can. The prototypical example is the Veronese surface  $S$  in the space  $\mathbb{P}^5$  of symmetric  $3 \times 3$ -matrices. Points on  $S$  are matrices of rank 1. The secant variety  $\text{Sec}_2(S)$  consists of matrices of rank  $\leq 2$ . Its expected dimension is five whereas the true dimension of  $S$  is only four. This means that  $S$  is  $k$ -defective for  $k = 2$ .

The following well-known result on higher secant varieties of a variety  $X$  allows us to show that  $X$  is not  $k$ -defective for any  $k$  by proving this for one particular  $k$  (see [1]):

**Proposition 6.** *Let  $X$  be a  $k'$ -defective subvariety of  $\mathbb{P}^d$  and  $k > k'$ . Then  $X$  is  $k$ -defective as long as  $\text{Sec}_k(X)$  is a proper subvariety of  $\mathbb{P}^d$ . In fact, the defectivity increases with  $k$ :*

$$(\dim(X) + 1) \cdot k - 1 - \dim(\text{Sec}_k(X)) > (\dim(X) + 1) \cdot k' - 1 - \dim(\text{Sec}_{k'}(X)). \quad (4)$$

*Proof.* By Terracini's Lemma, the dimension of the secant variety  $\text{Sec}_k(X)$  is the dimension of the span of the tangent spaces to  $X$  at  $k$  general points. Since  $X$  is  $k'$ -defective and  $k' < k$ , the linear span of  $k - k'$  general tangent spaces to the affine cone over  $X$  must intersect the span of  $k'$  such general tangent spaces in a positive-dimensional linear space. The dimension of that intersection is the difference of the left hand side minus the right hand side in (4).  $\square$

**Corollary 7.** *If a surface  $X \subset \mathbb{P}^d$  is defective then  $X$  is  $k$ -defective for some  $k \geq (d - 2)/3$ .*

*Proof.* We proceed by induction on  $k$ . If the surface  $X$  is  $(k - 1)$ -defective and  $k < (d - 2)/3$ , then  $\dim(\text{Sec}_k(X)) < 3k + 2 < d$ . So  $X$  is also  $k$ -defective, by Proposition 6.  $\square$

Our main geometric tool is Terracini's 1921 classification of all  $k$ -defective surfaces:

**Theorem 8.** *(Classification of  $k$ -defective surfaces) Let  $X \subset \mathbb{P}^N$  be a reduced, irreducible, non-degenerate projective surface that is  $k$ -defective. Then  $k \geq 2$  and either*

- (1)  $X$  is the quadratic Veronese embedding of a rational normal surface  $Y$  in  $\mathbb{P}^k$ ; or
- (2)  $X$  is contained in a cone over a curve, with apex a linear space of dimension  $\leq k - 2$ .

Furthermore, for general points  $x_1, \dots, x_k$  on  $X$  there is a hyperplane section tangent along a curve  $C$  that passes through these points. In case (1), the curve  $C$  is irreducible; in case (2), the curve  $C$  decomposes into  $k$  algebraically equivalent curves  $C_1, \dots, C_k$  with  $x_i \in C_i$ .

*Proof.* See [6, Theorem 1.3 (i),(ii)] and cases (i) and (ii) of the proof given there.  $\square$

Chiantini and Ciliberto offer a nice historical account of this theorem in the introduction to their article [6]. A modern proof follows from the more general result in [6, Theorem 1.1].

**Corollary 9.** *If the surface  $X = \mathcal{G}_{1,d}$  is  $k$ -defective then statement (2) in Theorem 8 holds.*

*Proof.* We need to rule out case (1) in Theorem 8. A rational normal surface is either a Hirzebruch surface or it is the cone over a rational curve. The former is smooth and the latter is singular at only one point. The same is true for the quadratic Veronese embedding of such a surface. By contrast, our surface  $\mathcal{G}_{1,d}$  is singular along a line, by Lemma 4.  $\square$

Our goal is now to rule out case (2) in Theorem 8. That proof will be much more involved. Our strategy is to set up a system of surfaces and morphisms between them, like this:

$$\begin{array}{ccc} S_d & \rightarrow & \bar{S}_d \subset \mathbb{P}^{N_d} \\ \downarrow & & \downarrow \\ \mathbb{P}^2 & & \mathcal{G}_{1,d} \subset \mathbb{P}^d \end{array} \quad (5)$$

The second row in (5) represents the rational map  $\phi : \mathbb{P}^2 \dashrightarrow \mathcal{G}_{1,d}$  that is given by the maximal minors of  $B_d$ . Above  $\mathbb{P}^2$  sits a smooth surface  $S_d$  which we shall construct by a sequence of blow-ups from  $\mathbb{P}^2$ . It will have the property that  $\phi$  lifts to a morphism on  $S_d$ . Curves of degree  $d$  in  $\mathbb{P}^2$  specify a divisor class  $H_d$  on  $S_d$ . The complete linear system  $|H_d|$  maps  $S_d$  onto a rational surface  $\bar{S}_d$  in  $\mathbb{P}^{N_d}$  where  $N_d = \dim(|H_d|)$ . The subsystem of  $|H_d|$  given by the  $d + 1$  maximal minors of  $B_d$  then defines the vertical map from  $\bar{S}_d$  onto  $\mathcal{G}_{1,d}$ . Our plan is to use the intersection theory on  $S_d$  to rule out the possibility (2) in Theorem 8.

**Lemma 10.** *Suppose that we have a diagram as in (5) and  $X = \mathcal{G}_{1,d}$  satisfies statement (2) in Theorem 8. Then, for any  $k$  general points  $x_1, \dots, x_k$  on the surface  $S_d$ , there exist linearly equivalent divisors  $D_1 \ni x_1, \dots, D_k \ni x_k$  and there exists a hyperplane section of  $\mathcal{G}_{1,d}$  in  $\mathbb{P}^d$ , with pullback  $H_d$  to  $S_d$ , such that  $H_d - 2D_1 - 2D_2 - \dots - 2D_k$  is effective on  $S_d$ .*

*Proof.* By part (2) of Theorem 8, there exist algebraically equivalent curves  $C_1, \dots, C_k$  on  $X$  that contain the images of the respective points  $x_1, \dots, x_k$ , and there is a hyperplane section  $H_X$  of  $X$  which contains and is singular along each  $C_i$ . Let  $H \subset S_d$  be the preimage of  $H_X$ , and let  $D_i \subset S_d$  be the preimage of  $C_i$ . Then  $x_i \in D_i$  for  $i = 1, \dots, k$ . Furthermore, the divisor  $H$  has multiplicity at least 2 along each  $D_i$ . Finally, since  $S_d$  is a rational surface, linear and algebraic equivalence of divisors coincide, and the lemma follows.  $\square$

We now construct the smooth surface  $S_d$ . Let  $V_d$  denote the  $(d+1)$ -dimensional vector space spanned by the maximal minors of the matrix  $B_d$  in (2). When  $d$  is odd these minors are

$$\begin{aligned}
b_{d,0} &= && z^d, \\
b_{d,1} &= && yz^{d-1}, \\
b_{d,2} &= && y^2z^{d-2} - xz^{d-1}, \\
b_{d,3} &= && y^3z^{d-3} - 3xyz^{d-2}, \\
&\dots && \dots \quad \dots \quad \dots \quad \dots \\
b_{d,d-1} &= && y^{d-1}z - \binom{d-1}{2}xy^{d-3}z^2 + \dots + a_{\binom{d-3}{2},d-1}x^{\frac{d-3}{2}}y^2z^{\frac{d-1}{2}} + a_{\binom{d-1}{2},d-1}x^{\frac{d-1}{2}}z^{\frac{d+1}{2}}, \\
b_{d,d} &= && y^d - \binom{d}{2}xy^{d-2}z + a_{(2,d)}x^2y^{d-4}z^2 + \dots + a_{\binom{d-1}{2},d}x^{\frac{d-1}{2}}yz^{\frac{d-1}{2}}.
\end{aligned}$$

When  $d$  is even, the maximal minors of the Hilbert-Burch matrix  $B_d$  are

$$\begin{aligned}
b_{d,0} &= && z^d, \\
b_{d,1} &= && yz^{d-1}, \\
b_{d,2} &= && y^2z^{d-2} - xz^{d-1}, \\
b_{d,3} &= && y^3z^{d-3} - 3xyz^{d-2}, \\
&\dots && \dots \quad \dots \quad \dots \quad \dots \\
b_{d,d-1} &= && y^{d-1}z - \binom{d-1}{2}xy^{d-3}z^2 + \dots + a_{\binom{d-4}{2},d-1}x^{\frac{d-4}{2}}y^3z^{\frac{d-2}{2}} + a_{\binom{d-2}{2},d-1}x^{\frac{d-2}{2}}yz^{\frac{d}{2}}, \\
b_{d,d} &= && y^d - \binom{d}{2}xy^{d-2}z + a_{(2,d)}x^2y^{d-4}z^2 + \dots + a_{\binom{d}{2},d}x^{\frac{d}{2}}z^{\frac{d}{2}}.
\end{aligned}$$

Here the  $a_{(i,j)}$  are rational constants. The point  $p = (1 : 0 : 0)$  is the only common zero of the forms  $b_{d,0}, \dots, b_{d,d}$ . All forms are singular at  $p$ , with the following lowest degree terms:

$$z^d, yz^{d-1}, z^{d-1}, yz^{d-2}, \dots, z^{(d+1)/2}, yz^{(d-1)/2} \quad \text{when } d \text{ is odd;} \quad (6)$$

$$z^d, yz^{d-1}, z^{d-1}, yz^{d-2}, \dots, yz^{d/2}, z^{d/2} \quad \text{when } d \text{ is even.} \quad (7)$$

Consider a general form in  $V_d$ . Then its lowest degree term at  $p$  is a linear combination of  $z^{(d+1)/2}$  and  $yz^{(d-1)/2}$  when  $d$  is odd, and it is a scalar multiple of  $z^{d/2}$  when  $d$  is even.

The forms  $b_{d,0}, \dots, b_{d,d}$  define a morphism  $\phi : \mathbb{P}^2 \setminus \{p\} \rightarrow \mathbb{P}^d$  that does not extend to  $p$ . Consider any map  $\pi : S' \rightarrow \mathbb{P}^2$  that is obtained by a sequence of blow-ups at smooth points,

starting with the blow-up of  $\mathbb{P}^2$  at  $p$ . Let  $E \subset S'$  be the preimage of  $p$ . The restriction of  $\pi$  to  $S' \setminus E$  is an isomorphism onto  $\mathbb{P}^2 \setminus \{p\}$ , and so  $\phi$  naturally defines a morphism  $S' \setminus E \rightarrow \mathbb{P}^d$ .

We now define our surface  $S_d$  in (5). It is the minimal surface  $S'$  such that  $S' \setminus E \rightarrow \mathbb{P}^d$  extends to a morphism  $\tilde{\phi} : S' \rightarrow \mathbb{P}^d$ . Here “minimal” refers to the number of blow-ups.

Let  $H_d$  be the strict transform on  $S_d$  of a curve in  $\mathbb{P}^2$  defined by a general form in  $V_d$ . The complete linear system  $|H_d|$  on  $S_d$  defines a morphism  $S_d \rightarrow \mathbb{P}^{N_d}$ , where  $N_d = \dim |H_d|$ . Let  $\tilde{S}_d \subset \mathbb{P}^N$  be the image. Then  $\tilde{\phi} : S_d \rightarrow \mathbb{P}^d$  is the composition of  $S_d \rightarrow \mathbb{P}^N$  and a linear projection to  $\mathbb{P}^d$  whose restriction to  $\tilde{S}_d$  is finite. Thus we now have the diagram in (5).

Relevant for proving Theorem 1 are the first two among the blow-ups that lead to  $S_d$ . The map  $\phi$  is not defined at  $p$ . More precisely,  $\phi$  is undefined at  $p$  and at its tangent direction  $\{z = 0\}$ . Let  $S_p \rightarrow \mathbb{P}^2$  be the blow-up at  $p$ , with exceptional divisor  $E_p$ . Let  $S_{p,z} \rightarrow S_p$  be the blow-up at the point on  $E_p$  corresponding to the tangent direction  $\{z = 0\}$  at  $p$ , with exceptional divisor  $E_z$ . To obtain  $S_d$  we need to blow up  $S_{p,z}$  in  $s$  further points for some  $s$ .

Now,  $S_d$  is a smooth rational surface. Let  $L$  be the class of a line pulled back to  $S_d$ , and let  $E_p, E_z, F_1, \dots, F_s$ , be the classes of the exceptional divisors of each blow-up, pulled back to  $S_d$ . The divisor class group of  $S_d$  is the free abelian group with basis  $L, E_p, E_z, F_1, \dots, F_s$ . The intersection pairing on this group is diagonal for this basis, with

$$L^2 = -E_p^2 = -E_z^2 = -F_1^2 = \dots = -F_s^2 = 1. \quad (8)$$

The intersection of two curves on the smooth surface  $S_d$ , having no common components, is a nonnegative integer. It is computed as the intersection pairing of their classes using (8).

**Lemma 11.** *Consider the linear system  $|H_d|$  on  $S_d$  that represents hyperplane sections of  $\mathcal{G}_{1,d} \subset \mathbb{P}^d$ , pulled back via the morphism  $\tilde{\phi}$ . Its class in the Picard group of  $S_d$  is given by*

$$\begin{aligned} H_d &= dL - \frac{d}{2}E_p - \frac{d}{2}E_z - c_1F_1 - c_2F_2 - \dots - c_sF_s & \text{when } d \text{ is even,} \\ H_d &= dL - \frac{d+1}{2}E_p - \frac{d-1}{2}E_z - c_1F_1 - c_2F_2 - \dots - c_sF_s & \text{when } d \text{ is odd.} \end{aligned}$$

Here  $c_1, c_2, \dots, c_s$  are positive integers whose precise value will not matter to us.

*Proof.* The forms in  $V_d$  define the preimages in  $\mathbb{P}^2$  of curves in  $|H_d|$ . The first three coefficients are seen from the analysis in (6) and (7). The general hyperplane in  $\mathbb{P}^d$  intersects the image of the exceptional curve  $F_i$  in finitely many points. Their number is the coefficient  $c_i$ .  $\square$

*Proof of the first part of Theorem 1.* Suppose that  $X = \mathcal{G}_{1,d}$  is  $k$ -defective for some  $k$ . By Corollary 7, we may assume that  $3k + 2 \geq d$ . By Corollary 9 and Lemma 10, the class of the linear system  $|H_d|$  in the Picard group of the smooth surface  $S_d$  can be written as

$$H_d = A + 2kD$$

where  $A$  is effective and  $D$  is the class of a curve that moves on  $S_d$ . This means that

$$D = aL - b_pE_p - b_zE_z - \sum_{i=1}^s c'_iF_i,$$



where  $a = D \cdot L$  is a positive integer and  $b_p, b_z, c'_1, \dots, c'_s$  are nonnegative integers.

Assume first that  $a \geq 2$ . We have the following chain of inequalities:

$$0 \leq L \cdot A = L \cdot H_d - 2k(L \cdot D) = d - 2ka \leq d - 4k \leq 2 - k.$$

This implies  $k \leq 2$ . The case  $k = 1$  being vacuous, we conclude that  $k = 2$  and hence  $d \leq 8$ . If  $d \leq 5$  then  $\text{Sec}_2(\mathcal{G}_{1,d}) = \mathbb{P}^d$  is easily checked. For  $d = 6$ , we know from [2, Theorem 1] that  $\text{Sec}_2(\mathcal{G}_{1,6})$  is a hypersurface of degree 39 in  $\mathbb{P}^6$ . If  $d \in \{7, 8\}$  then the secant variety  $\text{Sec}_2(\mathcal{G}_{1,d})$  is also 5-dimensional, by the computation with cumulants in [2, Proposition 13].

Next, suppose  $a = D \cdot L = 1$ . The divisor  $D$  is the strict transform on  $S_d$  of a line in  $\mathbb{P}^2$ . The multiplicity of this line at  $p$  is at most 1, i.e.  $0 \leq D \cdot E_p \leq 1$ . Furthermore,  $D \cdot E_z = 0$  because  $D$  moves. Suppose that  $D \cdot E_p = 0$  and  $d$  is even. Then we have  $d \geq 4k$  because

$$d/2 = H_d \cdot E_p = A \cdot E_p \leq A \cdot L \leq d - 2k.$$

Since  $d \leq 3k + 2$ , this implies  $k = 2$  and  $d = 8$ . This case has already been ruled out above. If  $D \cdot E_p = 0$  and  $d$  is odd, then the same reasoning yields  $(d + 1)/2 = A \cdot E_p \leq d - 2k$ . This implies  $3k + 2 \geq d \geq 4k + 1$ , which is impossible for  $k \geq 2$ .

It remains to examine the case  $D \cdot E_p = 1$ . Here, any curve linearly equivalent to  $D$  on  $S_d$  is the strict transform of a line in  $\mathbb{P}^2$  passing through  $p = (1 : 0 : 0)$ . Through a general point in the plane there is a unique such line, so it suffices to show that the doubling of any line through  $p$  is not a component of any curve defined by a linear combination of the  $b_{d,i}$ . In particular, it suffices to show that  $y^2$  is not a factor of any form in the vector space  $V_d$ .

To see this, we note that no monomial  $x^r y^s z^t$  appears in more than one of the forms  $b_{d,0}, b_{d,1}, \dots, b_{d,d}$ . Hence, in order for  $y^2$  to divide a linear combination of  $b_{d,0}, b_{d,1}, \dots, b_{d,d}$ , it must already divide one of the  $b_{d,i}$ . However, from the explicit expansions we see that  $y^2$  is not a factor of  $b_{d,i}$  for any  $i$ . This completes the proof of the first part in Theorem 1.  $\square$

### 3 Higher-dimensional Gaussians

We begin with the general definition of the moment variety for Gaussian mixtures. The coordinates on  $\mathbb{P}^N$  are the moments  $m_{i_1 i_2 \dots i_n}$ . The variety  $\text{Sec}_k(\mathcal{G}_{n,d})$  has the parametrization

$$\sum_{i_1, i_2, \dots, i_n \geq 0} \frac{m_{i_1 i_2 \dots i_n}}{i_1! i_2! \dots i_n!} t_1^{i_1} t_2^{i_2} \dots t_n^{i_n} = \sum_{\ell=1}^k \lambda_\ell \cdot \exp(t_1 \mu_{\ell 1} + \dots + t_n \mu_{\ell n}) \cdot \exp\left(\frac{1}{2} \sum_{i,j=1}^n \sigma_{\ell ij} t_i t_j\right). \quad (9)$$

This is a formal identity of generating functions in  $n$  unknowns  $t_1, \dots, t_n$ . The model parameters are the  $kn$  coordinates  $\mu_{\ell i}$  of the mean vectors, the  $k \binom{n+1}{2}$  entries  $\sigma_{\ell ij}$  of the covariance matrices, and the  $k$  mixture parameters  $\lambda_\ell$ . The latter satisfy  $\lambda_1 + \dots + \lambda_k = 1$ . This is a map from the space of model parameters into the affine space  $\mathbb{A}^N$  that sits inside  $\mathbb{P}^N$  as  $\{m_{00 \dots 0} = 1\}$ . We define  $\text{Sec}_k(\mathcal{G}_{n,d}) \subset \mathbb{P}^N$  as the projective closure of the image of this map.

In this section we focus on the case  $d = 3$ , that is, we examine the varieties defined by first, second and third moments of Gaussian distributions. The following is our main result.

**Theorem 12.** *The moment variety  $\mathcal{G}_{n,3}$  is  $k$ -defective for  $k \geq 2$  unless  $\text{Sec}_k(\mathcal{G}_{n,3})$  fills  $\mathbb{P}^N$ . In particular, for  $k = 2$ , the model has two more parameters than the dimension of the secant variety, i.e.  $n(n+3)+1 - \dim(\text{Sec}_2(\mathcal{G}_{n,3})) = 2$ . If  $n \geq 3$  and we fix distinct first coordinates  $\mu_{11}$  and  $\mu_{21}$  for the two mean vectors, then the remaining parameters are identified uniquely.*

This proves the second part of Theorem 1. We begin by studying the first interesting case.

**Example 13.** Let  $n = d = 3$  and  $k = 2$ . In words, we consider moments up to order three for the mixture of two Gaussians in  $\mathbb{R}^3$ . This case is special because the number of parameters coincides with the dimension of the ambient space:  $N = \frac{1}{2}kn(n+3)+k-1 = 19$ . The variety  $\text{Sec}_2(\mathcal{G}_{3,3})$  is the closure of the image of the map  $\mathbb{A}^{19} \rightarrow \mathbb{P}^{19}$  that is given by (9):

$$\begin{aligned}
m_{100} &= \lambda\mu_{11} + (1-\lambda)\mu_{21} \\
m_{010} &= \lambda\mu_{12} + (1-\lambda)\mu_{22} \\
m_{001} &= \lambda\mu_{13} + (1-\lambda)\mu_{23} \\
m_{200} &= \lambda(\mu_{11}^2 + \sigma_{111}) + (1-\lambda)(\mu_{21}^2 + \sigma_{211}) \\
m_{020} &= \lambda(\mu_{12}^2 + \sigma_{122}) + (1-\lambda)(\mu_{22}^2 + \sigma_{222}) \\
m_{002} &= \lambda(\mu_{13}^2 + \sigma_{133}) + (1-\lambda)(\mu_{23}^2 + \sigma_{233}) \\
m_{110} &= \lambda(\mu_{11}\mu_{12} + \sigma_{112}) + (1-\lambda)(\mu_{21}\mu_{22} + \sigma_{212}) \\
m_{101} &= \lambda(\mu_{11}\mu_{13} + \sigma_{113}) + (1-\lambda)(\mu_{21}\mu_{23} + \sigma_{213}) \\
m_{011} &= \lambda(\mu_{12}\mu_{13} + \sigma_{123}) + (1-\lambda)(\mu_{22}\mu_{23} + \sigma_{223}) \\
m_{300} &= \lambda(\mu_{11}^3 + 3\sigma_{111}\mu_{11}) + (1-\lambda)(\mu_{21}^3 + 3\sigma_{211}\mu_{21}) \\
m_{030} &= \lambda(\mu_{12}^3 + 3\sigma_{122}\mu_{12}) + (1-\lambda)(\mu_{22}^3 + 3\sigma_{222}\mu_{22}) \\
m_{003} &= \lambda(\mu_{13}^3 + 3\sigma_{133}\mu_{13}) + (1-\lambda)(\mu_{23}^3 + 3\sigma_{233}\mu_{23}) \\
m_{210} &= \lambda(\mu_{11}^2\mu_{12} + \sigma_{111}\mu_{12} + 2\sigma_{112}\mu_{11}) + (1-\lambda)(\mu_{21}^2\mu_{22} + \sigma_{211}\mu_{22} + 2\sigma_{212}\mu_{21}) \\
m_{201} &= \lambda(\mu_{11}^2\mu_{13} + \sigma_{111}\mu_{13} + 2\sigma_{113}\mu_{11}) + (1-\lambda)(\mu_{21}^2\mu_{23} + \sigma_{211}\mu_{23} + 2\sigma_{213}\mu_{21}) \\
m_{120} &= \lambda(\mu_{11}\mu_{12}^2 + \sigma_{122}\mu_{11} + 2\sigma_{112}\mu_{12}) + (1-\lambda)(\mu_{21}\mu_{22}^2 + \sigma_{222}\mu_{21} + 2\sigma_{212}\mu_{22}) \\
m_{102} &= \lambda(\mu_{11}\mu_{13}^2 + \sigma_{133}\mu_{11} + 2\sigma_{113}\mu_{13}) + (1-\lambda)(\mu_{21}\mu_{23}^2 + \sigma_{233}\mu_{21} + 2\sigma_{213}\mu_{23}) \\
m_{021} &= \lambda(\mu_{12}^2\mu_{13} + \sigma_{122}\mu_{13} + 2\sigma_{123}\mu_{12}) + (1-\lambda)(\mu_{22}^2\mu_{23} + \sigma_{222}\mu_{23} + 2\sigma_{223}\mu_{22}) \\
m_{012} &= \lambda(\mu_{12}\mu_{13}^2 + \sigma_{133}\mu_{12} + 2\sigma_{123}\mu_{13}) + (1-\lambda)(\mu_{22}\mu_{23}^2 + \sigma_{233}\mu_{22} + 2\sigma_{223}\mu_{23}) \\
m_{111} &= \lambda(\mu_{11}\mu_{12}\mu_{13} + \sigma_{112}\mu_{13} + \sigma_{113}\mu_{12} + \sigma_{123}\mu_{11}) \\
&\quad + (1-\lambda)(\mu_{21}\mu_{22}\mu_{23} + \sigma_{212}\mu_{23} + \sigma_{213}\mu_{22} + \sigma_{223}\mu_{21})
\end{aligned}$$

A direct computation shows that the  $19 \times 19$ -Jacobian matrix of this map has rank 17 for generic parameter values. Hence the dimension of  $\text{Sec}_2(\mathcal{G}_{3,3})$  equals 17. This is two less than the expected dimension of 19. We have here identified the smallest instance of defectivity.

Let  $m = (m_{ijk})$  be a valid vector of moments. Thus  $m$  is a point in  $\text{Sec}_2(\mathcal{G}_{3,3})$ . We assume that  $m \notin \mathcal{G}_{3,3}$ . Choose arbitrary but distinct complex numbers for  $\mu_{11}$  and  $\mu_{21}$ , while the other 17 model parameters remain unknowns. What we see above is a system of 19 polynomial equations in 17 unknowns. We claim that this system has a unique solution over  $\mathbb{C}$ . Hence, if  $m$  has its coordinates in  $\mathbb{Q}$  then that unique solution has its coordinates in  $\mathbb{Q}$ .

By solving the first equation, we obtain the mixture parameter  $\lambda$ . From the second and third equation we can eliminate  $\mu_{12}$  and  $\mu_{13}$ . Next, we observe that all 12 covariances  $\sigma_{ijk}$  appear linearly in our equations, so we can solve for these as well. We are left with a system

of truly non-linear equations in only two unknowns,  $\mu_{22}$  and  $\mu_{23}$ . A direct computation now reveals that this system has a unique solution that is rational expression in the given  $m_{ijk}$ .

Our computational argument shows that each general fiber of the natural parametrization of  $\text{Sec}_2(\mathcal{G}_{3,3})$  is birational to the affine plane  $\mathbb{A}^2$  whose coordinates are  $\mu_{11}$  and  $\mu_{21}$ . This establishes all assertions in Theorem 12 for the special case of trivariate Gaussians ( $n = 3$ ).

**Remark 14.** The second assertion in Theorem 12 holds for  $n = 2$  because there are 11 parameters and  $\text{Sec}_2(\mathcal{G}_{2,3}) = \mathbb{P}^9$ . However, the third assertion is not true for  $n = 2$  because the general fiber of the parametrization map  $\mathbb{A}^{11} \rightarrow \mathbb{P}^9$  is the union of three irreducible components. When  $\mu_{11}$  and  $\mu_{21}$  are fixed then the fiber consists of three points and not one.

*Proof of Theorem 12.* Suppose  $n \geq 4$  and let  $m \in \text{Sec}_2(\mathcal{G}_{n,3}) \setminus \mathcal{G}_{n,3}$ . Each moment  $m_{i_1 i_2 \dots i_n}$  has at most three non-zero indices. Hence, its expression in the model parameters involves at most three coordinates of the mean vectors and a block of size at most three in the covariance matrices. Let  $\mu_{11}$  and  $\mu_{21}$  be arbitrary distinct complex numbers. Then we can apply the rational solution in Example 13 for any 3-element subset of  $\{1, 2, \dots, n\}$  that contains 1. This leads to unique expressions for all model parameters in terms of the moments  $m_{i_1 i_2 \dots i_n}$ . In this manner, at most one system of parameters is recovered. This shows the third sentence in Theorem 12 is implied by the first two sentences. It is these two we shall now prove.

In the affine space  $\mathbb{A}^N = \{m_{000} = 1\} \subset \mathbb{P}^N$ , we consider the affine moment variety  $G_n^A := \mathcal{G}_{n,3} \cap \mathbb{A}^N$ . This has dimension  $M = \frac{1}{2}n(n+3)$ . The map from (9) that parametrizes the Gaussian moments is denoted  $\rho : \mathbb{A}^M \rightarrow \mathbb{A}^N$ . It is an isomorphism onto its image  $G_n^A$ .

Fix two points  $p = (\mu, \sigma)$  and  $p' = (\mu', \sigma')$  in  $\mathbb{A}^M$ . They determine the affine plane

$$A(p, p') = \{ (s\mu + (1-s)\mu', t\sigma + (1-t)\sigma') \mid s, t \in \mathbb{R} \} \subset \mathbb{A}^M.$$

Its image  $\rho(A(p, p'))$  is a surface in  $G_n^A \subset \mathbb{A}^N$ . The restrictions  $m_{i_1 \dots i_n}(s, t)$  of the moments to this surface are polynomials in  $s, t$  with coefficients that depend on the points  $p, p'$ . Since  $i_1 + \dots + i_n \leq 3$ , every moment  $m_{i_1 \dots i_n}(s, t)$  is a linear combination of the monomials  $1, s, t, st, s^2, s^3$ . Linearly eliminating these monomials, we obtain  $N-5$  linear relations among the moments when restricted to the plane  $A(p, p')$ . These relations define the affine span of the surface  $\rho(A(p, p'))$ . This affine space is therefore 5-dimensional. We denote it by  $\mathbb{A}_{p, p'}^5$ .

The monomials  $(b_1, b_2, b_3, b_4, b_5) = (s, t, st, s^2, s^3)$  serve as coordinates on  $\mathbb{A}_{p, p'}^5$ , modulo the affine-linear relations that define  $\mathbb{A}_{p, p'}^5$ . The image surface  $\rho(A(p, p'))$  is therefore contained in the subvariety of  $\mathbb{A}_{p, p'}^5$  that is defined by the  $2 \times 2$ -minors of the  $2 \times 4$ -matrix

$$\begin{pmatrix} 1 & b_2 & b_1 & b_4 \\ b_1 & b_3 & b_4 & b_5 \end{pmatrix} = \begin{pmatrix} 1 & t & s & s^2 \\ s & st & s^2 & s^3 \end{pmatrix}. \quad (10)$$

This variety is an irreducible surface, namely a scroll of degree 4. It hence equals  $\rho(A(p, p'))$ .

Let  $\bar{\sigma}$  denote the covariance matrix with entries  $\bar{\sigma}_{ij} = (\mu_i - \mu'_i)(\mu_j - \mu'_j)$ . We define

$$\mathbb{A}_{p, p'}^3 = \{ (\mu' + s(\mu - \mu'), \sigma' + t(\sigma - \sigma') + u\bar{\sigma}) \mid s, t, u \in \mathbb{R} \}.$$

Setting  $u = 0$  shows that this 3-space contains the plane  $A(p, p')$ . We claim that

$$\rho(\mathbb{A}_{p, p'}^3) \subseteq \mathbb{A}_{p, p'}^5. \quad (11)$$

On the image  $\rho(\mathbb{A}_{p,p'}^3)$ , each moment is a linear combination of the eight monomials  $1, s, s^2, s^3, t, st, u, su$ . A key observation is that, by our choice of  $\bar{\sigma}$ , these expressions are actually linear combinations of the six expressions  $1, s, s^2+u, s^3+3su, t, st$ . Indeed, the coefficient of  $s^2$  in the expansion of  $(\mu'_i + s(\mu_i - \mu'_i))(\mu'_j + s(\mu_j - \mu'_j))$  matches the coefficient  $\bar{\sigma}_{ij}$  of  $u$  in the expansion of second order moments. Likewise,  $s^2$  and  $u$  have equal coefficients in the third order moments. Analogously, the coefficient of the monomial  $s^3$  in the expansion of

$$(\mu'_i + s(\mu_i - \mu'_i))(\mu'_j + s(\mu_j - \mu'_j))(\mu'_k + s(\mu_k - \mu'_k))$$

is  $(\mu_i - \mu'_i)\bar{\sigma}_{jk} = (\mu_j - \mu'_j)\bar{\sigma}_{ik} = (\mu_k - \mu'_k)\bar{\sigma}_{ij}$ , which coincides with the corresponding coefficient of  $3su$  in the expansion of third order moments. From this we conclude that (11) holds.

Since  $\rho$  is birational,  $\rho(\mathbb{A}_{p,p'}^3)$  is a threefold in  $\mathbb{A}_{p,p'}^5$ . Since  $p$  and  $p'$  are arbitrary, these threefolds cover  $G_n^A$ . Through any point outside  $\rho(\mathbb{A}_{p,p'}^3)$  there is a 2-dimensional family of secant lines to  $\rho(\mathbb{A}_{p,p'}^3)$ . The same holds for  $G_n^A$ . Hence the 2-defectivity of  $\mathcal{G}_{n,3}$  is at least two.

To see that it is at most two, it suffices to find a point  $q$  in  $\text{Sec}_2(\mathcal{G}_{n,3})$  such that the variety of secant lines to  $\mathcal{G}_{n,3}$  through  $q$  is 2-dimensional. Let  $\mathcal{G}_{2,3}(1,2)$  denote the subvariety of  $\mathcal{G}_{n,3}$  defined by setting all parameters other than  $\mu_1, \mu_2, \sigma_{11}, \sigma_{12}, \sigma_{22}$  to zero. The span of  $\mathcal{G}_{2,3}(1,2) \cap \mathbb{A}^N$  is an affine 9-space  $\mathbb{A}^9(1,2)$  inside  $\mathbb{A}^N$ . Consider a general point  $q \in \mathbb{A}^9(1,2)$ . Then  $q \notin G_n^A$ . We claim that any secant to  $G_n^A$  through  $q$  is contained in  $\mathbb{A}^9(1,2)$ . A computation with Macaulay2 [8] shows that this is the case when  $n = 3$ . Explicitly, if  $q$  is any point whose moment coordinates vanish except those that involve only  $\mu_1, \mu_2, \sigma_{11}, \sigma_{12}, \sigma_{22}$ , then  $\mu_3 = \sigma_{13} = \sigma_{23} = \sigma_{33} = 0$ . In general, we may project any secant line through  $q$  to the span of any  $G_3^A \subset G_n^A$  defined by three indices  $1, 2, k$ . In each case, the secant lands in  $\mathbb{A}^9(1,2)$ , so it must already lie in this subspace before any of the projections. This argument proves the claim. In conclusion, we have shown that the 2-defectivity of the third order Gaussian moment variety  $\mathcal{G}_{n,3}$  is precisely two. This completes the proof of Theorem 12.  $\square$

We offer some remarks on the geometry underlying the proof of Theorem 12. Computations suggest that the inclusion (11) can be strengthened to the equality  $\rho^{-1}(\mathbb{A}_{p,p'}^5) = \mathbb{A}_{p,p'}^3$ . To better understand the threefold  $\rho(\mathbb{A}_{p,p'}^3)$ , we consider the maps

$$\begin{aligned} \tau : \mathbb{A}_{p,p'}^3 &\rightarrow \mathbb{A}^6 & : & (s, t, u) &\mapsto (s, t, st, s^2, s^3 + 3su, u), \\ \pi : \mathbb{A}^6 &\rightarrow \mathbb{A}_{p,p'}^5 & : & (a_1, \dots, a_6) &\mapsto (a_1, a_2, a_3, a_4 + a_6, a_5). \end{aligned}$$

The image  $\tau(\mathbb{A}_{p,p'}^3)$  in  $\mathbb{A}^6$  is the 3-fold scroll defined by the  $2 \times 2$  minors of the matrix

$$\begin{pmatrix} 1 & a_2 & a_1 & a_4 + 3a_6 \\ a_1 & a_3 & a_4 & a_5 \end{pmatrix}. \quad (12)$$

The composition  $\pi \circ \tau$  is the restriction of  $\rho$  to  $\mathbb{A}_{p,p'}^3$ . Hence  $\rho(\mathbb{A}_{p,p'}^3)$  is also a *quartic threefold scroll*. To find its equations in  $\mathbb{A}_{p,p'}^5$ , we set  $a_4 = b_4 - a_6$  and  $a_i = b_i$  for  $i \in \{1, 2, 3, 5\}$ , and then we eliminate  $a_6$  from the ideal of  $2 \times 2$ -minors of (12). The result is the system

$$b_1 b_2 - b_3 = 2b_1 b_3^2 + b_2^2 b_5 - 3b_2 b_3 b_4 = 2b_1^2 b_3 + b_2 b_5 - 3b_3 b_4 = 2b_1^3 - 3b_1 b_4 + b_5 = 0.$$

**Remark 15.** Fix a point  $q$  in the affine secant variety  $\text{Sec}_2(G_n^A)$ . The *entry locus*  $\Sigma_q$  is the closure of the set of points  $p \in G_n^A$  such that  $q$  lies on a secant line through  $p$ . Its preimage  $\rho^{-1}(\Sigma_q) \subset \mathbb{A}^M$  is the *parameter entry locus* at  $q$ . Since the defectivity is 2, the entry locus  $\Sigma_q$  is a surface. The same holds for the parameter entry locus  $\rho^{-1}(\Sigma_q)$ . Using computations, we found that, if  $q$  is on the secant spanned by  $p, p' \in G_n^A$ , then the entry locus  $\Sigma_q$  is a surface of degree 6 in  $\rho(\mathbb{A}_{p,p'}^3) \subset \mathbb{A}_{p,p'}^5$  while the parameter entry locus is a cubic surface in  $\mathbb{A}_{p,p'}^3$ .

We now come to the higher secant varieties of the Gaussian moment variety  $\mathcal{G}_{n,3}$ .

**Corollary 16.** *Let  $k \geq 2$  and  $n \geq 3k - 3$ . Then  $\mathcal{G}_{n,3}$  is  $k$ -defective.*

*Proof.* This is immediate from Theorem 12 and Proposition 6. □

$n$	$k$	$d$	par	$N$	exp	dim	$\delta$	par-dim
5	3	3	62	55	55	51	4	11
6	3	3	83	83	83	71	12	12
6	4	3	111	83	83	82	1	29
7	3	3	107	119	107	94	13	13
7	4	3	143	119	119	111	8	32
8	3	3	134	164	134	120	14	14
8	4	3	179	164	164	144	20	35
8	5	3	224	164	164	160	4	64
9	3	3	164	219	164	149	15	15
9	4	3	219	219	219	181	38	38
9	5	3	274	219	219	204	15	70
10	3	3	197	285	197	181	16	16
10	4	3	263	285	263	222	41	41
10	5	3	329	285	285	253	32	76
10	6	3	395	285	285	275	10	120

Table 1: Moment varieties of order  $d = 3$  for mixtures of  $k \geq 3$  Gaussians

Based on computations, like those in Table 1, we propose the following conjecture.

**Conjecture 17.** *For any  $n \geq 2$  and  $k \geq 1$ , we have*

$$\dim(\text{Sec}_k(\mathcal{G}_{n,3})) = \frac{1}{6}k [k^2 - 3(n+4)k + 3n(n+6) + 23] - (n+2), \quad (13)$$

for  $k = 1, 2, \dots, K$ , where  $K+1$  is the smallest integer such that the right hand side in (13) is larger than the ambient dimension  $\binom{n+3}{3} - 1$ .

For  $k = 1$  this formula evaluates to  $\dim(\mathcal{G}_{n,3}) = n(n+3)/2$ , as desired. Conjecture 17 also holds for  $k = 2$ . This is best seen by rewriting the identity (13) as follows:

$$\frac{1}{2}kn(n+3) + k - 1 - \dim(\text{Sec}_k(\mathcal{G}_{n,3})) = \frac{1}{2}(k-1)(k-2)n - \frac{1}{6}(k-1)(k^2 - 11k + 6).$$

This is the difference between the expected dimension and the true dimension of the  $k$ th secant variety. For  $k = 2$  this equals 2, independently of  $n$ , in accordance with Theorem 12.

Conjecture 17 was verified computationally for  $n \leq 15$ . Table 1 illustrates all cases for  $n \leq 10$ . Here,  $\text{exp} = \min(\text{par}, N)$  is the *expected dimension*, and  $\delta = \text{exp} - \text{dim}$  is the *defect*.

We also undertook a comprehensive experimental study for higher moments of multivariate Gaussians. The following two examples are the two smallest defective cases for  $d = 4$ .

**Example 18.** Let  $n = 8$  and  $d = 4$ . The Gaussian moment variety  $\mathcal{G}_{8,4}$  is 11-defective. The expected dimension of  $\text{Sec}_{11}(\mathcal{G}_{8,4})$  equals the ambient dimension  $N = 494$ , but this secant variety is actually a hypersurface in  $\mathbb{P}^{494}$ . It would be very nice to know its degree.

**Example 19.** Let  $n = 9$  and  $d = 4$ . The moment variety  $\mathcal{G}_{9,4}$  is 12-defective but it is not 11-defective. Thus the situation is much more complicated than that in Theorem 12, where defectivity always starts at  $k = 2$ . We do not yet have any theoretical explanation for this.

Table 2 shows the first few defective cases for Gaussian moments of order  $d = 4$ . It suggests a clear pattern, resulting in the following conjecture. We verified this for  $n \leq 14$ .

$n$	$k$	$d$	par	$N$	exp	dim	$\delta$	par-dim
8	11	4	494	494	494	493	1	1
9	12	4	659	714	659	658	1	1
9	13	4	714	714	714	711	3	3
10	13	4	857	1000	857	856	1	1
10	14	4	923	1000	923	920	3	3
10	15	4	989	1000	989	983	6	6
11	14	4	1091	1364	1091	1090	1	1
11	15	4	1169	1364	1169	1166	3	3
11	16	4	1247	1364	1247	1241	6	6
11	17	4	1325	1364	1325	1315	10	10
12	15	4	1364	1819	1364	1363	1	1
12	16	4	1455	1819	1455	1452	3	3
12	17	4	1546	1819	1546	1540	6	6
12	18	4	1637	1819	1637	1627	10	10
12	19	4	1728	1819	1728	1713	15	15
12	20	4	1819	1819	1819	1798	21	21

Table 2: A census of defective Gaussian moment varieties  $d = 4$

**Conjecture 20.** *The Gaussian moment variety  $\mathcal{G}_{n,4}$  is  $(n+3)$ -defective with defect  $\delta_{n+3} = 1$  for  $n \geq 8$ . Furthermore, for all  $r \geq 3$ , the  $(n+r)$ -defect of  $\mathcal{G}_{n,4}$  is equal to  $\delta_{n+r} = \binom{r-1}{2}$ , unless the number of model parameters exceeds the ambient dimension  $\binom{n+4}{4} - 1$ .*

## 4 Towards Equations and Degrees

We begin Section 4 by reminding the reader that the Veronese variety  $\mathcal{V}_{n,d}$  is a subvariety of  $\mathcal{G}_{n,d}$ . It is obtained by setting the covariance matrix in the parametrization equal to zero. The Gaussian moment variety can be thought of as a noisy version of the Veronese variety. Indeed, points on  $\mathcal{V}_{n,d}$  represent moments of order  $\leq d$  of Dirac measures, and points on its secant variety  $\text{Sec}_k(\mathcal{V}_{n,d})$  represent moments of finitely supported signed measures on  $\mathbb{R}^n$ .

The celebrated Alexander-Hirschowitz Theorem [4] characterizes defective Veronese varieties. It identifies all triples  $(n, d, k)$  such that a mixture of  $k$  Dirac measures on  $\mathbb{R}^n$  is not algebraically identifiable from its moments of order  $\leq d$ . This section is a first step towards a similar characterization for mixtures of  $k$  Gaussian measures on  $\mathbb{R}^n$ . The cases  $d = 3$  and  $d = 4$  for Gaussians, featured in Theorem 12 and Conjecture 20, are reminiscent of the case  $d = 2$  for Veronese varieties. At present we do not know any isolated deficient examples that would be analogous to the exceptional cases in the Alexander-Hirschowitz Theorem.

We wish to reiterate that the Gaussian moment varieties  $\mathcal{G}_{n,d}$  are much more complicated than the Veronese varieties  $\mathcal{V}_{n,d}$ . Beyond Proposition 3, their ideals are essentially unknown.

A well-known result in statistics states that, under reasonable hypotheses, probability distributions are determined by their moments. In addition, it is known (e.g. from [11]) that Gaussian mixtures are identifiable. Since their moments are polynomials in their parameters, Belkin and Sinha [3] concluded that (for  $k$  and  $n$  fixed) a finite set of moments is enough to recover the model parameters uniquely. In particular, the secant variety  $\text{Sec}_k(\mathcal{G}_{n,d})$  has the expected dimension for  $d \gg 0$  when  $k$  and  $n$  are fixed. This raises the following question:

**Problem 21.** *Let  $D(k, n)$  be the smallest integer such that the  $k$ -th mixtures of Gaussians on  $\mathbb{R}^n$  are algebraically identifiable from their moments of order  $\leq d$ . Find good upper bounds on  $D(k, n)$ . What are the best bounds that can be derived using algebraic geometry methods?*

For  $n \geq 2$  it is difficult to compute the prime ideal of the Gaussian moment variety  $\mathcal{G}_{n,d}$  in  $\mathbb{P}^N$ . One approach is to work on the affine open set  $\mathbb{A}^N = \{m_{00\dots 0} = 1\}$ . On that affine space,  $\mathcal{G}_{n,d}$  is a complete intersection defined by the vanishing of all cumulants  $k_{i_1 i_2 \dots i_n}$  whose order  $i_1 + i_2 + \dots + i_n$  is between 3 and  $d$ ; see [2, Remark 6]. Each such cumulant is a polynomial in the moments. Explicit formulas are obtained from the identity  $K = \log(M)$  of generating functions; see [2, eqn (8)]. The ideal of  $\mathcal{G}_{n,d}$  is then obtained from the ideal of cumulants by saturating with respect to  $m_{00\dots 0}$ . One example is featured in [2, eqn (7)].

We next exhibit an alternative representation of  $\mathcal{G}_{n,d} \cap \mathbb{A}^N$  as a determinantal variety. This is derived from Willink's recursion in [10]. It generalizes the matrix  $G_d$  in Proposition 3. We define the *Willink matrix*  $W_{n,d}$  as follows. Its rows are indexed by vectors  $u \in \mathbb{N}^n$  with  $|u| \leq d - 1$ . The matrix  $W_{d,n}$  has  $2n + 1$  columns. The first entry in the row  $u$  is the corresponding moment  $m_u$ . The next  $n$  entries in the row  $u$  are  $m_{u+e_1}, m_{u+e_2}, \dots, m_{u+e_n}$ . The last  $n$  entries in the row  $u$  are  $u_1 m_{u-e_1}, u_2 m_{u-e_2}, \dots, u_n m_{u-e_n}$ . Thus the Willink matrix  $W_{n,d}$  has format  $\binom{n+d-1}{d-1} \times (2n+1)$  and each entry is a scalar multiple of one of the moments. For  $n = 1$ , the  $d \times 3$ -matrix  $W_{1,d}$  equals the transpose of the matrix  $G_d$  after permuting rows.

**Proposition 22.** *The affine Gaussian moment variety  $\mathcal{G}_{n,d} \cap \mathbb{A}^N$  is defined by the vanishing of the  $(n+2) \times (n+2)$ -minors of the Willink matrix  $W_{n,d}$ .*

*Proof.* Suppose that the matrix  $W_{n,d}$  is filled with the moments of a Gaussian distribution on  $\mathbb{R}^n$ , and consider the  $n$  linearly independent vectors

$$\left(\mu_i, 0, \dots, 0, -1, 0, \dots, 0, \sigma_{1i}, \sigma_{2i}, \dots, \sigma_{ni}\right)^T \quad \text{for } i = 1, 2, \dots, n. \quad (14)$$

Here the entry  $-1$  appears in the  $(i+1)$ st coordinate. By [10, eqn (13)], these  $n$  vectors are in the kernel of  $W_{n,d}$ . Hence the rank of  $W_{n,d}$  is  $\leq n+1$ , and the  $(n+2)$ -minors are zero.

Conversely, let  $m$  be an arbitrary point in  $\mathbb{A}^N$  for which the matrix  $W_{n,d}$  has rank  $\leq n+1$ . The square submatrix indexed by the rows  $1, 2, \dots, n+1$  and the columns  $1, n+2, \dots, 2n+1$  has determinant equal to  $m_{00\dots 0}^{n+1} = 1$ . Hence the rank of  $W_{n,d}$  is exactly  $n+1$ . The kernel of the submatrix given by the first  $n+1$  rows is an  $n$ -dimensional space for which we can pick a basis of the form (14). The entries can be interpreted as the mean and the covariance matrix of a Gaussian distribution. The rank hypothesis on  $W_{n,d}$  now ensures that the  $n$  vectors in (14) are in the kernel of the full matrix  $W_{n,d}$ . This means that the higher moments satisfy the recurrences in [10, eqn (13)], and hence the chosen point  $m$  lies in  $\mathcal{G}_{n,d}$ .  $\square$

**Example 23.** Consider the moments of order at most four for a bivariate Gaussian. The variety  $\mathcal{G}_{2,4}$  has dimension 5 and degree 102 in  $\mathbb{P}^{14}$ . Its Willink matrix has format  $10 \times 5$ :

$$W_{2,4} = \begin{pmatrix} m_{00} & m_{01} & m_{10} & 0 & 0 \\ m_{01} & m_{02} & m_{11} & 0 & m_{00} \\ m_{10} & m_{11} & m_{20} & m_{00} & 0 \\ m_{02} & m_{03} & m_{12} & 0 & 2m_{01} \\ m_{11} & m_{12} & m_{21} & m_{01} & m_{10} \\ m_{20} & m_{21} & m_{30} & 2m_{10} & 0 \\ m_{03} & m_{04} & m_{13} & 0 & 3m_{02} \\ m_{12} & m_{13} & m_{22} & m_{02} & 2m_{11} \\ m_{21} & m_{22} & m_{31} & 2m_{11} & m_{20} \\ m_{30} & m_{31} & m_{40} & 3m_{20} & 0 \end{pmatrix}$$

The ideal of  $4 \times 4$ -minors of  $W_{2,4}$  is minimally generated by 657 quartics. Saturation with respect to the coordinate  $m_{00}$  yields the prime ideal of  $\mathcal{G}_{2,4}$ , as described in [2, Proposition 7].

One would expect that it is even more difficult to describe the prime ideals of the secant varieties  $\text{Sec}_k(\mathcal{G}_{n,d})$  for  $n \geq 2$ ,  $k > 1$ . Actually, it is already an open problem to find these ideals when  $n = 1$ ,  $k = 2$  and  $d \geq 8$ . We found in [2, Theorem 1] that  $\text{Sec}_2(\mathcal{G}_{1,6})$  is a hypersurface of degree 39 in  $\mathbb{P}^6$ . Its defining polynomial is the sum of 31154 monomials.

**Example 24.** Let  $n = 1$ ,  $k = 2$  and  $d = 7$ . The following results were obtained using methods from numerical algebraic geometry. The 5-dimensional variety  $\text{Sec}_2(\mathcal{G}_{1,7})$  has degree 105 in  $\mathbb{P}^7$ . The eight coordinate projections, defined algebraically by eliminating each one of  $m_{07}, m_{16}, \dots, m_{70}$  from the ideal of  $\text{Sec}_2(\mathcal{G}_{1,7})$ , are hypersurfaces in  $\mathbb{P}^6$ . Their degrees are 85, 99, 104, 95, 78, 66, 48 and 39 respectively. This suggests that there are no low degree generators in the ideal of  $\text{Sec}_2(\mathcal{G}_{1,7})$ . In fact, a state-of-the-art Gröbner basis computation by Jean-Charles Faugère shows that the smallest degree of such a minimal generator is 25.



With ideal generators out of reach, we first ask for the degrees of our secant varieties.

**Conjecture 25.** *For fixed  $k$  and  $n$ , the function  $d \mapsto \deg \text{Sec}_k(\mathcal{G}_{n,d})$  is a polynomial in  $d$ , starting from the smallest value of  $d$  where the secant variety does not fill the ambient space.*

The numerical `Macaulay2` [8] package `NumericalImplicitization.m2`, developed by Chen and Kileel [5], was very useful for us. It was able to compute the desired degrees in some interesting cases. These data points led us to Conjecture 25 and to the following result.

**Proposition 26.** *Suppose that Conjecture 25 holds for  $k = 2$  and  $n = 1$ . Then, for all  $d \geq 6$ , the degree of the  $d$ th moment variety for mixtures of two univariate Gaussians equals*

$$\deg \text{Sec}_2(\mathcal{G}_{1,d}) = \frac{(d+7)(d-4)(d-3)(d-2)}{8}. \quad (15)$$

*Proof.* Let  $X_d$  be a general variety defined by a Hilbert-Burch matrix  $B_d$  as in (2). Here ‘general’ means that the entries in  $B_d$  are generic linear forms in  $x, y, z$ . Using the double point formula in intersection theory [7, Sec. 9.3] for a general projection  $X_d \rightarrow \mathbb{P}^4$ , we compute

$$\deg \text{Sec}_2(X_d) = \frac{(d-4)(d-3)(d^2+5d-2)}{8}. \quad (16)$$

Since  $\mathcal{G}_{1,d}$  is singular, the degrees of its secant varieties are lower than (16), with a correction term accounting for the singular line in Lemma 4. The assumption that Conjecture 25 holds in our case implies that  $d \mapsto \deg \text{Sec}_2(\mathcal{G}_{1,d})$  is a polynomial function of degree at most 4. Our numerical computation shows that the degrees of  $\text{Sec}_2(\mathcal{G}_{1,d})$  for  $d = 6, \dots, 10$  are 39, 105, 225, 420 and 714. These are enough to interpolate, and we obtain the polynomial in (15).  $\square$

**Remark 27.** The zeroes of (15) at  $d = 2, 3, 4$  were not part of the interpolation but they are not unexpected. Also, substituting  $d = 5$  into (15) recovers the famous degree 9 that was found by Pearson in 1894 for identifying mixtures of two univariate Gaussians [2, Sec. 3]. Using `NumericalImplicitization.m2`, we verified the correctness of (15) up to  $d = 11$ .

Following this train of thought, and using the Le Barz classification formulas in [9], we compute an analogous formula to (16) for trisecants,  $k = 3$ , of a general smooth surface  $X_d$ :

$$\deg(\text{Sec}_3(X_d)) = \frac{(d-6)(d^5+3d^4-57d^3-43d^2+752d-512)}{48}.$$

Conjecture 25 now suggests that  $d \mapsto \deg \text{Sec}_3(\mathcal{G}_{1,d})$  is a polynomial function of degree 6. Unfortunately, we do not yet have numerical evidence for this. For instance, we do not even know the degree of  $\text{Sec}_3(\mathcal{G}_{1,9})$ . The formula yields the upper bound  $\deg(\text{Sec}_3(X_9)) = 2497$ .

We close with two more cases with  $n \geq 2$  for which we were able to compute the degrees.

**Example 28.** Let  $n = 2$  and  $d = 4$ . The 5-dimensional moment variety  $\mathcal{G}_{2,4}$  has degree 102 in  $\mathbb{P}^{14}$ . It is not defective. Its secant variety  $\text{Sec}_2(\mathcal{G}_{2,4})$  has dimension 11 and degree 538.

**Example 29.** We return to Example 13, so  $n = d = 3$ . The Gaussian moment variety  $\mathcal{G}_{3,3}$  has dimension 9 and degree 130 in  $\mathbb{P}^{19}$ . The number 130 was reported in [2, Sec. 2]. This variety is 2-defective. Its secant variety  $\text{Sec}_2(\mathcal{G}_{3,3})$  has dimension 17 and degree 79. We do not know its ideal generators. As in Example 24, we studied the degrees of its coordinate projections. The 20 coordinates on  $\mathbb{P}^{19}$  come in seven symmetry classes. Representatives are  $m_{000}, m_{100}, m_{200}, m_{110}, m_{300}, m_{201}, m_{111}$ . By omitting these coordinates, one at a time, we obtain hypersurfaces in  $\mathbb{P}^{18}$  whose degrees are 58, 63, 34, 42, 25, 34 and 40 respectively.

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## References

- [1] B. Ådlandsvik: *Varieties with an extremal number of degenerate higher secant varieties*, *J. reine angew. Math.* **392** (1988) 16-26.
- [2] C. Améndola, J.C. Faugère and B. Sturmfels: *Moment varieties of Gaussian mixtures*, *Journal of Algebraic Statistics* **7** (2016) 14-28.
- [3] M. Belkin and K. Sinha: *Polynomial learning of distribution families*, FOCS 2010, 51st Annual IEEE Symposium on Foundations of Computer Science (2010) 103–112.
- [4] M. Brambilla and G. Ottaviani: *On the Alexander-Hirschowitz theorem*, *J. Pure Appl. Algebra* **212** (2008) 1229–1251.
- [5] J. Chen and J. Kileel: *Numerical implicitization for Macaulay2*, [arXiv:1610.03034](https://arxiv.org/abs/1610.03034).
- [6] L. Chiantini and C. Ciliberto: *Weakly defective varieties*, *Transactions Amer. Math. Soc.* **354** (2002) 151–178.
- [7] W. Fulton: *Intersection Theory*, Springer-Verlag, New York (1984).
- [8] Daniel R. Grayson and Michael E. Stillman: *Macaulay2, a software system for research in algebraic geometry*, Available at <http://www.math.uiuc.edu/Macaulay2/>.
- [9] P. Le Barz: *Formules pour les triséchantes des surfaces algébriques*, *Enseign. Math.* (2) **33** (1987) 1–66.
- [10] R. Willink: *Normal moments and Hermite polynomials*, *Statistics and Probability Letters* **73** (2005) 271–275.
- [11] S. Yakowitz and J. Spragins: *On the identifiability of finite mixtures*, *Ann. Math. Statist.* **39** (1968) 209–214.

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