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Metric Algebraic Geometry

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Chapter 1

Historical Snapshot

Throughout this book, we will encounter many classical instances of the interplay of metric concepts with algebraic objects. In classical texts such as Salmon [133], metric properties of algebraic varieties were essential. This includes the curvature of algebraic curves and computing their arc lengths and areas using integral calculus. Conversely, many curves of interest were defined in terms of distances or angular conditions. This chapter provides an introduction to algebraic curves of the latter kind.

We denote the Euclidean distance between two real points P and Q by \overline{PQ} . Over the real numbers, the bilinear form $\langle P, Q \rangle := \sum_{i=1}^n P_i Q_i$ is an inner product and induces the Euclidean norm $\|P\| := \sqrt{\langle P, P \rangle}$. Thus, \overline{PQ} is short notation for $\|P - Q\|$. Throughout this volume, also when $P, Q \in \mathbb{C}^n$ are complex points, we write $\|P\| := \sqrt{\sum_{i=1}^n P_i^2}$ and $\overline{PQ} = \|P - Q\|$. However, over the complex numbers, $\|\cdot\|$ is *not* a norm. For instance, $\|(1, i)\| = 0$.

1.1 Polars

According to Salmon [133, §56], the following theorem was first proven by Roger Cotes (1682-1716) in his *Harmonia Mensurarum*:

Theorem 1.1 (Cotes [43]) Consider an algebraic plane curve C of degree n and a fixed point O in the plane. For any vector v through the point O , we denote by P_v the point on v whose distance to O satisfies

$$\frac{n}{OP_v} = \frac{1}{OR_1} + \frac{1}{OR_2} + \dots + \frac{1}{OR_n}, \quad (1.1)$$

where the points R_1, \dots, R_n are the intersection points of the line spanned by v with the curve C . Then the locus of all points P_v (for all vectors v through O) is a straight line (in fact, two straight lines, but we may choose one by restricting the vector v to a halfspace).

Salmon called this line the *polar line* of the curve C and the point O . For instance, if the curve C is a conic and O a point outside of C , then the polar line is spanned by the two points on C whose tangent line contains O ; see Figure 1.1.

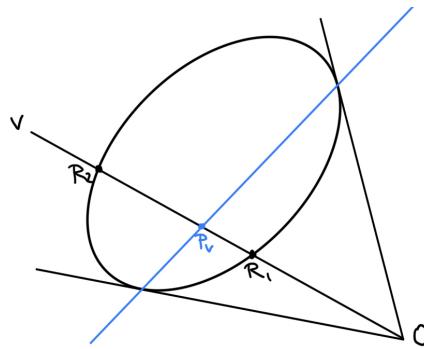


Fig. 1.1: A conic and its polar line (blue) with respect to the point O .

The relation (1.1) mean that the distance from O to P_v is the harmonic mean of the distances from O to the intersection points R_i . Rewriting it as

$$\sum_{i=1}^n \left(\frac{1}{\overline{OP_v}} - \frac{1}{\overline{OR_i}} \right) = 0, \quad (1.2)$$

we see that, in case the point O is at infinity, it specializes to

$$\sum_{i=1}^n \overline{P_v R_i} = 0.$$

Hence, Theorem 1.1 becomes:

Corollary 1.2 *Let C be a plane curve and \mathcal{L} a pencil of parallel lines. The locus of points P_L (for any $L \in \mathcal{L}$) whose signed distances to the intersection points of L with C sum to zero is a straight line.*

Salmon attributes this theorem to Newton¹ who called the resulting straight line the *diameter* of the curve C corresponding to the parallel-lines pencil \mathcal{L} [133, §51].

Remark 1.3 Another theorem on distances of a point to intersection points between a curve and lines that was first given by Newton in his *Enumeratio Linearum Tertii Ordinis* is the following: For a plane curve C of degree n , a point O in the plane, and two distinct lines passing through O , consider the ratio

$$\frac{\overline{OR_1} \cdot \overline{OR_2} \cdots \overline{OR_n}}{\overline{OS_1} \cdot \overline{OS_2} \cdots \overline{OS_n}}, \quad (1.3)$$

where R_1, R_2, \dots, R_n and S_1, S_2, \dots, S_n are the (complex) intersection points of the two lines with C . Then the ratio (1.3) is invariant under translations of the point O and the two intersecting lines [133, §46].

In [133, §57], Salmon generalizes the construction of polar lines to polar curves of higher order. Using the same notation as in Theorem 1.1, he shows that the locus of points P_v satisfying

$$\sum_{1 \leq i < j \leq n} \left(\frac{1}{\overline{OP_v}} - \frac{1}{\overline{OR_i}} \right) \left(\frac{1}{\overline{OP_v}} - \frac{1}{\overline{OR_j}} \right) = 0$$

instead of (1.1) is a conic, called the *polar conic* of the curve C and the point O . If O is at infinity, the polar conic is also referred to as the *diametral conic*. More generally, the locus of points P_v satisfying

$$\sum_{i_1 < \dots < i_k} \left(\frac{1}{\overline{OP_v}} - \frac{1}{\overline{OR_{i_1}}} \right) \left(\frac{1}{\overline{OP_v}} - \frac{1}{\overline{OR_{i_2}}} \right) \cdots \left(\frac{1}{\overline{OP_v}} - \frac{1}{\overline{OR_{i_k}}} \right) = 0$$

is the *polar curve* of order k associated with the curve C and the point O [133, §58]. If O is at infinity, that polar curve is called the *curvilinear diameter* of order k .

The polar curves can be expressed without involving distances. We write $f(x, y, z) = 0$ for the defining equation of the curve C in homogeneous coordinates. For $O = (a, b, c)$, we define the operator

$$\Delta_O := a \frac{\partial}{\partial x} + b \frac{\partial}{\partial y} + c \frac{\partial}{\partial z}.$$

Then, letting $n := \deg C$, the polynomial $\Delta_O^{n-k} f$ is the defining equation of the polar curve of order k [133, §63]. This metric-free approach is how polar curves are typically defined in more modern algebro-geometric literature; see Chapter 4.

¹ Cotes and Newton knew each other. In fact, Cotes edited the second edition of Newton's Principia before its publication.

By exploiting symmetry in Taylor series, Salmon also shows the following beautiful duality between polar curves that “may be written at pleasure” [133, §63] as:

$$\frac{1}{(n-k)!} \Delta_O^{n-k} f(x, y, z) = \frac{1}{k!} \Delta_P^k f(a, b, c),$$

where $P = (x, y, z)$. In particular, the polar curve of order k that is associated with the curve C and the point O is the locus of all points P such that the polar curve of order $n - k$ associated with C and P passes through O .

1.2 Foci

“we believe that it will be found that every point which has any special relation to any curve will be found either to be a singular point of the curve, or a focus of it” [133, §125]

An ellipse is the locus of points in a plane whose sum of distances to two fixed points in the plane is constant. The two points are the *foci* of the ellipse. In 1832, Plücker generalized the definition of foci to arbitrary plane curves as follows. Consider a circle in the plane. If we embed the plane into two dimensional projective space \mathbb{P}^2 by sending $(x, y) \in \mathbb{C}^2$ to $(x : y : 1)$ every circle passes through the two *circular points at infinity* $(1 : i : 0)$ and $(1 : -i : 0)$. In fact, a quadric is a circle if and only if it passes through the two circular points.

Definition 1.4 ([124]) Consider a plane curve C . A point F in the plane is a *focus* of the curve C if both lines spanned by the point F and the circular points at infinity are tangent to the curve C .

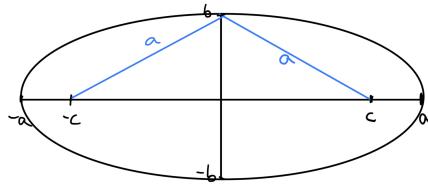


Fig. 1.2: The real foci of an ellipse with width $2a$ and height $2b$ ($a \geq b$) and its axes aligned with the x - and y -axis of the real affine plane are $(\pm\sqrt{a^2 - b^2}, 0)$.

Example 1.5 We determine the foci (in the sense of Plücker’s Definition 1.4) of an ellipse. Since the condition that a line in \mathbb{P}^2 passes through the point $(1 : \pm i : 0)$ is invariant under translations and rotations of the real affine plane $\{z \neq 0\} \subseteq \mathbb{P}^2$, we may translate and rotate the ellipse such that its two defining foci (whose sum of distances is constant along the ellipse) become $(c, 0)$ and $(-c, 0)$ in the real affine plane (with $c \geq 0$). Now the ellipse is the locus of points satisfying

$$\sqrt{(x - c)^2 + y^2} + \sqrt{(x + c)^2 + y^2} = 2a,$$

for some constant $a > 0$. From this, we see that the two points $(\pm a, 0)$ lie on the ellipse. Moreover, the ellipse intersects the y -axis at $(0, \pm b)$ such that $b^2 = a^2 - c^2$; see Figure 1.2. Hence, the width and height of the ellipse are $2a$ and $2b$, respectively, (with $a \geq b > 0$) and its defining equation can alternatively be written as

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1.$$

If the ellipse is not a circle (i.e., $a > b$), then there are two tangent lines to the ellipse that pass through the circular point at infinity $(1 : i : 0)$, namely the tangent lines at $P_+ := (a^2 : ib^2 : c)$ and $P_- := (-a^2 : -ib^2 : c)$. The tangent lines at the complex conjugates \bar{P}_+ and \bar{P}_- of the latter two points pass through the other circular point at infinity $(1 : -i : 0)$. The foci à la Plücker are the four points of intersection of the two tangent lines through $(1 : i : 0)$ with the two tangent lines through $(1 : -i : 0)$. Since the tangent lines at P_\pm and \bar{P}_\pm are a complex conjugated pair, they meet at a real point, namely $(\pm c : 0 : 1)$. This shows that the real foci we used to define the ellipse are indeed foci in the sense of Plücker's Definition 1.4. The other two foci are obtained by intersecting the tangent line at P_\pm with the tangent line at \bar{P}_\mp . They are the imaginary points $(0 : \mp ic : 1)$.

If the ellipse is a circle (i.e., $a = b$), it passes through the circular points at infinity. The tangent lines at those points are the only ones that pass through the circular points at infinity. They are given by $x \pm iy = 0$ and intersect at the origin $(0 : 0 : 1)$. The four foci of a general ellipse come together to a single point, namely the center of the circle.

In general, the number of foci of an algebraic plane curve depends on its *class*, that is the degree of its dual curve. The *dual projective plane* is the set of lines in the original projective plane \mathbb{P}^2 . The *dual curve* C^\vee of a plane curve $C \subseteq \mathbb{P}^2$ is the Zariski closure in the dual projective plane of the set of tangent lines at regular points of C . Hence, the degree of the dual curve C^\vee (equivalently, the class of C) is the number of tangent lines to C that pass through a generic point in the plane \mathbb{P}^2 .

A curve C of class m has m^2 complex foci (counted with multiplicity). Indeed, through each of the two circular points at infinity, there are m tangent lines to the curve C . The foci are the m^2 intersection points of these two sets of m lines. When the curve C is real, exactly m foci are real (namely, the intersection points of conjugate pairs of tangent lines) [133, §125].

There are several constructions that generalize ellipses in an obvious way. For instance, an *n -ellipse* is the locus of points in a plane whose sum of distances to n -fixed points in the plane is constant. n -ellipses were studied by Tschirnhaus in 1686 [145] and Maxwell in 1846 [107]. In general, n -ellipses are not algebraic, but semi-algebraic. In fact, they are special cases of spectrahedra [115].

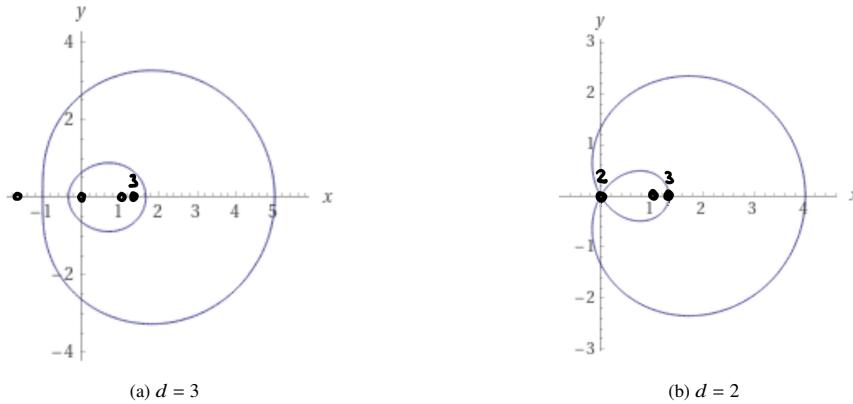


Fig. 1.3: Cartesian ovals with defining foci $F_1 = (0, 0)$, $F_2 = (1, 0)$ and weight $s = 2$ are described by $(-3(x^2 + y^2) + 8x + d^2 - 4)^2 - 4d^2(x^2 + y^2) = 0$. All six real foci are marked.

In the following, we discuss the Cartesian and the Cassini ovals that replace the *sum* of the distances in the definition of an ellipse with a weighted sum or a product, respectively. A *Cartesian oval* (named after Descartes who first studied them in his 1637 *La Géométrie* for their application to optics) is the locus of points in a plane whose weighted sum of distances to two fixed points is constant, i.e., it is the locus of points P that satisfy

$$\overline{PF_1} + s\overline{PF_2} = d,$$

where F_1 and F_2 are fixed points in the plane and s, d are fixed constants. In general, that Cartesian oval is not an algebraic curve, but it does satisfy a quartic equation. In fact, the real vanishing locus of that quartic polynomial is two nested ovals; see Figure 1.3a. Among the four possible equations

$$\overline{PF_1} \pm s\overline{PF_2} = \pm d, \quad (1.4)$$

exactly two have real solutions and those describe the ovals. Salmon shows that a quartic curve is a Cartesian oval if and only if it has cusps at the two circular points at infinity [133, §129]. By Plücker's formula [133, §72], it follows that the class of such a quartic is six (except in degenerate cases). Salmon determines the six real foci of Cartesian oval quartic curves [133, §129] (see also Basset [10, §273]): Three of them form a triple focus which is located at the intersection of the cusps' tangent lines. The remaining three foci lie on a straight line. Two of them are the points F_1 and F_2 that define the curve in (1.4). It was already observed by Chasles that in fact any two of the three single foci can be used to define the Cartesian oval by an equation of the form (1.4) [37, Note XXI]. If two of the three single foci come together, the Cartesian oval degenerates to a *Limaçon of Pascal*; see Figure 1.3b. Salmon further observes another interesting metric property of foci: Whenever a line meets a Cartesian oval in four points, the sum of their four distances from any of the three single foci is constant [133, §218].

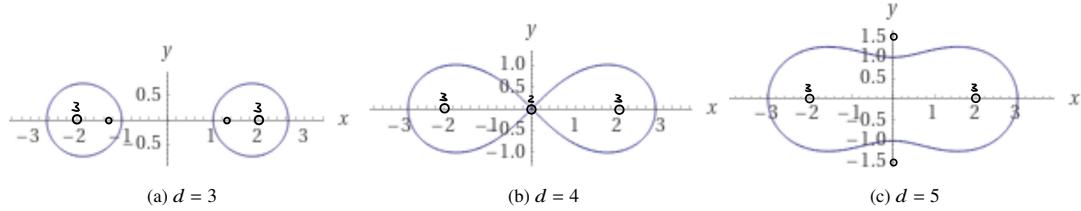


Fig. 1.4: Cassini ovals with defining foci $F_1 = (-2, 0), F_2 = (2, 0)$ and their remaining foci.

A *Cassini oval* (named after Cassini who studied them in 1693 [33]) is the locus of points in a plane whose product of distances to two fixed points F_1 and F_2 is constant. This is an algebraic curve defined by the real quartic polynomial

$$\overline{PF_1}^2 \cdot \overline{PF_2}^2 = d^2$$

for some constant d . The circular points at infinity are double points on each Cassini oval, and since these are the only singularities (except in degenerate cases), the class of a Cassini oval is eight in general [133, §219]. Basset [10, §247] explains that the two pairs of complex conjugated tangent lines at the two nodes intersect at F_1 and F_2 , respectively. Hence, those points are foci in the sense of Plücker's Definition 1.4. In fact, Basset shows that each of them is a triple focus (the reason being that the nodal tangents are stationary). To describe the remaining two real foci, we translate and rotate (as in Example 1.5) such that $F_1 = (c, 0)$ and $F_2 = (-c, 0)$. Then, the Cassini oval is defined by

$$\left((x - c)^2 + y^2 \right) \left((x + c)^2 + y^2 \right) = d^2.$$

If $d < c^2$, the real locus is two ovals. Otherwise, the real locus is connected, where the degenerate case $d = c^2$ is the *lemniscate of Bernoulli*; see Figure 1.4. In the case of two ovals, the remaining two real foci also lie on the x -axis; they are $(\pm \frac{1}{c} \sqrt{c^4 - d^2}, 0)$. If $d > c^2$, the two foci are $(0, \pm \frac{1}{c} \sqrt{d^2 - c^4})$ and lie on the y -axis. In the degenerate case $d = c^2$, they become a double focus at the origin.

1.3 Envelopes

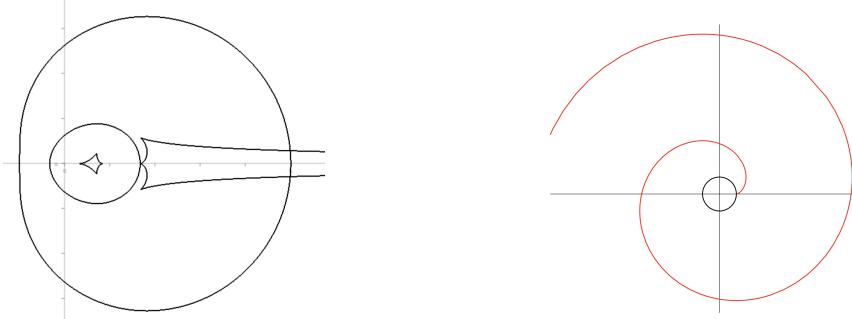
Given a one-dimensional algebraic family of lines in the plane, its *envelope* is a curve such that each of the given lines is tangent to the curve. Equivalently, in the dual projective plane, the family of lines is an algebraic curve \mathcal{L} and its dual curve \mathcal{L}^\vee is the envelope.



Fig. 1.5: Cubic curve $x^3 + 5x^2 + x - 1 - 2xy + y^3 = 0$ (blue) and the envelope $9xy + 15y - 1 = 0$ (red) of its diameters. The diameter (green) and diametral conic (yellow) are associated with the point $(2 : 1 : 0)$ at infinity.

Example 1.6 The diameters of a plane curve C form a one-dimensional family of lines. For a cubic curve C , the envelope of that family is the locus consisting of the centers of the diametral conics of C [133, §160]. For instance, for the cubic curve defined by $x^3 + y^3 + 5x^2 - 2xy + x - 1 = 0$, the diameter associated with the point $(a : b : 0)$ at infinity is the line given by $3a^2x + 3b^2y + 5a^2 - 2ab = 0$. The family of all diameters is the curve \mathcal{L} in the dual plane that is defined by $25x^2 - 4xy - 30x + 9 = 0$. Its dual curve \mathcal{L}^\vee , that is the envelope of the diameters, is $9xy + 15y - 1 = 0$. The diametral conic associated with $(a : b : 0)$ is $3a \left(x + \frac{5a-b}{3a} \right)^2 + 3b \left(y - \frac{a}{3b} \right)^2 + a - \frac{(5a-b)^2}{3a} - \frac{a^2}{3b} = 0$ and so its center $\left(\frac{-5a+b}{3a}, \frac{a}{3b} \right)$ lies on the envelope. In fact, the tangent line of the envelope at that point is the diameter associated with $(a : b : 0)$; see Figure 1.5.

Special instance of envelopes that are defined by metric properties are evolutes and caustics, both of which we will discuss in the remainder of this chapter. The *evolute* of a plane curve C is the envelope of its normals (i.e., the lines orthogonal to its tangent lines). Equivalently, the evolute is the locus of the centers of curvature (see Chapter 6.1 for an introduction on curvature). The study of evolutes goes back to Apollonius (ca. 200 BC) [148]. A recent discussion of evolutes can be found in [121]. The degree and



(a) The Cartesian oval from Figure 1.3a together with its evolute. (b) A circle with one of its parallel involutes.

Fig. 1.6: Evolute and involute.

class of the evolute of a general smooth curve of degree n are $3n(n - 1)$ [133, §119] and n^2 [133, §116], respectively. Moreover, its evolute has $\frac{n}{2}(3n - 5)(3n^2 - n - 6)$ double points, $3n(2n - 3)$ cusps, and no other singularities. For instance, the evolute of the Cartesian oval in Figure 1.3a is illustrated in Figure 1.6a. Its defining equation is

$$\begin{aligned}
 & 102036672x^{10}y^2 + 433655856x^8y^4 + 833407380x^6y^6 + 917059401x^4y^8 + 558336726x^2y^{10} + 143065521y^{12} \\
 & - 884317824x^9y^2 - 3106029888x^7y^4 - 4898885832x^5y^6 - 4008450240x^3y^8 - 1331276472xy^{10} + 3251316672x^8y^2 \\
 & + 9515584512x^6y^4 + 12088352844x^4y^6 + 6432939486x^2y^8 + 620191890y^{10} - 40310784x^9 - 6758774784x^7y^2 \\
 & - 16647933888x^5y^4 - 15962551632x^3y^6 - 4237194240xy^8 + 342641664x^8 + 9145229184x^6y^2 + 18728830368x^4y^4 \\
 & + 11743648812x^2y^6 + 961612425y^8 - 1239556608x^7 - 9234062208x^5y^2 - 14497919136x^3y^4 - 4640798304xy^6 \\
 & + 2495722752x^6 + 8064660672x^4y^2 + 8003654064x^2y^4 + 835700656y^6 - 3071831040x^5 - 6288399360x^3y^2 \\
 & - 2974296960xy^4 + 2390342400x^4 + 3772699200x^2y^2 + 540271200y^4 - 1173312000x^3 - 1396800000xy^2 \\
 & + 349920000x^2 + 228000000y^2 - 57600000x + 4000000 = 0.
 \end{aligned}$$

We will see in Chapter 6.1 that the finite cusps of the evolute correspond to the points of critical curvature of the original curve C . Salmon computes the length of an arc of the evolute as “the difference of the radii of curvature at its extremities” [133, §115]. The converse operation of computing the evolute is finding an *involute*, that is, for a given plane curve C , find any curve whose evolute is C . In contrast to evolutes, involutes of an algebraic curve are typically not unique (they are parallel curves / offset curves; see Section 7.2) and they might not be algebraic. For instance, the involute of a circle is a transcendental curve [133, §235] because it has infinitely many intersection points with any given line; see Figure 1.6b. Nevertheless, the foci of a plane curve are also foci of its evolute and involute [133, §127].

Caustics of plane curves come in two flavors. Let us imagine that a fixed point in the plane emits light. The light rays get reflected at each point of a given plane curve. The *caustic by reflection* is the envelope of the family of reflected rays. Similarly, the *caustic by refraction* is the envelope of the family of refracted rays. Figure 1.7 shows caustics of a circle when the light source is at infinity. Those curves can be commonly observed in real life, e.g., when the sun shines on a round glass.

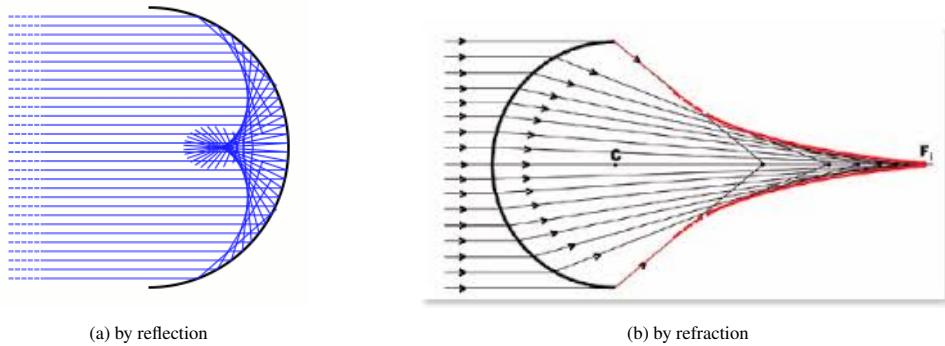


Fig. 1.7: Caustics of a circle with light source at infinity.

Chapter 2

Critical Equations

We consider a model $X_{\mathbb{R}}$ that is given as the zero set in \mathbb{R}^n of a collection $\{f_1, \dots, f_k\}$ of nonlinear polynomials in n unknowns x_1, \dots, x_n . Thus, $X_{\mathbb{R}}$ is a *real algebraic variety*. In order to apply algebraic methods, it is preferable to work with the complex algebraic variety $X \subset \mathbb{C}^n$ defined by the same polynomials. Thus $X_{\mathbb{R}}$ is the subset of real points in the complex variety X . We assume that X is irreducible, that $I_X = \langle f_1, \dots, f_k \rangle$ is its prime ideal, and that the set of nonsingular real points is Zariski dense in X . The $k \times n$ Jacobian matrix $\mathcal{J} = (\partial f_i / \partial x_j)$ has rank at most c at any point $x \in X$, where $c = \text{codim}(X)$. The point \mathbf{x} is *nonsingular* on X if the rank is exactly c . The variety X is called *smooth* if all its points are nonsingular. Elaborations on these hypotheses are found in many text books, including [111, Chapter 2].

The following optimization problem arises in many applications. Given a data point $\mathbf{u} \in \mathbb{R}^n \setminus X$, compute the distance to the model $X_{\mathbb{R}}$. Thus, we seek a point \mathbf{x}^* in $X_{\mathbb{R}}$ that is closest to \mathbf{u} . The answer depends on the chosen metric. We focus on the case when the metric is represented by a polynomial and \mathbf{x}^* is a smooth point on X . The optimal point \mathbf{x}^* is a solution to the *critical equations*. In optimization, these are also known as first-order conditions or KKT equations, and they arise from introducing Lagrange multipliers. We seek to compute all complex solutions to the critical equations. The set of these *critical points* is typically finite, and it includes all local maxima, all local minima and all saddle points.

2.1 Euclidean Distance Degree

We begin by discussing the *Euclidean distance (ED) problem*, which is as follows:

$$\underset{i=1}{\text{minimize}} \sum_{i=1}^n (x_i - u_i)^2 \text{ subject to } \mathbf{x} \in X. \quad (2.1)$$

Our first step is to derive the critical equations for (2.1). The *augmented Jacobian matrix* \mathcal{AJ} is the $(k+1) \times n$ matrix which is obtained by placing the row vector $(x_1 - u_1, \dots, x_n - u_n)$ atop the Jacobian matrix \mathcal{J} . We form the ideal generated by its $(c+1) \times (c+1)$ minors, we add the ideal of the model I_X , and we then saturate that sum by the ideal of $c \times c$ minors of \mathcal{J} . See [52, Eqn. (2.1)]. The result is the *critical ideal* $C_{X,\mathbf{u}}$ of the model X with respect to the given data point \mathbf{u} .

Example 2.1 (Plane curves) Let X be the plane curve defined by a polynomial $f(x_1, x_2)$ in two unknowns. We wish to compute the Euclidean distance from X to a given point $\mathbf{u} = (u_1, u_2) \in \mathbb{R}^2$. To this end, we form the augmented Jacobian matrix. This matrix is square of size 2×2 :

$$\mathcal{AJ} = \begin{pmatrix} x_1 - u_1 & x_2 - u_2 \\ \partial f / \partial x_1 & \partial f / \partial x_2 \end{pmatrix} \quad (2.2)$$

The critical ideal is obtained from f and the determinant of \mathcal{AJ} by performing a saturation step:

$$C_{X,\mathbf{u}} = \langle f, \det(\mathcal{AJ}) \rangle : \langle \partial f / \partial x_1, \partial f / \partial x_2 \rangle^\infty. \quad (2.3)$$

The ideal $C_{X,\mathbf{u}}$ lives in $\mathbb{R}[x_1, x_2]$. Frequently, the coefficients of f and the coordinates of \mathbf{u} are rational numbers, and in this case we can perform the computation purely symbolically in $\mathbb{Q}[x_1, x_2]$. The saturation step in (2.3) removes points that are singular on the curve $X = \mathcal{V}(f)$. If X is smooth then saturation is unnecessary, and we simply have $C_{X,\mathbf{u}} = \langle f, \det(\mathcal{AJ}) \rangle$.

In applications, we must expect singularities. For a concrete example take the cardioid

$$f = (x_1^2 + x_2^2 + x_2)^2 - (x_1^2 + x_2^2), \quad (2.4)$$

and fix a random point $\mathbf{u} = (u_1, u_2)$. See [52, Example 1.1]. The ideal $\langle f, \det(\mathcal{AJ}) \rangle$ is the intersection of $C_{X,\mathbf{u}}$ and an $\langle x_1, x_2 \rangle$ -primary ideal of multiplicity 3. The critical ideal $C_{X,\mathbf{u}}$ has three distinct complex zeros. We can express their coordinates in radicals in the given numbers u_1, u_2 .

The variety $\mathcal{V}(C_{X,\mathbf{u}})$ is the set of complex critical points of (2.1). For random data \mathbf{u} , this variety is a finite subset of \mathbb{C}^n , and it contains the optimal solution \mathbf{x}^* , provided the latter is attained at a smooth point of X . It was proved in [52] that the number of critical points, i.e. the cardinality of the variety $\mathcal{V}(C_{X,\mathbf{u}})$, is independent of \mathbf{u} , if we assume that the data point \mathbf{u} is sufficiently general. This number is called the *ED degree* of the variety X . In Example 2.1 we examined a plane curve of degree 4 whose ED degree equals 3. The ED degree of a variety X measures the difficulty of solving the ED problem (2.1) using exact algebraic methods. The ED degree is an important complexity measure in metric algebraic geometry.

Example 2.2 (Space curves) Fix $n = 3$ and let X be the curve in \mathbb{R}^3 defined by two general polynomials f_1 and f_2 of degrees d_1 and d_2 in three unknowns x_1, x_2, x_3 . The augmented Jacobian matrix is

$$\mathcal{AJ} = \begin{pmatrix} x_1 - u_1 & x_2 - u_2 & x_3 - u_3 \\ \partial f_1 / \partial x_1 & \partial f_1 / \partial x_2 & \partial f_1 / \partial x_3 \\ \partial f_2 / \partial x_1 & \partial f_2 / \partial x_2 & \partial f_2 / \partial x_3 \end{pmatrix}. \quad (2.5)$$

Fix a general data vector $\mathbf{u} \in \mathbb{R}^3$. Then the critical ideal equals $C_{X,\mathbf{u}} = \langle f_1, f_2, \det(\mathcal{AJ}) \rangle$. Hence the set of critical points is the intersection of three surfaces. These surfaces have degrees d_1, d_2 and $d_1 + d_2 - 1$. By Bézout's Theorem [111, Theorem 2.16], the expected number of solutions is the product of these degrees. Hence the ED degree of the curve X equals $d_1 d_2 (d_1 + d_2 - 1)$.

The same formula can be derived from a formula for general curves in terms of algebraic geometry data. Let X be a general smooth curve of degree d and genus g in any ambient space \mathbb{R}^n . By [52, Corollary 5.9], we have $\text{EDdegree}(X) = 3d + 2g - 2$. The above curve in 3-space has degree $d = d_1 d_2$ and genus $g = d_1^2 d_2 / 2 + d_1 d_2^2 / 2 - 2d_1 d_2 + 1$. We conclude that

$$\text{EDdegree}(X) = 3d + 2g - 2 = d_1 d_2 (d_1 + d_2 - 1).$$

This formula also covers the case of plane curves (cf. Example 2.1). Namely, if we set $d_1 = d$ and $d_2 = 1$ then we see that a general plane curve X of degree d has $\text{EDdegree}(X) = d^2$. In particular, a general plane quartic has ED degree 16. However, that number can drop a lot for curves that are special. For the cardioid in (2.4) the ED degree drops from 16 to 3.

Here is a general upper bound on the ED degree in terms of the given polynomials.

Proposition 2.3 *Let X be a variety of codimension c in \mathbb{R}^n whose ideal I_X is generated by polynomials $f_1, f_2, \dots, f_c, \dots, f_k$ of degrees $d_1 \geq d_2 \geq \dots \geq d_c \geq \dots \geq d_k$. Then*

$$\text{EDdegree}(X) \leq d_1 d_2 \cdots d_c \cdot \sum_{i_1+i_2+\cdots+i_c \leq n-c} (d_1 - 1)^{i_1} (d_2 - 1)^{i_2} \cdots (d_c - 1)^{i_c}. \quad (2.6)$$

Equality holds when X is a generic complete intersection of codimension c (hence $c = k$).

Proof This appears in [52, Proposition 2.6]. We can derive it as follows. Bézout's Theorem ensures that the degree of the variety X is at most $d_1 d_2 \cdots d_c$. The entries in the i th row of the matrix \mathcal{AJ} are polynomials of degrees $d_i - 1$. The degree of the variety of $(c+1) \times (c+1)$ minors of \mathcal{AJ} is at most the sum in (2.6). This follows from the Giambelli–Thom–Porteous formula, which expresses the degree of a determinantal variety in terms of symmetric functions. The intersection of that determinantal variety with X is our set of critical points, and the cardinality of that set is bounded by the product of the two degrees. Generically, that intersection is a complete intersection and the inequality (2.6) is attained. \square

Formulas or a priori bounds for the ED degree are important when studying exact solutions to the optimization problem (2.1). The paradigm is to compute all complex critical points, by either symbolic or numerical methods, and to then extract one's favorite real solutions among these. This leads, for instance, to all local minima in (2.1). The ED degree is an upper bound on the number of real critical points, but this bound is generally not tight.

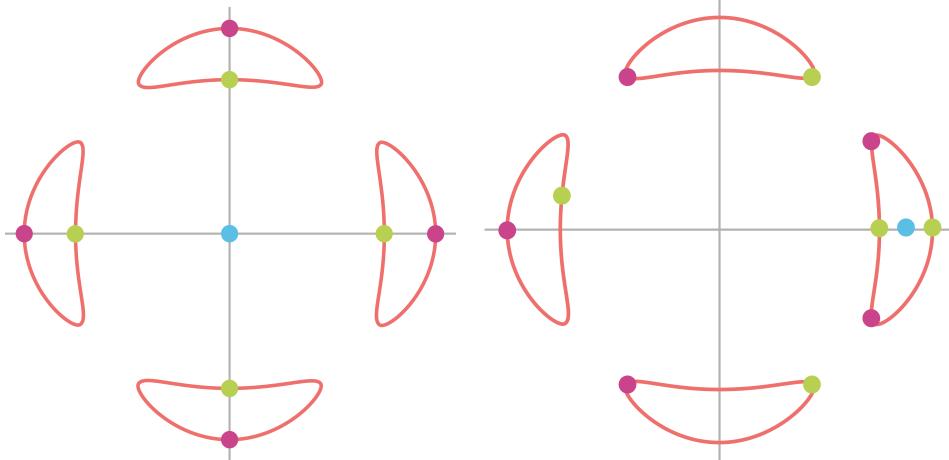


Fig. 2.1: ED problems on the Trott curve: configurations of eight (left) or ten (right) critical points. Data points are blue, local minimal are green, and local maxima are purple. The coordinates of the critical points are computed by solving the critical equations in (2.7).

Example 2.4 Consider the case $n = 2, c = 1, d_1 = 4$ in Proposition 2.3, where X is a generic quartic curve in the plane \mathbb{R}^2 . The number of complex critical points is $\text{EDdegree}(X) = 16$. But, they cannot be all real. For an illustration, consider the *Trott curve* $X = V(f)$, given by

$$f = 144(x_1^4 + x_2^4) - 225(x_1^2 + x_2^2) + 350x_1^2x_2^2 + 81.$$

This curve is shown in Figure 2.1. For general data $\mathbf{u} = (u_1, u_2)$ in \mathbb{R}^2 , the critical equations

$$f = \frac{\partial f}{\partial x_2}(x_1 - u_1) - \frac{\partial f}{\partial x_1}(x_2 - u_2) = 0. \quad (2.7)$$

have distinct 16 complex solutions, and these are all critical points in X . Since the Trott curve is smooth, the saturation step in (2.3) is not needed when computing the ideal $C_{X,\mathbf{u}}$.

The ED degree 16 is an upper bound for the number of real critical points of the optimization problem (2.1) for any data point \mathbf{u} . The actual number of real critical points depends heavily on the specific location of \mathbf{u} . For data \mathbf{u} near the origin, eight of the 16 points in $V(C_{X,\mathbf{u}})$ are real. For $\mathbf{u} = (\frac{7}{8}, \frac{1}{100})$, which is inside the rightmost oval, there are 10 real critical points. The two scenarios are shown in Figure 2.1. Local minima are green, while local maxima are purple. Finally, consider $\mathbf{u} = (2, \frac{1}{100})$, which lies to the right of the rightmost oval. Here, the number of real critical points is 12.

In general, our task is to compute the complex zeros of the critical ideal $C_{X,\mathbf{u}}$. Algorithms for this computation can be either symbolic or numerical. Symbolic methods usually rest on the construction of a Gröbner basis, to be followed by a floating point computation to extract the solutions. In recent years, numerical methods have become popular. These are based on homotopy continuation. Two notable

packages are `Bertini` [12] and `HomotopyContinuation.jl` [27]. The ED degree is important here because it indicates how many paths need to be tracked to solve (2.1). We next illustrate current capabilities.

Example 2.5 Suppose X is defined by $c = k = 3$ random polynomials in $n = 7$ variables, for a range of degrees d_1, d_2, d_3 . The table below lists the ED degree in each case, and the times used by `HomotopyContinuation.jl` to compute and certify all critical points in \mathbb{C}^7 .

$d_1 \ d_2 \ d_3$	3 2 2	3 3 2	3 3 3	4 2 2	4 3 2	4 3 3	4 4 2	4 4 3
EDdegree	1188	3618	9477	4176	10152	23220	23392	49872
Solving (sec)	3.849	21.06	61.51	31.51	103.5	280.0	351.5	859.3
Certifying (sec)	0.390	1.549	4.653	2.762	7.591	17.16	21.65	50.07

Here we represent $C_{X,\mathbf{u}}$ by a system of 10 equations in 10 variables. In addition to the three equations $f_1 = f_2 = f_3 = 0$ in x_1, \dots, x_7 , we take the seven equations $(1, y_1, y_2, y_3) \cdot \mathcal{AJ} = 0$. Here y_1, y_2, y_3 are new variables. These additional equations ensure that the 4×7 matrix \mathcal{AJ} has rank ≤ 3 . This formulation avoids the listing of all $\binom{7}{4} = 35$ maximal minors. It is the preferred representation of determinantal varieties in the setting of numerical algebraic geometry.

The timings above refer to computing all complex solutions to the system of 10 equations in 10 variables. They include the certification step [26] that proves correctness and completeness. These computations were performed using `HomotopyContinuation.jl` v2.5.6 on a 16 GB MacBook Pro with an Intel Core i7 processor working at 2.6 GHz. They suggest that our critical equations can be solved fast and reliably, with proof of correctness, when the ED degree is less than 50000. When the ED degree exceeds 50000, success with numerical path tracking will depend on the specific structure of the family. A key player on the geometric side is the discriminant of the problem. If that is well-behaved, then even larger ED degrees are feasible. A successful application to a physics problem is reported in [142, Table 1].

2.2 Low Rank Matrix Approximation

When the ED problem (2.1) arises in an application, one often considers varieties of matrices of low rank that are constrained to have a special structure. Sometimes these matrices are flattenings of tensors. This version of the problem was studied in the article [118], which focuses on Hankel matrices, Sylvester matrices and generic subspaces of matrices, and which uses a weighted version of the Euclidean metric. In this section we offer a brief introduction to this special case of our general ED problem.

Our point of departure is the following low-rank approximation problem for rectangular matrices:

$$\text{minimize } \|A - U\|_\Lambda^2 = \sum_{i=1}^m \sum_{j=1}^n \lambda_{ij} (a_{ij} - u_{ij})^2 \quad \text{subject to} \quad \text{rank}(A) \leq r. \quad (2.8)$$

In this problem, we are given a real *data matrix* $U = (u_{ij})$ of format $m \times n$, and we wish to find a real matrix $A = (a_{ij})$ of rank at most r that is closest to U in a weighted Frobenius norm. The entries of the *weight matrix* $\Lambda = (\lambda_{ij})$ are positive real numbers. If $m \leq n$ and the weight matrix Λ is the all-one matrix $\mathbf{1}$, then the solution to (2.8) is given by the *singular value decomposition*

$$U = T_1 \cdot \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_m) \cdot T_2.$$

Here T_1, T_2 are orthogonal matrices, and $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_m$ are the singular values of U . The following well-known theorem from numerical linear algebra concerns the variety X of $m \times n$ matrices of rank $\leq r$.

Theorem 2.6 (Eckart-Young) *The closest matrix of rank $\leq r$ to the given matrix U equals*

$$U^* = T_1 \cdot \text{diag}(\sigma_1, \dots, \sigma_r, 0, \dots, 0) \cdot T_2. \quad (2.9)$$

This is the unique local minimum. All complex critical points are real. They are found by substituting zeros for $m - r$ of the entries of $\text{diag}(\sigma_1, \dots, \sigma_m)$. Hence, $\text{EDdegree}(X) = \binom{m}{r}$.

For general weights Λ , the situation is more complicated. In particular, there can be complex critical points and multiple local minima. We discuss a small instance in Example 2.8.

First, let us define the problem of *structured low-rank approximation*. In this problem, we are given a linear subspace $\mathcal{L} \subset \mathbb{R}^{m \times n}$, and a data matrix $U \in \mathcal{L}$, and we wish to solve the restricted problem:

$$\text{minimize } \|A - U\|^2 = \sum_{i=1}^m \sum_{j=1}^n \lambda_{ij} (a_{ij} - u_{ij})^2 \text{ subject to } A \in \mathcal{L} \text{ and } \text{rank}(A) \leq r. \quad (2.10)$$

A best-case scenario for $\Lambda = \mathbf{1}$ would be the following: if U lies in \mathcal{L} then so does the SVD solution U^* in (2.9). This happens for some linear subspaces \mathcal{L} , including symmetric and circulant matrices. However, most subspaces \mathcal{L} of $\mathbb{R}^{m \times n}$ do not enjoy this property, and finding the global optimum in (2.10) can be quite difficult, even for $\Lambda = \mathbf{1}$. The article [118] studies this optimization problem for both generic and special subspaces \mathcal{L} . It rests on [52] and uses tools from algebraic geometry.

As before, our primary task is to compute the number of complex critical points of (2.10). Thus, we seek to find the Euclidean distance degree (ED degree) of the determinantal variety

$$\mathcal{L}_{\leq r} := \{A \in \mathcal{L} : \text{rank}(A) \leq r\}.$$

This variety is always regarded as a subvariety of the matrix space $\mathbb{R}^{m \times n}$. We use the Λ -weighted Euclidean distance coming from $\mathbb{R}^{m \times n}$. We write $\text{EDdegree}_\Lambda(\mathcal{L}_{\leq r})$ for the Λ -weighted Euclidean distance degree of the variety $\mathcal{L}_{\leq r}$. Thus $\text{EDdegree}_\Lambda(\mathcal{L}_{\leq r})$ is the number of complex critical points of the problem (2.10) for data matrices U that are generic in \mathcal{L} . The importance of the weights Λ is highlighted in [52, Example 3.2], for the seemingly harmless situation when \mathcal{L} is the space of all symmetric matrices in $\mathbb{R}^{n \times n}$.

Of special interest are the *unit ED degree*, when $\Lambda = \mathbf{1}$ is the all-one matrix, and the *generic ED degree*, denoted $\text{EDdegree}_{\text{gen}}(\mathcal{L}_{\leq r})$, when the weight matrix Λ is generic. The generic ED degree is given by a formula that rests on intersection theory. See [52, Theorem 7.7] and Theorem 2.9 below. Indeed, choosing the positive weights λ_{ij} to be generic ensures that the projective closure of $\mathcal{L}_{\leq r}$ has transversal intersection with the isotropic quadric

$$\{A \in \mathbb{P}^{mn-1} : \sum_{i=1}^m \sum_{j=1}^n \lambda_{ij} a_{ij}^2 = 0\}.$$

We next present two examples that illustrate the concepts above. These can then also serve as examples for Theorem 2.9 below, as seen by the Macaulay2 calculation in Example 2.15.

Example 2.7 Let $m = n = 3$ and $\mathcal{L} \subset \mathbb{R}^{3 \times 3}$ the 5-dimensional space of Hankel matrices:

$$A = \begin{bmatrix} a_0 & a_1 & a_2 \\ a_1 & a_2 & a_3 \\ a_2 & a_3 & a_4 \end{bmatrix}, \quad U = \begin{bmatrix} u_0 & u_1 & u_2 \\ u_1 & u_2 & u_3 \\ u_2 & u_3 & u_4 \end{bmatrix} \quad \text{and} \quad \Lambda = \begin{bmatrix} \lambda_0 & \lambda_1 & \lambda_2 \\ \lambda_1 & \lambda_2 & \lambda_3 \\ \lambda_2 & \lambda_3 & \lambda_4 \end{bmatrix}.$$

Our goal in (2.10) is to solve the following constrained optimization problem for $r = 1, 2$:

$$\begin{aligned} & \text{minimize } \lambda_0(a_0 - u_0)^2 + 2\lambda_1(a_1 - u_1)^2 + 3\lambda_2(a_2 - u_2)^2 + 2\lambda_3(a_3 - u_3)^2 + \lambda_4(a_4 - u_4)^2 \\ & \text{subject to } \text{rank}(X) \leq r. \end{aligned}$$

This can be rephrased as an unconstrained optimization problem. For instance, for rank $r = 1$, we get a one-to-one parametrization of $\mathcal{L}_{\leq 1}$ by setting $a_i = st^i$. Our optimization problem is as follows:

$$\text{Minimize } \lambda_0(s - u_0)^2 + 2\lambda_1(st - u_1)^2 + 3\lambda_2(st^2 - u_2)^2 + 2\lambda_3(st^3 - u_3)^2 + \lambda_4(st^4 - u_4)^2.$$

The ED degree is the number of critical points with $t \neq 0$. We consider three weight matrices:

$$\mathbf{1} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}, \quad \Omega = \begin{bmatrix} 1 & 1/2 & 1/3 \\ 1/2 & 1/3 & 1/2 \\ 1/3 & 1/2 & 1 \end{bmatrix}, \quad \Theta = \begin{bmatrix} 1 & 2 & 2 \\ 2 & 2 & 2 \\ 2 & 2 & 1 \end{bmatrix}.$$

Here Ω gives the usual Euclidean metric when \mathcal{L} is identified with \mathbb{R}^5 . The last weight matrix Θ arises from identifying \mathcal{L} with the space of symmetric $2 \times 2 \times 2 \times 2$ -tensors. We compute

$$\begin{aligned} \text{EDdegree}_\mathbf{1}(\mathcal{L}_{\leq 1}) &= 6, & \text{EDdegree}_\Omega(\mathcal{L}_{\leq 1}) &= 10, & \text{EDdegree}_\Theta(\mathcal{L}_{\leq 1}) &= 4, \\ \text{EDdegree}_\mathbf{1}(\mathcal{L}_{\leq 2}) &= 9, & \text{EDdegree}_\Omega(\mathcal{L}_{\leq 2}) &= 13, & \text{EDdegree}_\Theta(\mathcal{L}_{\leq 2}) &= 7. \end{aligned}$$

In both cases, Ω exhibits the generic behavior, so we have $\text{EDdegree}_{\text{gen}}(\mathcal{L}_{\leq r}) = \text{EDdegree}_\Omega(\mathcal{L}_{\leq r})$. We refer to [118, Sections 3 and 4] for larger Hankel matrices and formulas for their ED degrees.

Example 2.8 Let $m = n = 3, r = 1$ but now take $\mathcal{L} = \mathbb{R}^{3 \times 3}$. Thus, we are considering the weighted rank-one approximation problem for 3×3 -matrices. We know from [52, Example 7.10] that $\text{EDdegree}_{\text{gen}}(\mathcal{L}_{\leq 1}) = 39$. We take a circulant data matrix and a circulant weight matrix:

$$U = \begin{bmatrix} -59 & 11 & 59 \\ 11 & 59 & -59 \\ 59 & -59 & 11 \end{bmatrix} \quad \text{and} \quad \Lambda = \begin{bmatrix} 9 & 6 & 1 \\ 6 & 1 & 9 \\ 1 & 9 & 6 \end{bmatrix}.$$

This instance has 39 complex critical points. Of these, 19 are real, and 7 are local minima:

$$\begin{aligned} &\begin{bmatrix} 0.0826 & 2.7921 & -1.5452 \\ 2.7921 & 94.3235 & -52.2007 \\ -1.5452 & -52.2007 & 28.8890 \end{bmatrix}, \begin{bmatrix} -52.2007 & 28.8890 & -1.5452 \\ 2.7921 & -1.5452 & 0.0826 \\ 94.3235 & -52.2007 & 2.7921 \end{bmatrix}, \begin{bmatrix} -52.2007 & 2.7921 & 94.3235 \\ 28.8890 & -1.5452 & -52.2007 \\ -1.5452 & 0.0826 & 2.7921 \end{bmatrix}, \\ &\begin{bmatrix} -29.8794 & 36.2165 & -27.2599 \\ -32.7508 & 39.6968 & -29.8794 \\ 39.6968 & -48.1160 & 36.2165 \end{bmatrix}, \begin{bmatrix} -48.1160 & 36.2165 & 39.6968 \\ 36.2165 & -27.2599 & -29.8794 \\ 39.6968 & -29.8794 & -32.7508 \end{bmatrix}, \begin{bmatrix} -29.8794 & -32.7508 & 39.6968 \\ 36.2165 & 39.6968 & -48.1160 \\ -27.2599 & -29.8794 & 36.2165 \end{bmatrix}, \\ &\begin{bmatrix} -25.375 & -25.375 & -25.375 \\ -25.375 & -25.375 & -25.375 \\ -25.375 & -25.375 & -25.375 \end{bmatrix}. \end{aligned}$$

The first three are the global minima in our ED distance problem. The last matrix is the local minimum where the objective function has the largest value: note that each entry equals $-203/8$. The entries of the first six matrices are algebraic numbers of degree 10 over \mathbb{Q} . For instance, the two upper left entries 0.0826 and -48.1160 are among the four real roots of the irreducible polynomial

$$\begin{aligned} &164466028468224x^{10} + 27858648335954688x^9 + 1602205386689376672x^8 + 7285836260028875412x^7 \\ &- 2198728936046680414272x^6 - 14854532690380098143152x^5 + 2688673091228371095762316x^4 \\ &+ 44612094455115888622678587x^3 - 41350080445712457319337106x^2 \\ &+ 27039129499043116889674775x - 1977632463563766878765625. \end{aligned}$$

Here, the critical ideal in $\mathbb{Q}[x_{11}, x_{12}, \dots, x_{33}]$ is not prime. It is the intersection of six maximal ideals. Their degrees over \mathbb{Q} are 1, 2, 6, 10, 10, 10. The sum of these numbers equals $39 = \text{EDdegree}_{\text{gen}}(\mathcal{L}_{\leq 1})$.

Explicit formulas are derived in [118, Section 3] for $\text{EDdegree}_{\text{gen}}(\mathcal{L}_{\leq r})$ when \mathcal{L} is a generic subspace of $\mathbb{R}^{m \times n}$. This covers the four cases that arise by pairing affine subspaces or linear subspaces with either unit weights or generic weights. One important feature of determinantal varieties is they are not complete intersections. Their ED degrees are much smaller than suggested by the upper bound in Proposition 2.3.

2.3 Invitation to Polar Degrees

We have introduced the ED degree of an algebraic variety X as a complexity measure for the ED problem in (2.1). The number 39 in the previous example served as an illustration on how the ED degree controls the number of critical points. But a deeper understanding is needed. In this section, we develop the algebro-geometric roots of the ED degree, which will then yield more advanced algorithms for finding it.

Theorem 2.9 *If the given variety X meets both the hyperplane at infinity and the isotropic quadric transversally, then $\text{EDdegree}(X)$ equals the sum of the polar degrees of the projective closure of X .*

We shall explain all the terms used in this theorem. First of all, the *projective closure* of our affine real variety $X \subset \mathbb{C}^n$ is its Zariski closure in complex projective space \mathbb{P}^n , which we also denote by X . Algebraically, \mathbb{P}^n is obtained from \mathbb{C}^n by adding one homogenizing coordinate x_0 . We identify the affine space \mathbb{C}^n with the open subset $\{\mathbf{x} \in \mathbb{P}^n : x_0 \neq 0\}$. Its set complement $\{\mathbf{x} \in \mathbb{P}^n : x_0 = 0\} \simeq \mathbb{P}^{n-1}$ is the *hyperplane at infinity* inside \mathbb{P}^n . The hypersurface $\{\mathbf{x} \in \mathbb{P}^{n-1} : \sum_{i=1}^n x_i^2 = 0\}$ is called the *isotropic quadric*. It lives in the hyperplane at infinity and it has no real points. The hypothesis in Theorem 2.9 means that the intersection of X with these two loci is reduced and has the expected dimension.

Theorem 2.9 appears in [52, Proposition 6.10]. The hypothesis is stated in precise terms in [52, equation (6.4)]. It holds for all varieties X after a general linear change of coordinates.

If we are given a real projective variety X in \mathbb{P}^n from the start, then we also consider the ED problem for its affine cone in \mathbb{R}^{n+1} . The data vector now equals $\mathbf{u} = (u_0, u_1, \dots, u_n)$, and the augmented Jacobian is redefined so as to respect the fact that all polynomials are homogeneous. The general formula for this matrix and the homogeneous critical ideal appears in [52, equation (2.7)].

For a curve $X \subset \mathbb{P}^2$ with defining polynomial $f(x_0, x_1, x_2)$, the augmented Jacobian is

$$\mathcal{AJ} = \begin{pmatrix} u_0 & u_1 & u_2 \\ x_0 & x_1 & x_2 \\ \partial f / \partial x_0 & \partial f / \partial x_1 & \partial f / \partial x_2 \end{pmatrix},$$

and the homogeneous critical ideal in $\mathbb{R}[x_0, x_1, x_2]$ is computed as follows:

$$C_{X,\mathbf{u}} = \langle f, \det(\mathcal{AJ}) \rangle : (\langle \partial f / \partial x_0, \partial f / \partial x_1, \partial f / \partial x_2 \rangle \cdot (x_1^2 + x_2^2))^\infty. \quad (2.11)$$

The critical points are given by the variety $\mathcal{V}(C_{X,\mathbf{u}})$ in \mathbb{P}^2 , whose cardinality is $\text{EDdegree}(X)$. The factor $(x_1^2 + x_2^2)$ in the saturation step (2.11) is the isotropic quadric. It is needed whenever the hypothesis of Theorem 2.9 is not satisfied. Namely, it removes any extraneous component that may arise from non-transversal intersection of the curve X with the isotropic quadric.

Example 2.10 (Cardioid) We consider the homogeneous version of the cardioid in Example 2.1:

$$f = (x_1^2 + x_2^2 + x_0 x_2)^2 - x_0^2 (x_1^2 + x_2^2). \quad (2.12)$$

The projective curve $X = \mathcal{V}(f)$ has three singular points, namely that at the origin $\mathcal{V}(x_1, x_2)$ in $\mathbb{C}^2 = \{x_0 \neq 0\}$ and the two points in the isotropic quadric $\mathcal{V}(x_1^2 + x_2^2)$ in $\mathbb{P}^1 = \{x_0 = 0\}$.

The homogeneous critical ideal $C_{X,\mathbf{u}}$ is generated by three cubics, and it defines seven points in \mathbb{P}^2 . Hence the projective cardioid X has $\text{EDdegree}(X) = 7$. This is also the ED degree of the affine cardioid in (2.4) but only after a linear change of coordinates. Even a fairly modest change of coordinates can have dramatic impact. For instance, if we replace x_1 by $2x_1$ in (2.4) then the ED degree jumps from 3 to 7.

We now offer a first definition of the polar degrees of a projective variety $X \subset \mathbb{P}^n$. Recall that points \mathbf{h} in the dual projective space $(\mathbb{P}^n)^\vee$ represent hyperplanes in the primal space \mathbb{P}^n . Namely, we identify \mathbf{h} with the hyperplane $\{\mathbf{x} \in \mathbb{P}^n : h_0x_0 + \dots + h_nx_n = 0\}$. We are interested in all pairs (\mathbf{x}, \mathbf{h}) in $\mathbb{P}^n \times (\mathbb{P}^n)^\vee$ such that \mathbf{x} is a nonsingular point of X and \mathbf{h} is tangent to X at \mathbf{x} . The Zariski closure of this set is the *conormal variety* $N_X \subset \mathbb{P}^n \times (\mathbb{P}^n)^\vee$. It is known that N_X has dimension $n - 1$, and if X is irreducible then so is N_X . The image of N_X under projection onto the second factor is the dual variety X^\vee . The role of $x \in \mathbb{P}^n$ and $h \in (\mathbb{P}^n)^\vee$ can be swapped. The following biduality relations [65, §I.1.3] hold:

$$N_X = N_{X^\vee} \quad \text{and} \quad (X^\vee)^\vee = X.$$

The conormal variety is an object of algebraic geometry that offers the theoretical foundations for various aspects of duality in optimization, including primal-dual algorithms.

Example 2.11 For a plane curve $X = \mathcal{V}(f)$ in \mathbb{P}^2 , the conormal variety N_X is a curve in $\mathbb{P}^2 \times (\mathbb{P}^2)^\vee$. Its ideal is derived from the ideal that is generated by f and the 2×2 minors of

$$\begin{pmatrix} h_0 & h_1 & h_2 \\ \partial f / \partial x_0 & \partial f / \partial x_1 & \partial f / \partial x_2 \end{pmatrix}$$

By saturation, we remove singularities and points on the isotropic quadric, to arrive at $C_{X,\mathbf{u}}$.

For instance, if f is the homogeneous cardioid in (2.12) then X^\vee is the cubic defined by

$$16h_0^3 - 27h_0h_1^2 - 24h_0^2h_2 - 15h_0h_2^2 - 2h_2^3.$$

The ideal of N_X has ten minimal generators. In addition to the above generators of bidegrees $(4, 0)$ and $(0, 3)$, we find the quadric $x_0h_0 + x_1h_1 + x_2h_2$ of bidegree $(1, 1)$, three cubics of bidegree $(2, 1)$ like $x_1^2h_1 - 3x_2^2h_1 - x_0x_1h_2 + 4x_1x_2h_2$, and four cubics of bidegree $(1, 2)$.

We now finally come to the polar degrees. The product of two projective spaces $\mathbb{P}^n \times (\mathbb{P}^n)^\vee$ serves as the ambient space for our primal-dual approach to the ED problem. We now consider its cohomology ring:

$$H^*(\mathbb{P}^n \times (\mathbb{P}^n)^\vee, \mathbb{Z}) = \mathbb{Z}[s, t]/\langle s^{n+1}, t^{n+1} \rangle.$$

The class of the conormal variety N_X in this cohomology ring is a binary form of degree $n+1 = \text{codim}(N_X)$ whose coefficients are nonnegative integers:

$$[N_X] = \delta_1(X)s^n t + \delta_2(X)s^{n-1}t^2 + \delta_3(X)s^{n-2}t^3 + \dots + \delta_n(X)st^n.$$

The coefficients $\delta_i(X)$ of this binary form are called the *polar degrees* of X .

Remark 2.12 The polar degrees satisfy $\delta_i(X) = \#(N_X \cap (L \times L'))$, where $L \subset \mathbb{P}^n$ and $L' \subset (\mathbb{P}^n)^\vee$ are general linear subspaces of dimensions $n+1-i$ and i respectively. This geometric interpretation implies that $\delta_i(X) = 0$ for $i < \text{codim}(X^\vee)$ and for $i > \dim(X) + 1$. Moreover, the first and last polar degree are the classical degrees for the dual pair of varieties:

$$\delta_i(X) = \text{degree}(X) \text{ for } i = \dim(X) + 1 \text{ and } \delta_i(X) = \text{degree}(X^\vee) \text{ for } i = \text{codim}(X^\vee). \quad (2.13)$$

Example 2.13 Let $X \subset \mathbb{P}^2$ be the cardioid in (2.12). The curve $N_X \subset \mathbb{P}^2 \times (\mathbb{P}^2)^\vee$ has the class

$$[N_X] = \text{degree}(X^\vee) \cdot s^2t + \text{degree}(X) \cdot st^2 = 3 \cdot s^2t + 4 \cdot st^2.$$

Thus the polar degrees of the cardioid are 3 and 4. Their sum 7 is the ED degree.

Example 2.14 Let X be a general surface of degree d in \mathbb{P}^3 . Its dual X^\vee is a surface of degree $d(d-1)^2$ in $(\mathbb{P}^3)^\vee$. The conormal variety N_X is a surface in $\mathbb{P}^3 \times (\mathbb{P}^3)^\vee$, with class

$$[N_X] = d(d-1)^2 s^3t + d(d-1) s^2t^2 + d st^3.$$

The sum of the three polar degrees equals $\text{EDdegree}(X) = d^3 - d^2 + d$; see Proposition 2.3.

Theorem 2.9 allows us to compute the ED degree for many interesting varieties, e.g. using Chern classes [52, Theorem 5.8]. This is relevant for applications in machine learning [28] which rest on low-rank approximation of matrices and tensors with special structure [118].

Example 2.15 (Determinantal varieties) Let $X_r \subset \mathbb{P}^{m^2-1}$ be the variety of $m \times m$ matrices $x = (x_{ij})$ of rank $\leq r$. By [140], the conormal variety N_X is cut out by nice matrix equations:

$$N_X = \{(\mathbf{x}, \mathbf{h}) \in \mathbb{P}^{m^2-1} \times \mathbb{P}^{m^2-1} : \text{rank}(\mathbf{x}) \leq r, \text{rank}(\mathbf{h}) \leq m-r, \mathbf{x} \cdot \mathbf{h} = 0 \text{ and } \mathbf{h} \cdot \mathbf{x} = 0\}.$$

In particular, the duality relation $(X_r)^\vee = X_{m-r}$ holds among determinantal varieties. Typing the above formula into Macaulay2, we compute the polar degrees for $r = 1$ and $m = 3$:

```
QQ[x11,x12,x13,x21,x22,x23,x31,x32,x33,h11,h12,h13,h21,h22,h23,h31,h32,h33,
Degrees=> {{1,0},{1,0},{1,0},{1,0},{1,0},{1,0},{1,0},{1,0},{1,0},
{0,1},{0,1},{0,1},{0,1},{0,1},{0,1},{0,1},{0,1},{0,1}};
x = matrix {{x11,x12,x13},{x21,x22,x23},{x31,x32,x33}};
h = matrix {{h11,h12,h13},{h21,h22,h23},{h31,h32,h33}};
I = minors(2,x) + minors(3,h) + minors(1,x*h) + minors(1,h*x);
isPrime(I), codim(I), degree I
multidegree(I)
```

The code starts with the bigraded coordinate ring of $\mathbb{P}^8 \times \mathbb{P}^8$. It verifies that N_X has codimension 9 and that I is its prime ideal. The last command computes the polar degrees:

$$[N_X] = 3s^8t + 6s^7t^2 + 12s^6t^3 + 12s^5t^4 + 6s^4t^5. \quad (2.14)$$

After verifying (2.13), one concludes that $\text{EDdegree}(X_1) = 3+6+12+12+6 = 39$. Indeed, after changing coordinates, the EDdegree for 3×3 -matrices of rank 1 equals 39. We saw this already in Example 2.8, where 39 critical points were found by a numerical computation.

The primal-dual set-up of conormal varieties allows for a very elegant formulation of the critical equations. This will be presented in the next theorem. We now assume that X is an irreducible variety defined by homogeneous polynomials in n variables. Thus X is an affine cone in \mathbb{C}^n . Its dual $Y = X^\vee$ is the affine cone over the dual of the projective variety given by X . Thus Y is also an affine cone in \mathbb{C}^n . In this setting, the conormal variety N_X is viewed as an affine variety of dimension n in \mathbb{C}^{2n} . The homogeneous ideals of these cones are precisely those discussed above.

Theorem 2.16 *The ED problems for X and Y coincide, and we have $\text{EDdegree}(X) = \text{EDdegree}(Y)$. Given a general data point $\mathbf{u} \in \mathbb{R}^n$, the critical equations for this ED problem are:*

$$(\mathbf{x}, \mathbf{h}) \in N_X \quad \text{and} \quad \mathbf{x} + \mathbf{h} = \mathbf{u}. \quad (2.15)$$

Proof See [52, Theorem 5.2]. □

It is instructive to verify Theorem 2.16 for Example 2.15. For any data matrix \mathbf{u} of size $m \times m$, the sum in (2.15) is a special decomposition of \mathbf{u} , namely \mathbf{x} of rank r plus \mathbf{h} of rank $m - r$. By the Eckhart-Young Theorem, it arises from zeroing out complementary singular values σ_i in the two matrices \mathbf{x} and \mathbf{h} .

In general, there is no free lunch, even with a simple formulation like (2.15). The difficulty lies in computing the ideal of the conormal variety N_X . However, this should be thought of as a preprocessing step, to be carried out only once per model X . If an efficient presentation of N_X is available, our task is to solve the system $\mathbf{x} + \mathbf{h} = \mathbf{u}$ of n linear equations in $2n$ coordinates for the n -dimensional affine variety N_X .

The discussion so far was restricted to the Euclidean norm. But, we can measure distances in \mathbb{R}^n with any other norm $\|\cdot\|$. Our optimization problem (2.1) extends naturally:

$$\text{minimize } \|\mathbf{x} - \mathbf{u}\| \text{ subject to } \mathbf{x} \in X. \quad (2.16)$$

The unit ball $B = \{\mathbf{x} \in \mathbb{R}^n : \|\mathbf{x}\| \leq 1\}$ is a centrally symmetric convex body. Conversely, every centrally symmetric convex body B defines a norm, and we can paraphrase the previous optimization problem as:

$$\text{minimize } \lambda \text{ subject to } \lambda \geq 0 \text{ and } (\mathbf{u} + \lambda B) \cap X \neq \emptyset. \quad (2.17)$$

If the boundary of the unit ball B is smooth and algebraic then we can express the critical equations for the corresponding norm as a polynomial system. This is derived as before, but we now replace the first row of the augmented Jacobian matrix \mathcal{AJ} with the gradient of the map $\mathbb{R}^n \rightarrow \mathbb{R}$, $\mathbf{x} \mapsto \|\mathbf{x} - \mathbf{u}\|$.

Chapter 3

Computations

In this chapter we study two computational approaches to solve a system of polynomial equations. A system of m polynomial equations in n variables is a system of the form

$$F(\mathbf{x}) = \begin{pmatrix} f_1(\mathbf{x}) \\ \vdots \\ f_m(\mathbf{x}) \end{pmatrix} = 0,$$

where $f_1, \dots, f_m \in \mathbb{C}[\mathbf{x}] := \mathbb{C}[x_1, \dots, x_n]$. If $n = m$, we call $F(\mathbf{x})$ a *square system*. If $n > m$, we call $F(\mathbf{x})$ *underdetermined*. If $n < m$, we call $F(\mathbf{x})$ *overdetermined*. In this chapter we will mostly focus on square systems.

Example 3.1 In the previous chapter we have considered constrained optimization problems of the form $\min_{\mathbf{x} \in \mathbb{R}^n : f(\mathbf{x})=0} g(\mathbf{x})$, where f and g are polynomials in n variables $\mathbf{x} = (x_1, \dots, x_n)$. To solve this problem one can compute the solutions of the critical equations $f(\mathbf{x}) = \frac{\partial f}{\partial x_1} - \lambda \frac{\partial g}{\partial x_1} = \dots = \frac{\partial f}{\partial x_n} - \lambda \frac{\partial g}{\partial x_n} = 0$. This is a square system in the $n + 1$ variables (\mathbf{x}, λ) . \diamond

Solving the system of equations $F(\mathbf{x}) = 0$ means that we compute *all* points $\mathbf{z} = (z_1, \dots, z_n) \in \mathbb{C}^n$ such that $F(\mathbf{z}) = 0$. The first is how to find an appropriate *data structure* to represent a solution. In fact, $F(\mathbf{z}) = 0$ is already *implicit* represented by its equation. Some information can be read off this representation. For instance, if $F(\mathbf{z}) = 0$ and F has rational coefficients, we know that \mathbf{z} is an algebraic number. On the other hand, other information like whether or not \mathbf{z} is real is not directly accessible from this implicit representation.

The goal of this lecture is to discuss two data structures for representing solutions of systems of polynomial equations: the first is *Gröbner bases* and the second is *approximate zeros*.

3.1 Gröbner Bases

We use the notation $\mathbf{x}^\alpha := x_1^{\alpha_1} \cdots x_n^{\alpha_n}$ for the exponent vector $\alpha = (\alpha_1, \dots, \alpha_n) \in \mathbb{N}^n$. In fact, we can identify monomials with their exponent vectors. A monomial ordering $>$ on $\mathbb{C}[\mathbf{x}]$ is then defined by a total order $>$ on \mathbb{N}^n that satisfies (1) if $\alpha > \beta$, then $\alpha + \gamma > \beta + \gamma$ for every $\gamma \in \mathbb{N}^n$ and (2) every nonempty subset of \mathbb{N}^n has a smallest element under $>$ (see, e.g., [44, Chapter 2 §2, Definition 1]).

Example 3.2 The Lex (Lexicographic) order is defined by setting $\alpha >_{\text{Lex}} \beta$, if $\alpha_j - \beta_j > 0$ for $\alpha, \beta \in \mathbb{N}^n$, where $j := \min\{i \mid \alpha_i \neq \beta_i\}$ is the first index where α and β are not equal. For instance, $x_1^2 x_2 > x_1 x_2 x_3^3$. Intuitively speaking, the Lex order views a polynomial $f \in \mathbb{C}[\mathbf{x}]$ as a polynomial in x_1 with coefficients that are polynomials in x_2 , which has coefficients that are polynomials in x_3 , and so on. \diamond

Every monomial order induces the notion of *leading term* of a polynomial. Let $f = \sum_{i=1}^k c_i \mathbf{x}^{\alpha_i} \in \mathbb{C}[\mathbf{x}]$, where $\alpha_1 > \alpha_2 > \dots > \alpha_k$ and $c_1 \neq 0$. Then, $\text{LT}(f) := c_1 \mathbf{x}^{\alpha_1}$. The *leading term ideal* of an ideal $I \subset \mathbb{C}[x_1, \dots, x_n]$ is defined as

$$\text{LT}(I) := \langle \{\text{LT}(f) \mid f \in I \setminus \{0\}\} \rangle.$$

Next comes the definition of a Gröbner basis.

Definition 3.3 (Gröbner basis) Let $I \subset \mathbb{C}[x_1, \dots, x_n]$ be an ideal and $>$ be a monomial order. A subset $G = \{g_1, \dots, g_m\} \subset I$ is called a *Gröbner basis* for I with respect to $>$, if its leading terms generate the leading term ideal; i.e., if

$$\langle \text{LT}(g_1), \dots, \text{LT}(g_m) \rangle = \text{LT}(I).$$

Remark 3.4 If G is a Gröbner basis for an ideal I , then $I = \langle G \rangle$ (see [44, Chapter 2 §5, Corollary 6]), hence the name ‘‘basis’’. A Gröbner basis defines a notion of *normal form* of an ideal. More specifically, let $I \subset \mathbb{C}[\mathbf{x}]$ be an ideal and let $G = \{g_1, \dots, g_m\}$ be a Gröbner basis for I . Then for every $f \in \mathbb{C}[\mathbf{x}]$ there is a unique $r \in \mathbb{C}[\mathbf{x}]$, such that $f = g + r$ with $g \in I$ and no term of r is divisible by any of $\text{LT}(g_1), \dots, \text{LT}(g_m)$ (see [44, Chapter 2 §6, Proposition 1]). The remainder can be computed using the division algorithm.

The following example is [44, Chapter 2 §8, Example 2]. It illustrates how Gröbner bases can be used to solve systems of polynomial equations.

Example 3.5 Consider the system of polynomial equations

$$F(x, y, z) = \begin{pmatrix} x^2 + y^2 + z^2 - 1 \\ x^2 + z^2 - y \\ x - z \end{pmatrix} = 0.$$

We compute a Gröbner basis of the ideal $I = \langle x^2 + y^2 + z^2 - 1, x^2 + z^2 - y, x - z \rangle$ relative to the Lex order with $x > y > z$ using Macaulay2 [67].

```
R = QQ[x, y, z, MonomialOrder => Lex];
f = x^2 + y^2 + z^2 - 1;
g = x^2 + z^2 - y;
h = x - z;
I = ideal {f, g, h};
G = gb I
gens G
```

This computes the Gröbner basis $G = \{x - z, y - 2z^2, 4z^4 - 2z^2 - 1\}$. Because $I = \langle G \rangle$, we can solve $F(x, y, z) = 0$ by solving the system of equations given by G . Notice that the third polynomial in G only depends on z , the second only on y and z , and the third only on x and z . Thus, we can reduce solving $F(x, y, z) = 0$ to solving 3 univariate polynomial equations. This gives us the 4 solutions $(z, 2z^2, z)$, where z iterates through the 4 roots of $4z^4 - 2z^2 - 1$. \diamond

The reason why using the Lex order in Example 3.5 works well is the *Elimination Theorem*. To state the theorem, let $I \subset \mathbb{C}[\mathbf{x}]$ be an ideal. We denote for every $0 \leq j < n$ the ideal $I_j := I \cap \mathbb{C}[x_j, \dots, x_n]$. The ideal I_j is called the j -th *elimination ideal* of I . It consists of those polynomials in I that only contain the variables x_j, \dots, x_n . For a proof of the next theorem see [44, Chapter 3, §1, Theorem 1].

Theorem 3.6 (The Elimination Theorem) Let $I \subset \mathbb{C}[\mathbf{x}]$ be an ideal and G be a Gröbner basis for I with respect to the lex order with $x_1 > \dots > x_n$. Then

$$G_j := G \cap \mathbb{C}[x_{j+1}, \dots, x_n]$$

is a Gröbner basis of the j -th elimination ideal of I .

For us the most important consequence of the Elimination Theorem is that, if a system of polynomial equations $F(\mathbf{x}) = (f_1(\mathbf{x}), \dots, f_n(\mathbf{x})) = 0$ has finitely many solutions, the j -th elimination will not be empty for $1 \leq j \leq n$. Consequently, we can solve $F(\mathbf{x}) = 0$ by computing a Gröbner basis for the Lex order and then sequentially solving univariate equations. We can compute zeros of univariate polynomials by computing eigenvalues of the associated *companion matrix*. If $f(x) = x^d + \sum_{i=0}^{d-1} c_i x^i$ is a univariate polynomial we have $f(x) = 0$ if and only if x is an eigenvalue of the companion matrix

$$\begin{pmatrix} 0 & \cdots & 0 & -a_0 \\ 1 & \cdots & 0 & -a_1 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & 1 & -a_{d-1} \end{pmatrix}.$$

Sometimes we are not interested in the solutions of $F(\mathbf{x}) = 0$ per se, but only in the how many solutions there are. Gröbner bases naturally carry this information: Suppose $I \subset \mathbb{C}[\mathbf{x}]$ is an ideal and $>$ a monomial order. Recall that a monomial $\mathbf{x}^\alpha \notin \text{LT}(I)$ is called a *standard monomial* of I relative to $>$. The next result shows how to get the number of solutions of $F(\mathbf{x}) = 0$ from a Gröbner basis; see [141, Proposition 2.1].

Proposition 3.7 *Let $I \subset \mathbb{C}[\mathbf{x}]$ be an ideal. Let $>$ be a term order and \mathcal{B} be the set of standard monomials of I relative to $>$. Then, \mathcal{B} is finite if and only if $V(I)$ is finite, and $\#\mathcal{B}$ equals the number of points in $V(I)$ counting multiplicities.*

Example 3.8 In Example 3.5 there are four standard monomials. Namely, $1, z, z^2$ and z^3 . This is why we have four solutions of the system $F(x, y, z) = 0$. \diamond

We have now understood how to solve systems of polynomials with finitely many zeros using Gröbner bases. What about systems whose zero set contains positive dimensional component? In this case, the n -th elimination ideal must necessarily be empty. To cope with this case one can remove positive dimensional components using ideal saturation. Let $I, J \subset \mathbb{C}[\mathbf{x}]$ be two ideals. The *saturation* of I by J is the ideal

$$I : J^\infty := \{f \in \mathbb{C}[\mathbf{x}] \mid \text{there is } \ell > 0 \text{ with } f \cdot g^\ell \in I \text{ for all } g \in J\}.$$

Saturation is the ideal analogue of removing components on the level of varieties. We have

$$V(I : J^\infty) = \overline{V(I) \setminus V(J)}; \quad (3.1)$$

see [44, Chapter 4 §4, Corollary 11].

Recall that a solution to a square system $F(\mathbf{x}) = (f_1(\mathbf{x}), \dots, f_n(\mathbf{x})) = 0$ is called *regular*, if the Jacobian determinant $\det\left(\frac{\partial f_i}{\partial x_j}\right)$ does not vanish at that solution. There can be only finitely many regular zeros of a system of polynomial equations, and a finite union of points is Zariski closed. Consequently, if we saturate $I = \langle f_1, \dots, f_n \rangle$ by $J = \left\langle \det\left(\frac{\partial f_i}{\partial x_j}\right)\right\rangle$, we can use the strategy from above to solve $F(\mathbf{x}) = 0$.

Example 3.9 Consider the following system of 2 polynomials in 2 variables

$$F(x, y) = \begin{pmatrix} (x-1) \cdot (x-2) \cdot (x^2 + y^2 - 1) \\ (y-1) \cdot (y-3) \cdot (x^2 + y^2 - 1) \end{pmatrix} = 0.$$

It has 4 regular solutions $(1, 1), (1, 3), (2, 1), (2, 3)$ and the circle $x^2 + y^2 - 1$ as positive dimensional component. We use Macaulay2 [67] to saturate the ideal generated by F .

```
R = QQ[x, y, MonomialOrder => Lex];
f = (x-1) * (x-2) * (x^2+y^2-1);
g = (y-1) * (y-3) * (x^2+y^2-1);
I = ideal {f, g};
Jac = matrix{{diff(x, f), diff(x, g)}, {diff(y, f), diff(y, g)}};
J = ideal det(Jac)
K = saturate(I, J)
```

This returns the ideal $K = \langle y^2 - 4y + 3, x^2 - 3x + 2 \rangle$. In fact, these two generators already form a Gröbner basis for K . Their joint zero set consists of the 4 solutions from Example 3.5. \diamond

Next, we state two propositions related to elimination and saturation of ideals with parameters, and one lemma on Gröbner bases of parameterized ideals. For this, let $\mathbf{x} = (x_1, \dots, x_n)$ and $\mathbf{p} = (p_1, \dots, p_k)$ two sets of variables, and $\mathbb{C}[\mathbf{x}, \mathbf{p}] := \mathbb{C}[x_1, \dots, x_n, p_1, \dots, p_k]$. We regard \mathbf{p} as variables for *parameters*. For a fixed parameter $\mathbf{q} \in \mathbb{C}^k$ we denote the surjective ring homomorphism

$$\phi_{\mathbf{q}} : \mathbb{C}[\mathbf{x}, \mathbf{p}] \rightarrow \mathbb{C}[\mathbf{x}], \quad f(\mathbf{x}; \mathbf{p}) \mapsto f(\mathbf{x}; \mathbf{q}). \quad (3.2)$$

Proposition 3.10 Consider an ideal $I \subset \mathbb{C}[\mathbf{x}, \mathbf{p}]$ and let $G = \{g_1, \dots, g_m\}$ be a Gröbner basis for I relative to Lex order $x_1 > \dots > x_n > p_1 > \dots > p_k$. For $1 \leq i \leq m$ with $g_i \notin \mathbb{C}[\mathbf{p}]$, write g_i in the form $g_i = c_i(\mathbf{p})\mathbf{x}^{\alpha_i} + h_i$, where all terms of h_i are strictly smaller than \mathbf{x}^{α_i} . Let $\mathbf{q} \in V(I \cap \mathbb{C}[\mathbf{p}]) \subseteq \mathbb{C}^k$, such that $c_i(\mathbf{q}) \neq 0$ for all $g_i \notin \mathbb{C}[\mathbf{p}]$. Then,

$$\phi_{\mathbf{q}}(G) = \{\phi_{\mathbf{q}}(g_i) \mid g_i \notin \mathbb{C}[\mathbf{p}]\}$$

is a Gröbner basis for the ideal $\phi_{\mathbf{q}}(I) \subset \mathbb{C}[\mathbf{x}]$.

Proof See, e.g., [44, Chapter 4 §7, Theorem 2]. \square

Proposition 3.11 Let $I \subset \mathbb{C}[\mathbf{x}, \mathbf{p}]$ be an ideal and $J = \langle h \rangle$ a principal ideal in the same ring. Let u be an additional variable and $K := \langle 1 - u \cdot h \rangle$. Then,

$$I : J^\infty = (I + K) \cap \mathbb{C}[\mathbf{x}, \mathbf{p}].$$

Furthermore, if G is a Gröbner basis of $I + K$ relative to the Lex order $u > x_1 > \dots > x_n > p_1 > \dots > p_k$, then $G \cap \mathbb{C}[\mathbf{x}, \mathbf{p}]$ is a Gröbner basis of $I : J^\infty$.

Proof See, e.g., [44, Chapter 4 §4, Theorem 14]. \square

The following is [19, Lemma 2.5].

Lemma 3.12 Let $I \subset \mathbb{C}[\mathbf{x}, \mathbf{p}]$ be an ideal and $J = \langle h \rangle \subset \mathbb{C}[\mathbf{x}, \mathbf{p}]$ be a principal ideal, such that $(I : J^\infty) \cap \mathbb{C}[\mathbf{p}] = \{0\}$. Let $G = \{g_1, \dots, g_s\}$ be a Gröbner basis of $I : J^\infty$ with respect to the Lex order $x_1 > \dots > x_n > p_1 > \dots > p_k$. There is a proper subvariety $\Delta \subsetneq \mathbb{C}^k$ such that for all $\mathbf{q} \notin \Delta$ the set $\{\phi_{\mathbf{q}}(g_1), \dots, \phi_{\mathbf{q}}(g_s)\}$ is a Gröbner basis for $\phi_{\mathbf{q}}(I) : \phi_{\mathbf{q}}(J)^\infty$ and none of the leading terms of g_1, \dots, g_s vanish when evaluated at \mathbf{q} . In particular, $\phi_{\mathbf{q}}(I : J^\infty) = \phi_{\mathbf{q}}(I) : \phi_{\mathbf{q}}(J)^\infty$ for all $\mathbf{q} \notin \Delta$.

Proof Let u be an additional variable and, as in Proposition 3.11, denote the ideal $K := \langle 1 - u \cdot h \rangle$. By Proposition 3.11, we have $I : J^\infty = (I + K) \cap \mathbb{C}[\mathbf{x}, \mathbf{p}]$. Since $(I : J^\infty) \cap \mathbb{C}[\mathbf{p}] = \{0\}$, we therefore have

$$(I + K) \cap \mathbb{C}[\mathbf{p}] = \{0\}. \quad (3.3)$$

This shows $V((I + K) \cap \mathbb{C}[\mathbf{p}]) = \mathbb{C}^k$ and we may therefore apply Proposition 3.10 to $I + K$ without putting any restrictions on \mathbf{q} . As in Proposition 3.10, we augment the Lex order by letting u be the largest variable. Let $\bar{G} := \{g_1, \dots, g_r\}$ be a Gröbner basis of $I + K$ relative to this order. It follows from (3.3) that we have $g_1, \dots, g_r \notin \mathbb{C}[\mathbf{p}]$. We write each g_i in the form $g_i = c_i(\mathbf{p})u^\beta \mathbf{x}^{\alpha_i} + h_i$, where all terms of h_i are strictly smaller than $u^\beta \mathbf{x}^{\alpha_i}$, and define the hypersurface

$$\Delta := \{\mathbf{q} \in \mathbb{C}^k \mid c_1(\mathbf{q}) \cdots c_r(\mathbf{q}) = 0\}. \quad (3.4)$$

In the following, let $\mathbf{q} \in \mathbb{C}^k \setminus \Delta$. By Proposition 3.10, $\phi_{\mathbf{q}}(\bar{G}) = \{\phi_{\mathbf{q}}(g_1), \dots, \phi_{\mathbf{q}}(g_r)\}$ is a Gröbner basis for

$$\phi_{\mathbf{q}}(I + K) = \phi_{\mathbf{q}}(I) + \phi_{\mathbf{q}}(K) = \phi_{\mathbf{q}}(I) + (1 - u \cdot \phi_{\mathbf{q}}(h)).$$

Without restriction, the first $s \leq r$ elements in \bar{G} are those that do not depend on the variable u . We denote $G := \{g_1, \dots, g_s\} = \bar{G} \cap \mathbb{C}[\mathbf{x}, \mathbf{p}]$. It follows from Proposition 3.11 that G is a Gröbner basis of $I : J^\infty$. Because $\mathbf{q} \notin \Delta$, none of the leading terms in \bar{G} when evaluated at \mathbf{q} vanish. Consequently,

$$\phi_{\mathbf{q}}(G) \cap \mathbb{C}[\mathbf{x}] = \phi_{\mathbf{q}}(\bar{G}) \cap \mathbb{C}[\mathbf{x}].$$

Therefore, $\phi_{\mathbf{q}}(G) = \{\phi_{\mathbf{q}}(g_1), \dots, \phi_{\mathbf{q}}(g_s)\}$ is a Gröbner basis of $\phi_{\mathbf{q}}(I) : \phi_{\mathbf{q}}(J)^\infty$ by Proposition 3.11. \square

Equation (3.4) leads to the following corollary.

Corollary 3.13 *Given an ideal $I = \langle f_1, \dots, f_n \rangle \subset \mathbb{C}[\mathbf{x}, \mathbf{p}]$ and a principal ideal $J = \langle h \rangle \subset \mathbb{C}[\mathbf{x}, \mathbf{p}]$, the discriminant Δ in Lemma 3.12 is found by computing a Lex Gröbner basis for $I + \langle 1 - u \cdot h \rangle$, where $u > x_1 > \dots > x_n > p_1 > \dots > p_k$. The product of the leading coefficients $c_i(\mathbf{p})$ of this Gröbner basis gives us an equation for Δ .*

3.2 The Parameter Continuation Theorem

We use the theory of Gröbner bases to prove that a square system of polynomials equations with parameters has a “degree”. More specifically, we prove the *Parameter Continuation Theorem* by Morgan and Sommese [113]. For this we consider the polynomial ring $\mathbb{C}[\mathbf{x}, \mathbf{p}] := \mathbb{C}[x_1, \dots, x_n, p_1, \dots, p_k]$. We interpret \mathbf{x} as variables and \mathbf{p} as parameters.

Definition 3.14 Let $f_1(\mathbf{x}; \mathbf{p}), \dots, f_n(\mathbf{x}; \mathbf{p}) \in \mathbb{C}[\mathbf{x}, \mathbf{p}]$. We call the image of the polynomial map

$$\mathbb{C}^k \mapsto \mathbb{C}[\mathbf{x}]^n, \quad \mathbf{p}_0 \mapsto F(\mathbf{x}; \mathbf{p}_0) = \begin{pmatrix} f_1(\mathbf{x}; \mathbf{p}_0) \\ \vdots \\ f_n(\mathbf{x}; \mathbf{p}_0) \end{pmatrix}.$$

a family of polynomial systems. In other words, a family $\mathcal{F} = \{F(\mathbf{x}; \mathbf{p}) \mid \mathbf{p} \in \mathbb{C}^k\}$ consists of n polynomials in n variables that depend polynomially on k parameters.

Example 3.15 The family of univariate quadratic polynomials is $\mathcal{F} = \{x^2 + ax + b \mid a, b \in \mathbb{C}\}$. Here, the parameters are $\mathbf{p} = (a, b) \in \mathbb{C}^2$. \diamond

We fix a family of polynomial systems \mathcal{F} depending on k parameters $\mathbf{p} = (p_1, \dots, p_k)$. Recall that a zero of $F(\mathbf{x}; \mathbf{p}) = (f_1(\mathbf{x}; \mathbf{p}), \dots, f_n(\mathbf{x}; \mathbf{p})) \in \mathcal{F}$ is called a *regular zero*, if the Jacobian determinant $\det\left(\frac{\partial f_i}{\partial x_j}\right)_{1 \leq i, j \leq n}$ does not vanish. The next theorem implies that for almost all parameters \mathbf{p} the number of regular solutions is the same.

Theorem 3.16 (The Parameter Continuation Theorem) *Let \mathcal{F} be a family of polynomial systems that consists of systems of n polynomials in n variables depending on k parameters. For $\mathbf{p} \in \mathbb{C}^k$ denote*

$$N(\mathbf{p}) := \#\{\mathbf{x} \in \mathbb{C}^n \mid \mathbf{x} \text{ is a regular zero of } F(\mathbf{x}; \mathbf{p})\}.$$

Let $N := \sup_{\mathbf{p} \in \mathbb{C}^k} N(\mathbf{p})$. Then, $N < \infty$ and there exists a proper algebraic subvariety $\Delta \subseteq \mathbb{C}^k$, called discriminant, such that $N(\mathbf{p}) = N$ for $\mathbf{p} \notin \Delta$.

Proof We recall the proof from [19]. Another proof can also be found in the textbook [138].

Suppose $\mathcal{F} = \{F(\mathbf{x}; \mathbf{p}) \mid \mathbf{p} \in \mathbb{C}^k\}$, where $F(\mathbf{x}; \mathbf{p}) = (f_1(\mathbf{x}; \mathbf{p}), \dots, f_n(\mathbf{x}; \mathbf{p})) \in \mathcal{F}$. Let

$$I = \langle f_1, \dots, f_n \rangle \quad \text{and} \quad J := \langle \det\left(\frac{\partial f_i}{\partial x_j}\right) \rangle.$$

If $N = 0$, then no system in \mathcal{F} has regular zeros. In this case, the statement is true. We now assume $N > 0$. By (3.1), $V(I : J^\infty)$ contains all $(\mathbf{x}, \mathbf{q}) \in \mathbb{C}^n \times \mathbb{C}^k$ such that \mathbf{x} is a regular zero of $F(\mathbf{x}; \mathbf{q})$. Since $N > 0$, we therefore have $V(I : J^\infty) \neq \emptyset$. Let $(\mathbf{x}, \mathbf{q}) \in V(I : J^\infty)$. The Implicit Function Theorem implies that there is a Euclidean open neighbourhood U of \mathbf{q} such that $F(\mathbf{x}; \mathbf{q})$ has regular zeros for all $\mathbf{q} \in U$. Consequently, $(I : J^\infty) \cap \mathbb{C}[\mathbf{p}] = \{0\}$, so we can apply Lemma 3.12.

We denote $I_{\mathbf{q}} = \phi_{\mathbf{q}}(I)$ and $J_{\mathbf{q}} = \phi_{\mathbf{q}}(J)$. Let $G = \{g_1, \dots, g_s\}$ be a Gröbner basis of $I : J^\infty$ relative to the Lex order where $x_1 > \dots > x_n > p_1 > \dots > p_k$. By Lemma 3.12, there is a proper algebraic subvariety $\Delta \subsetneq \mathbb{C}^k$ such that $\phi_{\mathbf{q}}(G) = \{\phi_{\mathbf{q}}(g_1), \dots, \phi_{\mathbf{q}}(g_s)\}$ is a Gröbner basis for $I_{\mathbf{q}} : J_{\mathbf{q}}^\infty$ and none of the leading terms of g_1, \dots, g_s vanish when evaluated at \mathbf{q} . This implies that the leading monomials of $I_{\mathbf{q}} : J_{\mathbf{q}}^\infty$ are constant on $\mathbb{C}^k \setminus \Delta$. Let

$$\mathcal{B}_{\mathbf{q}} := \{\text{standard monomials of } I_{\mathbf{q}} : J_{\mathbf{q}}^\infty\}.$$

Then what we have shown is that $\mathcal{B}_{\mathbf{q}}$ is constant on $\mathbb{C}^k \setminus \Delta$. On the other hand, by (3.1) and since the union of finitely many points is Zariski closed, we have $V(I : J^\infty) = V(I) \setminus V(J)$. Proposition 3.7 and the fact that regular zeros have multiplicity one imply that

$$N(\mathbf{q}) = \#\mathcal{B}_{\mathbf{q}}.$$

This shows that $N(\mathbf{q})$ is constant on $\mathbb{C}^k \setminus \Delta$. The Implicit Function Theorem implies that for all $\mathbf{q} \in \mathbb{C}^k$ there exists a Euclidean neighbourhood U of \mathbf{q} such that $N(\mathbf{q}) \leq N(\mathbf{q}')$ for all $\mathbf{q}' \in U$. Since Δ is a proper subvariety of \mathbb{C}^k and thus lower-dimensional, we have $N = N(\mathbf{q}) < \infty$ for $\mathbf{q} \in \mathbb{C}^k \setminus \Delta$. \square

We can use the algorithm in Corollary 3.13 to compute the discriminant. Observe that this algorithm also returns the discriminant when $F(\mathbf{x}; \mathbf{p}) = 0$ has non-regular solutions for *all* parameters \mathbf{p} . By contrast, computing resultants would not give the desired result, because the resultant will be constant and equal to zero.

Example 3.17 Recall from Example 3.15 the family $\mathcal{F} = \{x^2 + ax + b \mid a, b \in \mathbb{C}\}$. Here, the parameters are $\mathbf{p} = (a, b) \in \mathbb{C}^2$. A polynomial in this family has $N = 2$ regular zeros unless $a^2 - 4b = 0$. \diamond

Example 3.18 The critical equations for the ED problem in (2.1) have parameters \mathbf{u} . In this case, N is the Euclidean Distance Degree. \diamond

Example 3.19 We slightly modify the system from Example 3.9 and consider

$$F(x, y; a) = \begin{pmatrix} (x-1) \cdot (x-2) \cdot (x^2 + y^2 - 1) \\ (y-1) \cdot (y-a) \cdot (x^2 + y^2 - 1) \end{pmatrix} = 0,$$

where $a \in \mathbb{C}$ is a parameter. If $a \notin \{0, 1, \pm\sqrt{-3}\}$, we have $N = 4$ regular solutions. Let us compute the discriminant using the algorithm in Corollary 3.13. We use the Macaulay2 code from [19].

```
R = QQ[u, x, y, a, MonomialOrder => Lex];
f = (x-1) * (x-2) * (x^2+y^2-1);
g = (y-1) * (y-a) * (x^2+y^2-1);
I = ideal {f, g};
Jac = matrix{{diff(x, f), diff(x, g)}, {diff(y, f), diff(y, g)}};
K = ideal {1 - u * det(Jac)};
G = gens gb (I+K)
E = (entries(G))#0

P = QQ[a][u, x, y, MonomialOrder => Lex]
result = apply(E, t -> leadCoefficient(sub(t, P)))
factor(product result)
```

The result is the polynomial $a^6 \cdot (a-1)^4 \cdot (a^2+3)^2 \cdot g(a)$, where $g(a) = (a+1) \cdot (a^7 - 2a^6 + 8a^5 - 14a^4 + 23a^3 - 32a^2 + 32a - 32)$. The zeros of the additional factor $g(a)$ give system that also have 4 regular solutions. However, Theorem 3.16 only states that if a parameter is outside the discriminant, it has the maximal number of regular zeros, but not the reverse implication. \diamond

3.3 Polynomial Homotopy Continuation

In Section 3.1 we have seen how to use Gröbner bases to reduce solving $F(\mathbf{x}) = 0$ to the problem of sequentially computing zeros of univariate polynomials. Another approach is *polynomial homotopy continuation* (PHC). This is a numerical method for computing the regular zeros of a square system of polynomial equations. The textbook of Sommese and Wampler [138] provides a detailed introduction to the theory of polynomial homotopy continuation. We also refer to the overview article [11].

The goal in polynomial homotopy continuation is to compute *approximate zeros*. The definition goes back to Smale (see [17, §8, Definition 1]).

Definition 3.20 (Approximate Zeros) Let $F(\mathbf{x})$ be a square system of polynomial equations in n variables, and write $JF(\mathbf{x})$ for its (square) Jacobian matrix. A point $\mathbf{z} \in \mathbb{C}^n$ is called \mathbf{z} an *approximate zero* of F , if the sequence of Newton iterates $\mathbf{z}_{k+1} := \mathbf{z}_k - JF(\mathbf{x})^{-1}F(\mathbf{x})$ starting at $\mathbf{z}_0 := \mathbf{z}$ converges to a zero of F .

An approximate zero \mathbf{z} of a system F is in a precise sense close to an actual zero \mathbf{x} of F . Applying the Newton operator to \mathbf{z} we can get as close to \mathbf{x} as we want. Therefore, we can approximate \mathbf{x} to any desired accuracy.

Suppose now that $F(\mathbf{x}) = 0$ is a system of polynomial equations that we want to solve. The idea in homotopy continuation is to find a family \mathcal{F} and parameters $\mathbf{p}, \mathbf{q} \in \mathbb{C}^k$ with the following properties:

- $F(\mathbf{x}) = F(\mathbf{x}; \mathbf{p})$;
- $G(\mathbf{x}) := F(\mathbf{x}; \mathbf{q})$ is a system whose solutions are known or can be computed by other means.

Then one chooses a (piecewise) smooth path $\gamma(t)$ in \mathbb{C}^k with $\gamma(0) = \mathbf{p}$ and $\gamma(1) = \mathbf{q}$, defines the *parameter homotopy*

$$H(\mathbf{x}, t) := F(\mathbf{x}; \gamma(t))$$

and *tracks* the solutions of $F(\mathbf{x}; \mathbf{q}) = 0$ to $F(\mathbf{x}; \mathbf{p})$ along the homotopy H . This means that we use numerical algorithms to solve the *ODE initial value problem*

$$\left(\frac{d}{dx} H(\mathbf{x}, t) \right) \frac{d\mathbf{x}}{dt} + \frac{d}{dt} H(\mathbf{x}, t) = 0, \quad \mathbf{x}(0) = \mathbf{z}, \quad (3.5)$$

where the initial value \mathbf{z} is a zero of $G(\mathbf{x})$. In this setting $G(\mathbf{x}) = F(\mathbf{x}; \mathbf{q})$ is called *start system* and $F(\mathbf{x}) = F(\mathbf{x}; \mathbf{p})$ is called *target system*. The output of the numerical solver is then an approximate zero of $F(\mathbf{x})$. In implementations one often uses piecewise linear paths.

The next proposition explains why polynomial homotopy continuation works and when the initial value problem from (3.5) is well-posed. The proof of the proposition crucially relies on the Parameter Continuation Theorem (Theorem 3.16).

Proposition 3.21 Let \mathcal{F} be a family of polynomial systems with parameters $\mathbf{p} \in \mathbb{C}^k$. Let N and Δ be as in Theorem 3.16, and assume that $N > 0$. Given $\mathbf{q} \in \mathbb{C}^k \setminus \Delta$ and $\mathbf{p} \in \mathbb{C}^k$, then for almost all $\mathbf{p}_{\text{mid}} \in \mathbb{C}^k$ the piecewise linear path

$$\gamma(t) = \begin{cases} (2t-1)\mathbf{q} + 2(1-t)\mathbf{p}_{\text{mid}}, & \text{if } \frac{1}{2} \leq t \leq 1 \\ 2t\mathbf{p}_{\text{mid}} + (1-2t)\mathbf{p}, & \text{if } 0 < t \leq \frac{1}{2} \end{cases}$$

satisfies:

1. $\gamma((0, 1]) \cap \Delta = \emptyset$.
2. The homotopy $H(\mathbf{x}, t) := F(\mathbf{x}; \gamma(t))$ defines N smooth curves $\mathbf{x}(t)$ with the property that $H(\mathbf{x}(t), t) = 0$ for $0 < t \leq 1$. These curves are called *solution paths*.
3. As $t \rightarrow 0$, the limits of the solution paths include all regular solutions of $F(\mathbf{x}; \mathbf{p}) = 0$.
4. If moreover $\gamma(0) \notin \Delta$, then every solution path $\mathbf{x}(t)$ converges for $t \rightarrow 0$ to a regular zero of $F(\mathbf{x}; \mathbf{p})$.

Proof If $N > 0$, the discriminant $\Delta \subsetneq \mathbb{C}^k$ is a proper complex subvariety. Therefore, Δ is of complex codimension at least 1, hence of real codimension at least 2. This implies that for general $\mathbf{p}_{\text{mid}} \in \mathbb{C}^k$ the path $\gamma(t)$ does not intersect Δ for $t \in (0, 1]$. This proves the first item.

Since $\mathbf{q} = \gamma(0) \notin \Delta$, the implicit function theorem implies that there exists a neighborhood $\mathcal{U}_0 \subset \mathbb{C}^k$ of \mathbf{q} and a smooth *solution map* $s_0 : \mathcal{U}_0 \rightarrow \mathbb{C}^n$ with $F(s(\mathbf{p}), \mathbf{p}) = 0$ for all $\mathbf{p} \in \mathcal{U}_0$. Let

$$t_0 := \min \{t \in [0, 1] \mid \gamma(t) \in \overline{\mathcal{U}_0}\},$$

where $\overline{\mathcal{U}_0}$ is the Euclidean closure of \mathcal{U}_0 . If $t_0 > 0$, $\gamma(t_0) \notin \Delta$ and we can repeat the construction for the new start system $F(\mathbf{x}; \gamma(t_0))$. Eventually, we obtain an open cover

$$(0, 1] = \bigcup_{i \in \mathcal{I}} \mathcal{U}_i$$

for some index set \mathcal{I} , together with smooth solution maps $s_i : \mathcal{U}_i \rightarrow \mathbb{C}^n$. Taking a partition of unity $(\rho_i(t))_{i \in \mathcal{I}}$ relative to this cover we set

$$\mathbf{x}(t) := \sum_{i \in \mathcal{I}} \rho_i(t) \cdot (s_i \circ \gamma)(t), \quad t \in (0, 1].$$

By construction, $\mathbf{x}(t)$ is smooth and has the property that $H(\mathbf{x}(t), t) = 0$. Furthermore, as $t \rightarrow 0$ the solution path $\mathbf{x}(t)$ either converges to a point \mathbf{z} or diverges as $\|\mathbf{x}_i(t)\| \rightarrow \infty$. In the first situation, by continuity, \mathbf{z} is a zero of $F(\mathbf{x}, \gamma(0)) = F(\mathbf{x}, \mathbf{p})$ (not necessarily regular).

By Theorem 3.16, $F(\mathbf{x}; \mathbf{q})$ has N regular zeros. The construction above yields N solution paths $\mathbf{x}_1(t), \dots, \mathbf{x}_N(t)$. Smoothness implies that $\mathbf{x}_i(t) \neq \mathbf{x}_j(t)$ for $i \neq j$ and all $t \in (0, 1]$. This proves the second item. Furthermore, for every regular zero of $F(\mathbf{x}; \mathbf{q})$ we also find a (local) solution map, which connects to exactly one of the smooth paths $\mathbf{x}_1(t), \dots, \mathbf{x}_N(t)$. This implies the third and fourth item. \square

Example 3.22 We use `HomotopyContinuation.jl` [23] to solve the system of polynomial equations from Example 3.5.

```
using HomotopyContinuation
@var x y z;
f = x^2 + y^2 + z^2 - 1;
g = x^2 + z^2 - y;
h = x - z;
F = System([f; g; h], variables = [x; y; z])
solve(F)
```

This returns the solutions (here displayed with only the 4 most significant digits)

$$\begin{aligned} & (0.556 + 0.0\sqrt{-1}, 0.618 - 0.0\sqrt{-1}, 0.556 + 0.0\sqrt{-1}), \\ & (-0.0 - 0.899\sqrt{-1}, -1.618 + 0.0\sqrt{-1}, -0.0 - 0.899\sqrt{-1}), \\ & (-0.556 - 0.0\sqrt{-1}, 0.618 + 0.0\sqrt{-1}, -0.556 + 0.0\sqrt{-1}), \\ & (0.0 + 0.899\sqrt{-1}, -1.618 + 0.0\sqrt{-1}, -0.0 + 0.899\sqrt{-1}). \end{aligned}$$

These are numerical approximations of the solutions in Example 3.5. \diamond

Remark 3.23 Numerical computations are not exact computations and therefore can produce errors. This is hence also true for polynomial homotopy continuation. It is possible, though, to *certify* the output of PHC. Certification means that we obtain a computer proof that we have indeed computed an approximate zero. There are various certification methods. Current implementations are [22, 70, 103].

Corollary 3.24 A general system of polynomials $F(\mathbf{x}) = (f_1(\mathbf{x}), \dots, f_n(\mathbf{x}))$ in n variables has

$$N = d_1 \cdots d_n$$

isolated zeros in \mathbb{C}^n , where $d_i = \deg f_i$. (The number $d_1 \cdots d_n$ is also called Bézout number of F .)

Proof We consider the family $\mathcal{F}_{\text{Bézout}}$ of polynomial systems $F(\mathbf{x}) = (f_1(\mathbf{x}), \dots, f_n(\mathbf{x}))$ with $d_i = \deg f_i$. The parameters are the coefficients of the polynomials f_1, \dots, f_n . Here, we can use the start system

$$G(\mathbf{x}) = \begin{pmatrix} x_1^{d_1} - 1 \\ \vdots \\ x_n^{d_n} - 1 \end{pmatrix}.$$

This system has the $d_1 \cdots d_n$ many zeros $(\xi_1^{k_1}, \dots, \xi_n^{k_n})$, where $\xi_i := \exp(2\pi\sqrt{-1}/d_i)$ is the d_i -th root of unity and k_i ranges from 1 to d_i . One calls $G(x)$ the *total degree start system*. It neither has non-regular zeros nor zeros at infinity. Together with Proposition 3.21 this implies that $G(\mathbf{x})$ has the maximal number $N = d_1 \cdots d_n$ of regular zeros in $\mathcal{F}_{\text{Bézout}}$. \square

Remark 3.25 Corollary 3.24 is not yet a complete proof of Bézout's theorem, because it misses that for $F \in \Delta$ the number of zeros counted with multiplicities is also $d_1 \cdots d_n$.

Corollary 3.24 implies that one can use the total degree start system for homotopy continuation in the family of system of polynomials with fixed degree pattern.

Example 3.26 The system $F(x, y, z) = (x^2 + y^2 + z^2 - 1, x^2 + z^2 - y, x - z)$ from Example 3.22 consists of three polynomials in degrees $d_1 = 2, d_2 = 2$ and $d_3 = 1$. We have shown that the number of zeros of F is the Bézout number $N = d_1 \cdot d_2 \cdot d_3 = 4$. In `HomotopyContinuation.jl` [23] we can use the total degree start system by setting the following flag:

```
solve(F; start_system = :total_degree)
```

\diamond

Example 3.27 Let $A \subset \mathbb{N}^n$ be a finite set and denote $\mathcal{F}_A := \{\sum_{\alpha \in A} c_\alpha \mathbf{x}^\alpha \mid c_\alpha \in \mathbb{C}\}$. An element in \mathcal{F}_A is called a *sparse polynomial*, since only the monomials with exponent vector in A appear. For finite subsets $A_1, \dots, A_n \subset \mathbb{N}^n$ we consider the family $\mathcal{F}_{\text{sparse}} := \mathcal{F}_{A_1} \times \cdots \times \mathcal{F}_{A_n}$. The parameters in this family are the coefficients of the n sparse polynomials of a system in $\mathcal{F}_{\text{sparse}}$. For $1 \leq i \leq n$ let P_i be the convex hull of A_i ; the polytope P_i is called *Newton polytope* of F_{A_i} . Let $\text{MV}(P_1, \dots, P_n)$ denote the mixed volume of these n polytopes. The BKK Theorem [15, 16] asserts that a general $F \in \mathcal{F}_{\text{sparse}}$ has $n! \cdot \text{MV}(P_1, \dots, P_n)$ many zeros in the torus $(\mathbb{C}^*)^n$. Provided a general $F \in \mathcal{F}_{\text{sparse}}$ only has zeros with nonzero entries the maximal number of regular zeros in $\mathcal{F}_{\text{sparse}}$ therefore is

$$N = n! \cdot \text{MV}(P_1, \dots, P_n).$$

For instance, consider the system of polynomial equations

$$F(x, y) = \begin{pmatrix} a + bx + cy + dxy \\ \alpha + \beta x + \gamma y + \delta xy \end{pmatrix} \in \mathcal{F}_{\text{sparse}},$$

where $\mathbf{p} = (a, b, c, d, \alpha, \beta, \gamma, \delta) \in \mathbb{C}^8$ are parameters. Both polynomials in F have as Newton polytopes the unit cube. The mixed volume of two unit cubes is equal to 1. Therefore, the BKK Theorem implies that $F(x, y) = 0$ has $N = 2$ solutions for general parameters $\mathbf{p} \in \mathbb{C}^8$.

The article [83] provides an algorithm to compute an explicit start system for $\mathcal{F}_{\text{sparse}}$, called *polyhedral start system*. See also the summary in [11, Section 3]. \diamond

Chapter 4

Polar Degrees

We compare three definitions of *polar degrees*, in terms of non-transversal intersections, Schubert varieties and the Gauss map, and conormal varieties. The latter approach was used in Chapter 2.3. We discuss the key properties of polar degrees under projective duality and explain how polar degrees are related with Chern classes.

We work over an algebraically closed field of characteristic zero.

4.1 Polar Varieties

Example 4.1 Imagine that you look at an algebraic surface $X \subseteq \mathbb{P}^3$ from a point $V \in \mathbb{P}^3$. If you would want to sketch the surface from your point of view, you would draw its *contour curve* $P(X, V)$; see Figure 4.1. The contour curve consists of all points p on the surface X such that the line spanned by V and p is tangent at p . The *first polar degree* $\mu_1(X)$ of the surface X is the degree of the contour curve for a generic point V .

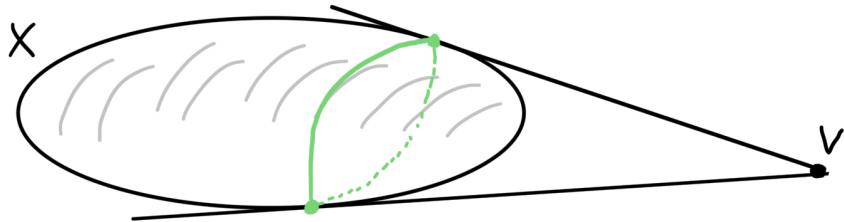


Fig. 4.1: Green contour curve when the ellipsoid X is viewed from the point V .

Now we change the setting slightly and imaging that our viewing of the surface X is not centered at a point but at a line $V \subseteq \mathbb{P}^3$. This time our contour set $P(X, V)$ consists of all point p on the surface X such that the plane spanned by the point p and the line V is tangent at p ; see Figure 4.2. For a generic line V , the contour set $P(X, V)$ is finite, and the *second polar degree* is its cardinality. \diamond

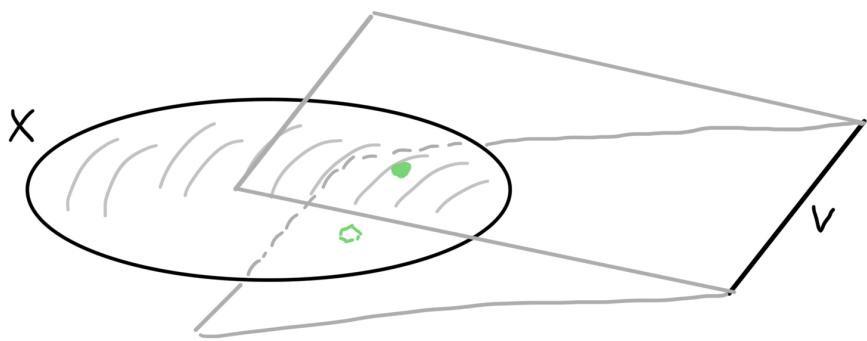


Fig. 4.2: The green contour set consists of two points when the ellipsoid X is viewed from the line V .

The contour sets described in the example above are also known as *polar varieties*. To define polar varieties in general, we need to fix some conventions and notations. For instance, the dimension of the empty set is considered to be -1 . Given projective subspaces $V, W \subseteq \mathbb{P}^n$, their projective span (equivalently, their join) is denoted by $V + W \subseteq \mathbb{P}^n$. If V and W are disjoint in projective space then we have

$$\dim(V + W) = \dim(V) + \dim(W) + 1$$

Given a projective variety $X \subseteq \mathbb{P}^n$, we write $\text{Reg}(X)$ for its regular locus. The *embedded tangent space* of X at $p \in \text{Reg}(X)$ is

$$\mathbb{T}_p X := \left\{ v \in \mathbb{P}^n \mid \forall f \in I(X) : \sum_{i=0}^n \frac{\partial f}{\partial x_i}(p) \cdot v_i = 0 \right\}.$$

We recall that a projective subspace $W \subseteq \mathbb{P}^n$ is said to intersect X *non-transversely* at $p \in \text{Reg}(X)$ if $p \in W$ and $\dim(W + \mathbb{T}_p X) < n$. For instance, if X is a smooth curve in \mathbb{P}^3 , then every line that intersects it does so non-transversely, while the tangent planes of X are the only planes that meet X non-transversely.

Definition 4.2 Let $X \subseteq \mathbb{P}^n$ be an irreducible projective variety. The *polar variety* of X with respect to a projective subspace $V \subseteq \mathbb{P}^n$ is

$$P(X, V) := \overline{\{p \in \text{Reg}(X) \setminus V \mid V + p \text{ intersects } X \text{ at } p \text{ non-transversely}\}}.$$

For every $i \in \{0, \dots, \dim X\}$, there is an integer $\mu_i(X)$ that is equal to the degree of $P(X, V)$ for almost all projective subspaces $V \subseteq \mathbb{P}^n$ with $\dim V = \text{codim } X - 2 + i$. The nonnegative integer $\mu_i(X)$ is called the *i-th polar degree* of X .

Example 4.3 A surface $X \subseteq \mathbb{P}^3$ has three polar degrees. For $i = 0, 1, 2$, the generic subspace V in Definition 4.2 is empty, a point, or a line, respectively. We saw the latter two cases in Example 4.1. For the case $i = 0$, we observe that $P(X, \emptyset) = X$. So, the 0-th polar degree $\mu_0(X)$ is the degree of the surface X . \diamond

Example 4.4 The last observation that $\mu_0(X) = \deg(X)$ is true in general. If $i = 0$, the dimension of the generic subspace V in Definition 4.2 is $\text{codim } X - 2$. Hence, we have for every $p \in \text{Reg}(X)$ that

$$\begin{aligned} \dim((V + p) + \mathbb{T}_p X) &= \dim(V + \mathbb{T}_p X) = \dim V + \dim X - \dim(V \cap \mathbb{T}_p X) \\ &\leq (\text{codim } X - 2) + \dim X + 1 = n - 1, \end{aligned}$$

which means that $V + p$ intersects X at p non-transversely. Therefore, we conclude that $P(X, V) = X$ and $\mu_0(X) = \deg(X)$. \diamond

We will now give a second definition of polar varieties in terms of the Gauss map and Schubert varieties. For that fix a projective subspace $V \subseteq \mathbb{P}^n$. We observe that $V + p$ intersects X at $p \in \text{Reg}(X)$ non-transversely (i.e., $n > \dim((V + p) + \mathbb{T}_p X) = \dim V + \dim X - \dim(V \cap \mathbb{T}_p X)$) if and only if

$$\dim(V \cap \mathbb{T}_p X) > \dim V - \text{codim } X. \tag{4.1}$$

Since $\dim V - \text{codim } X$ is the expected dimension of the intersection of the two projective subspaces V and $\mathbb{T}_p X$, condition (4.1) means that the tangent space $\mathbb{T}_p X$ meets V in an unexpectedly large dimension. Such subspaces are collected in simple instances of *Schubert varieties*:

$$\Sigma_m(V) := \{T \in \text{Gr}(m, \mathbb{P}^n) \mid \dim(V \cap T) > \dim V - n + m\}.$$

If $m = \dim X$, then condition (4.1) is equivalent to $\mathbb{T}_p X \in \Sigma_m(V)$. Hence, the *Gauss map*

$$\begin{aligned}\gamma_X : X &\dashrightarrow \mathrm{Gr}(m, \mathbb{P}^n), \\ p &\longmapsto \mathbb{T}_p X\end{aligned}$$

pulls the Schubert variety $\Sigma_m(V)$ back to the polar variety $P(X, V)$, i.e.,

$$P(X, V) = \overline{\gamma_X^{-1}(\Sigma_{\dim X}(V))}.$$

4.2 Projective Duality

We recall that there is a one-to-one correspondence between hyperplanes H in the \mathbb{P}^n and points H^\vee in the dual projective space $(\mathbb{P}^n)^*$. The *dual variety* of a projective variety $X \subseteq \mathbb{P}^n$ consists of all tangent hyperplanes of X :

$$X^\vee := \overline{\{H^\vee \in (\mathbb{P}^n)^* \mid \exists p \in \mathrm{Reg}(X) : \mathbb{T}_p X \subseteq H\}}.$$

Theorem 4.5 (Biduality theorem, [66]) Let $X \subseteq \mathbb{P}^n$ be a projective variety over an algebraically closed field of characteristic zero. Moreover, let $p \in \mathrm{Reg}(X)$ and $H^\vee \in \mathrm{Reg}(X^\vee)$. The hyperplane H is tangent to X at the point p if and only if the hyperplane p^\vee is tangent to X^\vee at the point H^\vee . In particular, $(X^\vee)^\vee = X$.

Example 4.6 If X is a projective subspace of \mathbb{P}^n , then X^\vee is a projective subspace of $(\mathbb{P}^n)^*$ with $\dim X^\vee = n - 1 - \dim X$. In particular, we have that $(\mathbb{P}^n)^\vee = \emptyset$.

Example 4.7 Let us revisit the example in Figure 4.2 that illustrates the polar variety $P(X, V)$ of a surface $X \subseteq \mathbb{P}^3$ and a generic line V . The tangent planes passing through the line V correspond in $(\mathbb{P}^3)^*$ to points on the dual variety X^\vee that are contained in the line V^\vee ; see Figure 4.3. Hence, if the dual variety is a surface as well, then its degree is given by the second polar degree of X , i.e., $\mu_2(X) = \deg(X^\vee)$. Otherwise, if the dual variety X^\vee is of smaller dimension, the line V^\vee misses it and $\mu_2(X) = 0$.

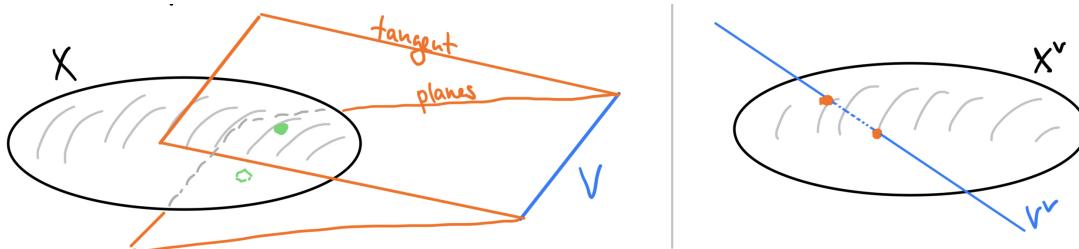


Fig. 4.3: $\mu_2(X) = \deg(X^\vee)$ holds for pairs of dual surfaces in projective 3-space ($q_i = (\mathbb{T}_p X)^\vee$).

In the setting of Figure 4.1, the polar variety $P(X, V)$ of a surface $X \subseteq \mathbb{P}^3$ and a generic point V is a curve. Thus, its degree ($= \mu_1(X)$) is computed by intersecting it with a generic plane H . The polar curve consists of all points on X whose tangent plane contains the point V , i.e., $P(X, V) = \overline{\{p \in \mathrm{Reg}(X) \mid V \in \mathbb{T}_p X\}}$. Hence, the first polar degree $\mu_1(X)$ counts all (regular) points $p \in X$ such that

$$p \in H \text{ and } V \in \mathbb{T}_p X. \quad (4.2)$$

The tangent planes at those points correspond to points $q := (\mathbb{T}_p X)^\vee$ in the dual projective space. By the biduality theorem, those points satisfy $\mathbb{T}_q X^\vee = p^\vee$ if the dual variety X^\vee is a surface. Hence, in that case, the two conditions in (4.2) are equivalent to

$$H^\vee \in \mathbb{T}_q X^\vee \text{ and } q \in V^\vee. \quad (4.3)$$

Comparing now (4.3) with (4.2), we see that the point-plane pair (H^\vee, V^\vee) imposes the same conditions on the points $q \in X^\vee$ as the point-plane pair (V, H) imposes on the points $p \in X$; see also Figure 4.4. Due to the genericity of (V, H) , we conclude that $\mu_1(X) = \mu_1(X^\vee)$ if X^\vee is a surface. If X^\vee is a curve, then $\mathbb{T}_q X^\vee \subseteq p^\vee$ and so the only conditions imposed by (4.2) on the points $q \in X^\vee$ is that they must lie in V^\vee , i.e., $\mu_1(X) = |X^\vee \cap V^\vee| = \deg(X^\vee) = \mu_0(X^\vee)$. Finally, if X^\vee is a point (i.e., X is a plane), then $\mu_1(X) = 0$. \diamond

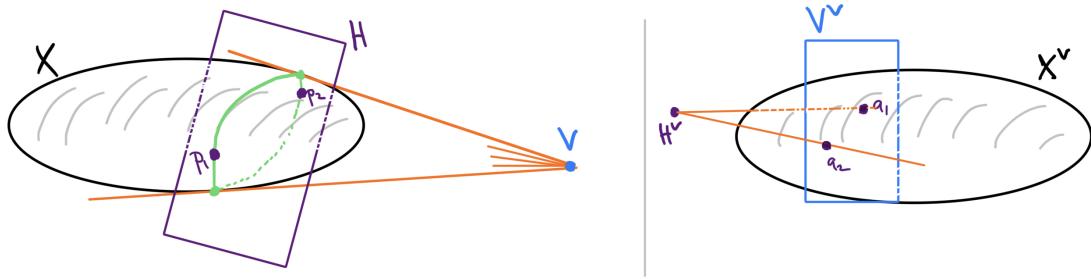


Fig. 4.4: $\mu_1(X) = \mu_1(X^\vee)$ holds for pairs of dual surfaces in projective 3-space.

The relations between the polar degrees of a variety and its dual that we observed in the previous example are true in more generality. More specifically, the list of polar degrees of a projective variety X is exactly the list of polar degrees of its dual variety X^\vee in reversed order. As seen in Example 4.4, the first non-zero entry in that list is $\deg(X)$, and so its last non-zero entry is $\deg(X^\vee)$. We summarize these key properties of polar degrees:

Proposition 4.8 ([76]) *Let X be an irreducible projective variety, and let $\alpha(X) := \dim X - \operatorname{codim} X^\vee + 1$.*

- (a) $\mu_i(X) > 0 \iff 0 \leq i \leq \alpha(X)$.
- (b) $\mu_0(X) = \deg X$.
- (c) $\mu_{\alpha(X)}(X) = \deg X^\vee$.
- (d) $\mu_i(X) = \mu_{\alpha(X)-i}(X^\vee)$.

The ideas discussed in Example 4.7 can be turned into formal proofs for almost all assertions in Proposition 4.8 (only the direction “ \Leftarrow ” in (a) is rather tricky). Another strategy is to first establish the relation of the polar degrees with the *conormal variety* of the projective variety $X \subseteq \mathbb{P}^n$:

$$\mathcal{N}_X := \overline{\{(p, H^\vee) \in \mathbb{P}^n \times (\mathbb{P}^n)^* \mid p \in \operatorname{Reg}(X), \mathbb{T}_p X \subseteq H\}}.$$

The projection of the conormal variety \mathcal{N}_X onto the first resp. second factor is the variety X resp. its dual X^\vee . Moreover, by the biduality theorem, we have that

$$\mathcal{N}_{X^\vee} = \{(H^\vee, p) \mid (p, H^\vee) \in \mathcal{N}_X\}. \quad (4.4)$$

Independently of the dimension of X , the dimension of the conormal variety is always $n - 1$. Hence, the *multidegree* of the conormal variety is given by its intersections with $L_1 \times L_2$, where $L_1 \subseteq \mathbb{P}^n$ and $L_2 \subseteq (\mathbb{P}^n)^*$ are generic subspaces with $\dim L_1 + \dim L_2 = \text{codim } \mathcal{N}_X = n + 1$. We denote the entries of that multidegree by

$$\delta_j(X) := |\mathcal{N}_X \cap (L_1 \times L_2)|, \text{ for generic } L_1, L_2 \text{ with } \dim L_2 = j, \dim L_1 = n + 1 - j.$$

We saw in Section 2.3 that the multidegree is the cohomology class of the conormal variety \mathcal{N}_X .

Proposition 4.9 ([91, Prop. (3) on page 187] or [64, Lem. (2.23) on page 169]) *The multidegree agrees with the polar degrees. More precisely, we have $\delta_j(X) = \mu_i(X)$, where $i := \dim X + 1 - j$.*

This proposition together with (4.4) implies immediately Proposition 4.8(d) and hence using Example 4.4 also (b) and (c). The direction “ \Rightarrow ” in Proposition 4.8(a) can also be deduced directly from the definition of the $\delta_j(X)$.

Before we present an idea of proof for Proposition 4.9, we revisit our running example.

Example 4.10 We see from Figure 4.4 and the conditions (4.2) and (4.3) that the first polar degree of a surface X in \mathbb{P}^3 is computed as $\mu_1(X) = |\mathcal{N}_X \cap (H \times V^\vee)| = \delta_2(X)$. In other words, Proposition 4.8 holds for surfaces X in \mathbb{P}^3 .

Proof (Sketch for Proposition 4.9) Let $L_1 \subseteq \mathbb{P}^n$ and $L_2 \subseteq (\mathbb{P}^n)^*$ be generic subspaces of dimensions $n + 1 - j$ and j , respectively. Setting $V := L_2^\vee$, we start by observing that V has the correct dimension to be used in the computation of the i -th polar degree (where $i = \dim X + 1 - j$), since $\dim V = n - j - 1 = \text{codim } X - 2 + i$.

Now we consider a generic pair $(p, H^\vee) \in \mathcal{N}_X \cap (\mathbb{P}^n \times L_2)$. The point $p \in X$ is regular and both its tangent space $\mathbb{T}_p X$ and $V = L_2^\vee$ are contained in the hyperplane H . In particular, we have $\dim(V + \mathbb{T}_p X) < n$ and so p is in the polar variety $P(X, V)$. In fact, the projection $\mathcal{N}_X \cap (\mathbb{P}^n \times L_2) \rightarrow P(X, V)$ onto the first factor is birational. Hence, $\mu_i(X) = \deg P(X, V) = |P(X, V) \cap L_1| = |\mathcal{N}_X \cap (L_1 \times L_2)| = \delta_j(X)$. \square

4.3 Chern Classes

Chern classes are topological invariants associated with vector bundles on smooth manifolds or varieties. For a smooth, irreducible projective variety X , its polar degrees can be computed from its Chern classes (see Proposition 4.11).

To a vector bundle \mathcal{E} on X of rank r , we associate the Chern classes $c_0(\mathcal{E}), \dots, c_r(\mathcal{E})$, which are formally elements in the *Chow ring* of X . Chern classes are easiest understood when the vector bundle \mathcal{E} is globally generated. In that case, the Chern class $c_{r+1-j}(\mathcal{E})$ is the element in the Chow ring of X that is associated with the following degeneracy locus:

$$D(\sigma_1, \dots, \sigma_j) := \{x \in X \mid \sigma_1(x), \dots, \sigma_j(x) \text{ are linearly dependent}\},$$

where $\sigma_1, \dots, \sigma_j : X \rightarrow \mathcal{E}$ are j general global sections. For the purpose of this section, it is not crucial to understand the Chow ring. It suffices for us to understand the *degree* of $c_{r+1-j}(\mathcal{E})$. This is defined to be the degree of the degeneracy locus $D(\sigma_1, \dots, \sigma_j)$ for general σ_i . For instance, the degree of the *top Chern class* $c_r(\mathcal{E})$ is the degree of the vanishing locus of a single general global section.

There are some calculation rules that allow us to compute Chern classes of more complex vector bundles. Most notably, the *Whitney sum formula* states for a short exact sequence $0 \rightarrow \mathcal{E}' \rightarrow \mathcal{E} \rightarrow \mathcal{E}'' \rightarrow 0$ of

vector bundles that $c_k(\mathcal{E}) = \sum_{i+j=k} c_i(\mathcal{E}')c_j(\mathcal{E}'')$; see [63, Theorem 3.2]. The Chern class $c_k(X)$ of X is an abbreviation for the Chern class $c_k(\mathcal{T}X)$ of its tangent bundle $\mathcal{T}X$.

Proposition 4.11 ([76, eq. (3)]) *Let X be a smooth, irreducible projective variety, and let $m := \dim X$. Then,*

$$\mu_i(X) = \sum_{k=0}^i (-1)^k \binom{m-k+1}{m-i+1} \deg(c_k(X)).$$

This formula can also be reverted to express degrees of Chern classes in terms of polar degrees:

$$\deg(c_k(X)) = \sum_{i=0}^k (-1)^i \binom{m-i+1}{m-k+1} \mu_i(X). \quad (4.5)$$

Remark 4.12 Both formulas also hold for singular varieties, after replacing the classical Chern classes with Chern-Mather classes. That result is due to R. Piene (see [123, Theorem 3] or [122]).

An important difference between polar degrees and Chern classes is the following: Polar degrees are projective invariants of the embedded variety $X \subseteq \mathbb{P}^n$. This holds also more generally for the *polar classes*, i.e., the rational equivalence classes (in the Chow ring of X) of the polar varieties. Chern classes are even *intrinsic invariants* of the variety X , i.e., they do not depend on the embedding of X in projective space.

Example 4.13 Let X be a smooth, irreducible projective variety.

- a) We see from (4.5) that $\deg(c_0(X)) = \mu_0(X) = \deg X$.
- b) The top Chern class of X coincides with its topological Euler characteristic: $\deg(c_m(X)) = \chi(X)$, where $m = \dim X$.
- c) If X is a curve, then $\chi(X) = 2 - 2g(X)$, where $g(X)$ denotes the genus. Moreover, we see from (4.5) that $\deg(c_1(X)) = 2\deg X - \mu_1(X)$. Hence, we conclude:

$$2\deg X - \mu_1(X) = 2 - 2g(X). \quad (4.6)$$

- d) If $X \subseteq \mathbb{P}^n$ is a rational curve, we can easily verify the relation (4.6):

- If X is a line, its dual variety is never a hypersurface, and so $\mu_1(X) = 0$.
- If X is a conic (i.e., $\deg X = 2$), its dual variety is (a cone over) a conic, and so $\mu_1(X) = \deg X^\vee = 2$.
- If X is a twisted cubic (i.e., $\deg X = 3$), its dual variety is (a cone over) the discriminant hypersurface of a cubic polynomial, and so $\mu_1(X) = \deg X^\vee$ is the degree of that discriminant, which is 4.
- More generally, if X is a rational normal curve of degree d , its dual variety is (a cone over) the discriminant hypersurface of a degree- d polynomial, and so $\mu_1(X) = \deg X^\vee$ is the degree of that discriminant, which is $2d - 2$.

Chapter 5

Wasserstein Distance

A fundamental problem in metric algebraic geometry is distance minimization. We seek a point in a variety X in \mathbb{R}^n that is closest to a given data point $\mathbf{u} \in \mathbb{R}^n$. Thus, we must solve the optimization problem

$$\text{minimize } \|\mathbf{x} - \mathbf{u}\| \text{ subject to } \mathbf{x} \in X. \quad (5.1)$$

In what follows, this minimum in (5.1) is always attained because X is non-empty and closed. Hence there exists at least one optimal solution. If that solution is unique then we denote it by \mathbf{x}^* .

In the previous chapter we discussed this problem for the Euclidean norm on \mathbb{R}^n . In what follows we study (5.1) in the case when the distance is given by a *polyhedral norm*. We will then focus on a particular class of polyhedral norms that arise from optimal transport theory. These are known as Wasserstein norms.

5.1 Polyhedral Norms

A norm $\|\cdot\|$ on the real vector space \mathbb{R}^n is a *polyhedral norm* if its unit ball is polyhedral:

$$B = \{\mathbf{x} \in \mathbb{R}^n : \|\mathbf{x}\| \leq 1\}.$$

More precisely, B is a centrally symmetric convex polytope. Conversely, every centrally symmetric convex polytope B in \mathbb{R}^n defines a polyhedral norm on \mathbb{R}^n . Using the unit ball, we can paraphrase (5.1) as follows:

$$\text{minimize } \lambda \text{ subject to } \lambda \geq 0 \text{ and } (\mathbf{u} + \lambda B) \cap X \neq \emptyset. \quad (5.2)$$

Familiar examples of polyhedral norms are $\|\cdot\|_\infty$ and $\|\cdot\|_1$. For these norms, the unit ball B is, respectively, the cube and the crosspolytope (a.k.a. generalized octahedron). Polyhedral norms are very important in optimal transport theory, where one uses a Wasserstein norm on the space of probability distributions. This will be our main application in this chapter, and it will be discussed in detail in the later sections.

We begin our discussion with a general polyhedral norm, that is, we allow B to be an arbitrary n -dimensional centrally symmetric polytope in \mathbb{R}^n . The boundary of B consists of faces whose dimensions range from 0 to $n - 1$. We use the dot \cdot for the standard inner product on \mathbb{R}^n . Recall that a subset F of the polytope B is a *face* if there exists a linear functional $\ell \in \mathbb{R}^n \setminus \{0\}$ such that

$$F = \{\mathbf{x} \in B : \ell \cdot \mathbf{x} \geq \ell \cdot \mathbf{y} \text{ for all } \mathbf{y} \in B\}. \quad (5.3)$$

The set of all faces, ordered by inclusion, is a partial ordered set, called the *face poset* of B . An important combinatorial invariant of our polytope B is its *f-vector* $f(B) = (f_0, f_1, \dots, f_{n-1})$. By definition, the i th coordinate f_i of the f-vector is the number of i -dimensional faces of B .

The dual of the unit ball B is also a centrally symmetric polytope, namely it is the set

$$B^* = \{\ell \in \mathbb{R}^n : \ell \cdot \mathbf{x} \leq 1 \text{ for all } \mathbf{x} \in B\}.$$

The norm $\|\cdot\|_*$ defined by the dual polytope B^* is dual to the norm $\|\cdot\|$ given by B . The f-vector of B^* is the reverse of the f-vector of B . More precisely, we have $f_i(B^*) = f_{n-1-i}(B)$ for $i = 0, 1, \dots, n - 1$.

Example 5.1 Fix the unit cube $B = [-1, 1]^n$. Its dual is the crosspolytope

$$B^* = \text{conv}\{\pm \mathbf{e}_1, \pm \mathbf{e}_2, \dots, \pm \mathbf{e}_n\} \subset \mathbb{R}^n.$$

Here \mathbf{e}_j is the j th standard basis vector. The number of i -dimensional faces of the cube is

$$f_i(B) = \binom{n}{i} \cdot 2^{n-i}.$$

The 3-dimensional crosspolytope is the octahedron. The 3-cube and the octahedron satisfy

$$f(B) = (8, 12, 6) \quad \text{and} \quad f(B^*) = (6, 12, 8).$$

These numbers govern the combinatorial structure of the norms $\|\cdot\|_\infty$ and $\|\cdot\|_1$ on \mathbb{R}^3 .

We now turn to the critical equations for the optimization problem given in (5.1) or (5.2). To derive these equations, a combinatorial stratification of the problem will be used. This is given by the face poset of the polytope B . Suppose that the variety X is in sufficiently general position in \mathbb{R}^n . This hypothesis implies that $(\mathbf{u} + \lambda^* B) \cap X = \{\mathbf{x}^*\}$ is a singleton for the optimal value λ^* in (5.2). The point $\frac{1}{\lambda^*}(\mathbf{x}^* - \mathbf{u})$ lies in boundary of the unit ball B . Hence it lies in the relative interior of a unique face F of the polytope B . Let L_F denote the linear span of F in \mathbb{R}^n . We have $\dim(L_F) = \dim(F) + 1$. Let ℓ be any linear functional on \mathbb{R}^n that attains its maximum over the polytope B at the face F . This means that (5.3) holds.

Lemma 5.2 *The optimal point \mathbf{x}^* in (5.1) is the unique solution to the optimization problem*

$$\text{Minimize } \ell(\mathbf{x}) \text{ subject to } \mathbf{x} \in (\mathbf{u} + L_F) \cap X. \quad (5.4)$$

Proof The general position hypothesis ensures that the affine space $\mathbf{u} + L_F$ intersects the real variety X transversally, and \mathbf{x}^* is a smooth point of that intersection. Moreover, \mathbf{x}^* is a minimum of the restriction of ℓ to the variety $(\mathbf{u} + L_F) \cap X$. By our hypothesis, this linear function is generic relative to the variety, so the number of critical points is finite and the function values are distinct. \square

Example 5.3 (Touching at a facet) Suppose that the face F is a facet of the unit ball B . Then $L_F = \mathbb{R}^n$, and ℓ is an outer normal vector to that facet, which is unique up to scaling. Here, the optimization problem (5.4) asks for the minimum of ℓ over X . This situation corresponds to the left diagram in Figure 5.1.

Example 5.4 (Touching at a vertex) Suppose F is a vertex of the unit ball B . This case arises when X is a hypersurface. It corresponds to the middle diagram in Figure 5.1. Here, the affine space $\mathbf{u} + L_F$ is the line that connects \mathbf{u} and \mathbf{x}^* . That line intersects X in a finite set of cardinality $\text{degree}(X)$. The optimal \mathbf{x}^* is the real point in that finite set at which the value of the linear form ℓ is minimal.

Problem (5.4) amounts to linear programming over a real variety. We now determine the algebraic degree of this optimization task when F is a face of codimension i . To this end, we replace the affine variety $X \subset \mathbb{R}^n$ by its closure in complex projective space \mathbb{P}^n . We retain the same symbol X for that projective variety. Consider the affine space $L = u + L_F$ in \mathbb{R}^n , and also identify it with its closure in \mathbb{P}^n . If the face F has codimension i then the linear space L has codimension $i - 1$. The following result assumes that this space is in general position relative to the variety X and relative to the isotropic quadric.

Theorem 5.5 *Let L be a general affine-linear space of codimension $i - 1$ in \mathbb{R}^n and let ℓ be a general linear form. The number of critical points of ℓ on $L \cap X$ is the polar degree $\delta_i(X)$.*

Proof This result appears in [36, Theorem 5.1]. The number of critical points of a linear form is the degree of the dual variety $(L \cap X)^\vee$. That degree coincides with the polar degree $\delta_i(X)$. \square

Example 5.6 Examples 5.3 and 5.4 explain Theorem 5.5 in the two extreme cases $i = 1$ and $i = n$. Touching at a vertex ($i = n$) can only happen when X is a hypersurface, and here $\delta_n(X) = \text{degree}(X)$. Touching at a facet ($i = 1$) can happen for varieties of any dimension, as long as the dual variety X^\vee is a hypersurface. In that case we have $\delta_1(X) = \text{degree}(X^\vee)$.

Theorem 5.5 offers a direct interpretation of each polar degree $\delta_i(X)$ in terms of optimization on X . This interpretation can be used as a definition of polar degrees. Some readers might prefer this.

Example 5.7 Consider the distance minimization problem in (5.1) and (5.2) where X is a general surface of degree d in \mathbb{R}^3 . The optimal face F of the unit ball B depends on the location of the data point \mathbf{u} . The algebraic degree of the solution \mathbf{x}^* equals $\delta_3(X) = d$ if $\dim(F) = 0$, it is $\delta_2(X) = d(d-1)$ if $\dim(F) = 1$, and it is $\delta_1(X) = d(d-1)^2$ if $\dim(F) = 2$. Here \mathbf{x}^* is the unique point in $(\mathbf{u} + \lambda^* B) \cap X$, where λ^* is the optimal value in (5.2). Figure 5.1 visualizes this scenario for $d = 2$ and $\|\cdot\|_\infty$. The variety X is the green sphere, which is a surface of degree $d = 2$. The unit ball for the norm $\|\cdot\|_\infty$ is the cube $B = [-1, 1]^3$. The picture shows the smallest λ^* such that $\mathbf{u} + \lambda^* B$ touches the sphere X . The cross marks the point of contact. This is the point \mathbf{x}^* in X which is closest in ∞ -norm to the green point \mathbf{u} in the center of the cube. Point of contact is either on a facet, or on an edge, or it is a vertex. The algebraic degree of \mathbf{x}^* is two in all three cases, i.e. we can write the solution \mathbf{x}^* in terms of the data \mathbf{u} by solving the quadratic formula. If the green surface in Figure 5.1 were a cubic surface then these polar degrees would be 3, 6 and 12.

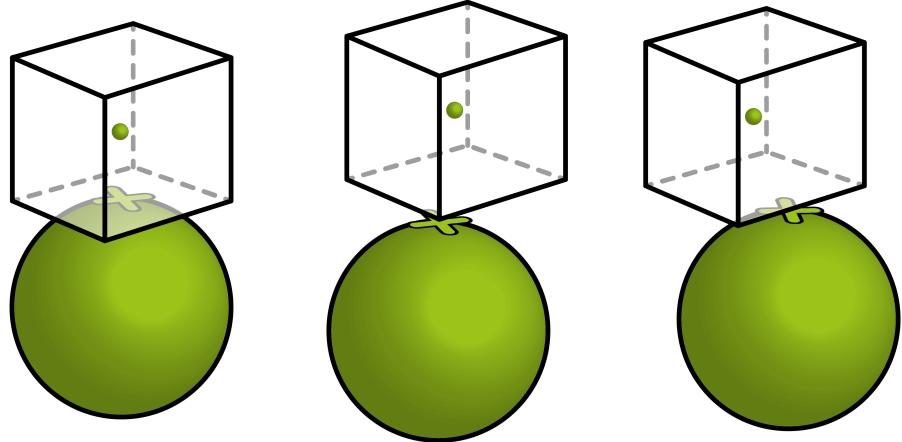


Fig. 5.1: The cube is an $\|\cdot\|_\infty$ ball around the green point u . The variety X is the sphere. The contact point x^* is marked with a cross. The optimal face F is a facet, vertex, or edge.

We have learned that the conormal variety N_X and its cohomology class $[N_X]$ are key players when it comes to reliably solving the distance minimization problem for a variety X . This applies not just to the Euclidean distance problem, but also to the analogous problem for polyhedral norms. The polar degrees $\delta_i(X)$ reveal precisely how many paths need to be tracked by numerical solvers like [12, 27] in order to find and certify [26] the optimal solution x^* in (5.1) or (5.4).

5.2 Optimal Transport and Independence Models

We now come to the main theme of this chapter, namely the Wasserstein distance to a given variety X . For us, X will be an independence model in a probability simplex, described algebraically by matrices or tensors of low rank, and we measure distances using Wasserstein metrics on that simplex. This is a class of polyhedral norms which are important in optimal transport theory. We now present the relevant definitions.

A probability distribution on the finite set $[n] = \{1, 2, \dots, n\}$ is a point ν in the simplex $\Delta_{n-1} = \{(\nu_1, \dots, \nu_n) \in \mathbb{R}_{\geq 0}^n : \sum_{i=1}^n \nu_i = 1\}$. We metrize this simplex by the *Wasserstein distance*. To define this

notion, we first turn the state space $[n]$ into a finite metric space by fixing a symmetric $n \times n$ matrix $d = (d_{ij})$ with nonnegative entries. These entries satisfy $d_{ii} = 0$ and $d_{ik} \leq d_{ij} + d_{jk}$ for all i, j, k . Given two probability distributions μ and ν in Δ_{n-1} , we consider the following linear programming problem, where $\mathbf{z} = (z_1, \dots, z_n)$ denotes the decision variables:

$$\text{Maximize } \sum_{i=1}^n (\mu_i - \nu_i) z_i \text{ subject to } |z_i - z_j| \leq d_{ij} \text{ for all } 1 \leq i < j \leq n. \quad (5.5)$$

The optimal value of (5.5), denoted $W_d(\mu, \nu)$, is the *Wasserstein distance* between μ and ν .

The optimal solution \mathbf{z}^* to problem (5.5) is known as the *optimal discriminator* for the two probability distributions μ and ν . It satisfies $W_d(\mu, \nu) = \langle \mu - \nu, \mathbf{z}^* \rangle$, and its coordinates z_i^* are weights on the state space $[n]$ that tell μ and ν apart. Here $\langle \cdot, \cdot \rangle$ is the standard inner product on \mathbb{R}^n . The linear program (5.5) is the *Kantorovich dual* of the *optimal transport problem*.

The feasible region of the linear program (5.5) is unbounded because it is invariant under translation by $\mathbf{1} = (1, 1, \dots, 1)$. It is compact after taking the quotient modulo the line $\mathbb{R}\mathbf{1}$:

$$P_d = \{ \mathbf{z} \in \mathbb{R}^n / \mathbb{R}\mathbf{1} : |z_i - z_j| \leq d_{ij} \text{ for all } 1 \leq i < j \leq n \}. \quad (5.6)$$

This $(n-1)$ -dimensional polytope is the *Lipschitz polytope* of the metric space $([n], d)$. In the field of tropical geometry, one calls P_d a *polytrope* because it is convex both classically and tropically.

The polytope P_d^* that is dual to P_d lies in the hyperplane perpendicular to the line $\mathbb{R}\mathbf{1}$. We call P_d^* the *root polytope* because its vertices are, up to scaling, the elements $\mathbf{e}_i - \mathbf{e}_j$ in the root system of Lie type A_{n-1} . More precisely, we have

$$P_d^* = \{ x \in \mathbb{R}^n : \max_{z \in P_d} \langle x, z \rangle \leq 1 \} = \text{conv} \left\{ \frac{1}{d_{ij}} (\mathbf{e}_i - \mathbf{e}_j) : 1 \leq i, j \leq n \right\}.$$

This is a centrally symmetric polytope since the finite metric space $([n], d)$ satisfies $d_{ij} = d_{ji}$.

Proposition 5.8 *The Wasserstein metric W_d on the probability simplex Δ_{n-1} is given by the polyhedral norm whose unit ball is the root polytope P_d^* .*

Proof Fix the polyhedral norm with unit ball P_d^* . The distance between μ and ν in this norm is the smallest real number λ such that $\mu \in \nu + \lambda P_d^*$, or, equivalently, $\frac{1}{\lambda}(\mu - \nu) \in P_d^*$. By definition of dual polytope, this minimal λ is the maximum inner product $\langle \mu - \nu, z \rangle$ over all points z in the dual $(P_d^*)^*$ of the unit ball. But this specifies the Lipschitz polytope, i.e. $(P_d^*)^* = P_d$. Hence the distance between μ and ν is equal to $W_d(\mu, \nu)$, which is the optimal value in (5.5). \square

Example 5.9 Let $n = 4$ and fix the finite metric space graph distance on the 4-cycle

$$d = \begin{pmatrix} 0 & 1 & 1 & 2 \\ 1 & 0 & 2 & 1 \\ 1 & 2 & 0 & 1 \\ 2 & 1 & 1 & 0 \end{pmatrix}. \quad (5.7)$$

The induced metric on the tetrahedron Δ_3 is given by the Lipschitz polytope

$$\begin{aligned} P_d &= \{ (x_1, x_2, x_3, x_4) \in \mathbb{R}^4 / \mathbb{R}\mathbf{1} : |x_1 - x_2| \leq 1, |x_1 - x_3| \leq 1, |x_2 - x_4| \leq 1, |x_3 - x_4| \leq 1 \} \\ &= \text{conv} \{ (1, 0, 0, -1), (1, 0, 0, -1), (\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}), (-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}), (0, 1, -1, 0), (0, -1, 1, 0) \}. \end{aligned}$$

Note that this 3-dimensional polytope is an octahedron. Therefore, its dual is a cube:

$$\begin{aligned} P_d^* &= \{(y_1, y_2, y_3, y_4) \in (\mathbb{R}\mathbf{1})^\perp : |y_1 - y_4| \leq 1, |y_2 - y_3| \leq 1, |y_2 + y_3| \leq 1\} \\ &= \text{conv}\{(1, -1, 0, 0), (1, 0, -1, 0), (0, 1, 0, -1), (0, 0, 1, -1) \\ &\quad (-1, 1, 0, 0), (-1, 0, 1, 0), (0, -1, 0, 1), (0, 0, -1, 1)\}. \end{aligned}$$

This is the unit ball for the Wasserstein metric on the tetrahedron Δ_3 that is induced by d . Measuring the distance from a point to a surface with respect to this metric is illustrated in Figure 5.1.

We wish to compute the Wasserstein distance from a given distribution μ to a fixed *discrete statistical model* $\mathcal{M} \subset \Delta_{n-1}$. This is the problem studied in [35, 36]. Our discussion serves as an introduction. As is customary in algebraic statistics, we assume that \mathcal{M} is defined by polynomials in v_1, \dots, v_n .

Our task is to solve the following optimization problem:

$$W_d(\mu, \mathcal{M}) := \min_{v \in \mathcal{M}} W_d(\mu, v) = \min_{v \in \mathcal{M}} \max_{x \in P_d} \langle \mu - v, x \rangle. \quad (5.8)$$

Computing this quantity means solving a non-convex optimization problem. Our aim is to study this problem and propose solution strategies, using methods from geometry, algebra and combinatorics. The analogous problem for the Euclidean metric was treated earlier.

We now present a detailed case study for the tetrahedron Δ_3 whose points are joint probability distributions of two binary random variables. The *2-bit independence model* $\mathcal{M} \subset \Delta_3$ consists of all nonnegative 2×2 matrices of rank one whose entries sum to one:

$$\begin{pmatrix} v_1 & v_2 \\ v_3 & v_4 \end{pmatrix} = \begin{pmatrix} pq & p(1-q) \\ (1-p)q & (1-p)(1-q) \end{pmatrix}, \quad (p, q) \in [0, 1]^2. \quad (5.9)$$

Thus, \mathcal{M} is the quadratic surface in the tetrahedron Δ_3 defined by the equation $v_1 v_4 = v_2 v_3$. The next theorem gives the optimal value function and the solution function for this independence model. We use the Wasserstein metric W_d that was defined in Example 5.9.

Theorem 5.10 *The Wasserstein distance from a distribution $\mu \in \Delta_3$ to the surface \mathcal{M} equals*

$$W_d(\mu, \mathcal{M}) = \begin{cases} 2\sqrt{\mu_1}(1 - \sqrt{\mu_1}) - \mu_2 - \mu_3 & \text{if } \mu_1 \geq \mu_4, \sqrt{\mu_1} \geq \mu_1 + \mu_2, \sqrt{\mu_1} \geq \mu_1 + \mu_3, \\ 2\sqrt{\mu_2}(1 - \sqrt{\mu_2}) - \mu_1 - \mu_4 & \text{if } \mu_2 \geq \mu_3, \sqrt{\mu_2} \geq \mu_1 + \mu_2, \sqrt{\mu_2} \geq \mu_2 + \mu_4, \\ 2\sqrt{\mu_3}(1 - \sqrt{\mu_3}) - \mu_1 - \mu_4 & \text{if } \mu_3 \geq \mu_2, \sqrt{\mu_3} \geq \mu_1 + \mu_3, \sqrt{\mu_3} \geq \mu_3 + \mu_4, \\ 2\sqrt{\mu_4}(1 - \sqrt{\mu_4}) - \mu_2 - \mu_3 & \text{if } \mu_4 \geq \mu_1, \sqrt{\mu_4} \geq \mu_2 + \mu_4, \sqrt{\mu_4} \geq \mu_3 + \mu_4, \\ |\mu_1\mu_4 - \mu_2\mu_3|/(\mu_1 + \mu_2) & \text{if } \mu_1 \geq \mu_4, \mu_2 \geq \mu_3, \mu_1 + \mu_2 \geq \sqrt{\mu_1}, \mu_1 + \mu_2 \geq \sqrt{\mu_2}, \\ |\mu_1\mu_4 - \mu_2\mu_3|/(\mu_1 + \mu_3) & \text{if } \mu_1 \geq \mu_4, \mu_3 \geq \mu_2, \mu_1 + \mu_3 \geq \sqrt{\mu_1}, \mu_1 + \mu_3 \geq \sqrt{\mu_3}, \\ |\mu_1\mu_4 - \mu_2\mu_3|/(\mu_2 + \mu_4) & \text{if } \mu_4 \geq \mu_1, \mu_2 \geq \mu_3, \mu_2 + \mu_4 \geq \sqrt{\mu_4}, \mu_2 + \mu_4 \geq \sqrt{\mu_2}, \\ |\mu_1\mu_4 - \mu_2\mu_3|/(\mu_3 + \mu_4) & \text{if } \mu_4 \geq \mu_1, \mu_3 \geq \mu_2, \mu_3 + \mu_4 \geq \sqrt{\mu_4}, \mu_3 + \mu_4 \geq \sqrt{\mu_3}. \end{cases}$$

The solution function $\Delta_3 \rightarrow \mathcal{M}$, $\mu \mapsto v^*(\mu)$ is given (with the same case distinction) by

$$v^*(\mu) = \begin{cases} (\mu_1, \sqrt{\mu_1} - \mu_1, \sqrt{\mu_1} - \mu_1, -2\sqrt{\mu_1} + \mu_1 + 1), \\ (\sqrt{\mu_2} - \mu_2, \mu_2, -2\sqrt{\mu_2} + \mu_2 + 1, \sqrt{\mu_2} - \mu_2), \\ (\sqrt{\mu_3} - \mu_3, -2\sqrt{\mu_3} + \mu_3 + 1, \mu_3, \sqrt{\mu_3} - \mu_3), \\ (-2\sqrt{\mu_4} + \mu_4 + 1, \sqrt{\mu_4} - \mu_4, \sqrt{\mu_4} - \mu_4, \mu_4), \\ (\mu_1, \mu_2, \mu_1(\mu_3 + \mu_4)/(\mu_1 + \mu_2), \mu_2(\mu_3 + \mu_4)/(\mu_1 + \mu_2)), \\ (\mu_1, \mu_1(\mu_2 + \mu_4)/(\mu_1 + \mu_3), \mu_3, \mu_3(\mu_2 + \mu_4)/(\mu_1 + \mu_3)), \\ (\mu_2(\mu_1 + \mu_3)/(\mu_2 + \mu_4), \mu_2, \mu_4(\mu_1 + \mu_3)/(\mu_2 + \mu_4), \mu_4), \\ (\mu_3(\mu_1 + \mu_2)/(\mu_3 + \mu_4), \mu_4(\mu_1 + \mu_2)/(\mu_3 + \mu_4), \mu_3, \mu_4). \end{cases}$$

The boundaries separating the various cases are given by the surfaces $\{\mu \in \Delta_3 : \mu_1 - \mu_4 = 0, \mu_1 + \mu_2 \geq \sqrt{\mu_1}, \mu_1 + \mu_3 \geq \sqrt{\mu_1}\}$ and $\{\mu \in \Delta_3 : \mu_2 - \mu_3 = 0, \mu_1 + \mu_2 \geq \sqrt{\mu_2}, \mu_2 + \mu_4 \geq \sqrt{\mu_2}\}$.

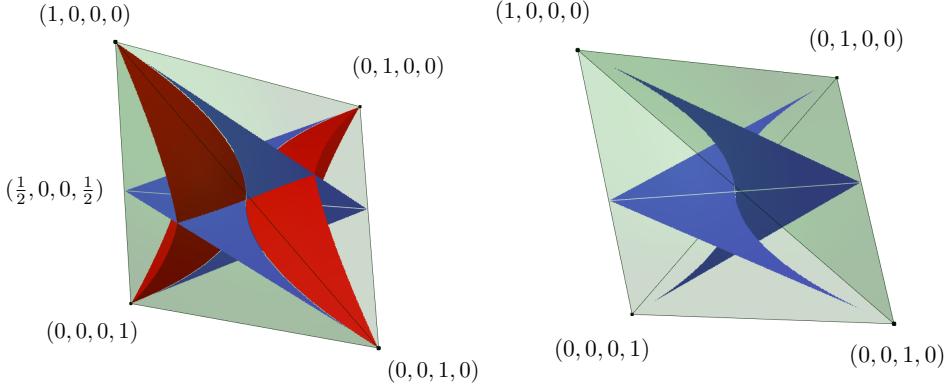


Fig. 5.2: The optimal value function of Theorem 5.10 subdivides the tetrahedron of probability distributions μ (left). The surfaces that separate the various cases are shown in blue (right).

Theorem 5.10 involves a distinction into eight cases. This division of Δ_3 is shown in Figure 5.2. Each of the last four cases breaks into two subcases, since the numerator in the formulas is the absolute value of $\mu_1\mu_4 - \mu_2\mu_3$. The sign of this 2×2 determinant matters for the pieces of our piecewise algebraic function. Thus, the tetrahedron Δ_3 is divided into 12 regions on which $\mu \mapsto W_d(\mu, \mathcal{M})$ is algebraic. We now explain how to visualize Figure 5.2. The red surface consists of eight pieces that, together with the blue surface, separate the eight cases (this surface is not the model). Four convex regions are enclosed between the red surfaces and the edges they meet. These regions represent the first four cases in Theorem 5.10. For instance, the region containing the points $(1, 0, 0, 0), (1/2, 0, 0, 1/2)$ corresponds to the first case. The remaining four regions are each bounded by two red and two blue pieces, and correspond to the last four cases. Each of these four regions is further split in two by the model. We do not depict this in our visualization. The two sides are determined by the sign of the determinant $\mu_1\mu_4 - \mu_2\mu_3$. The two blue surfaces in the right figure separate the various cases. These specify the points $\mu \in \Delta_3$ with more than one optimal solution. For the proof of Theorem 5.10 and a simpler example see [36]. For further details we refer to [35].

5.3 Wasserstein meets Segre-Veronese

Returning to the general case, let \mathcal{M} be a smooth variety in $\Delta_{n-1} \subset \mathbb{R}^n$. For any $\nu \in \Delta_{n-1}$, we seek its distance to \mathcal{M} under our polyhedral norm. As before, the optimal point ν^* determines a unique face F of the unit ball $B = P_d^*$. Given that face F , we now characterize optimality as in Lemma 5.2. Let \mathcal{F} be the set of all index pairs (i, j) such that the point $\frac{1}{d_{ij}}(\mathbf{e}_i - \mathbf{e}_j)$ is a vertex and it lies in F . Let ℓ_F be any linear functional on \mathbb{R}^n that attains its maximum over B at F . We work in the linear space spanned by the face:

$$L_F = \left\{ \sum_{(i,j) \in \mathcal{F}} \lambda_{ij} (\mathbf{e}_i - \mathbf{e}_j) : \lambda_{ij} \in \mathbb{R} \right\}. \quad (5.10)$$

The point ν^* on \mathcal{M} that is closest to μ is the solution of the following optimization problem:

$$\text{Minimize } \ell_F = \ell_F(\nu) \text{ subject to } \nu \in (\mu + L_F) \cap \mathcal{M}. \quad (5.11)$$

This is an optimization problem in the linear subspace L_F . With the notation in (5.10), the decision variables are λ_{ij} for $(i, j) \in \mathcal{F}$. The algebraic complexity of this problem is given by the polar degree (Theorem 5.5). The combinatorial complexity is governed by the facial structure of the Wasserstein ball $B = P_d^*$ associated to a finite metric space $([n], d)$. We now focus on the polar dual, the $(n-1)$ -dimensional Lipschitz polytope $B^* = P_d$. This polytope lives in $\mathbb{R}^n / \mathbb{R}\mathbf{1} \simeq \mathbb{R}^{n-1}$, and is defined in (5.6).

In the study of independence models $\mathcal{M} \subset \Delta_{n-1}$, the following metrics $([n], d)$ arise:

- The discrete metric on any finite set $[n]$ where $d_{ij} = 1$ for distinct i, j .
- The L_0 -metric on the Cartesian product $[m_1] \times \cdots \times [m_k]$ where $d_{ij} = \#\{l : i_l \neq j_l\}$. Here $i = (i_1, \dots, i_k)$ and $j = (j_1, \dots, j_k)$ are elements in that Cartesian product.
- The L_1 -metric on the Cartesian product $[m_1] \times \cdots \times [m_k]$ where $d_{ij} = \sum_{l=1}^k |i_l - j_l|$.

For the last two metrics, the number of states of the relevant independence models is $n = m_1 \cdots m_k$. To compute Wasserstein distances, we need to describe the Lipschitz polytope P_d as explicitly as possible. All three metrics above are *graph metrics*. This means that there exists an undirected simple graph G with vertex set $[n]$ such that d_{ij} is the length of the shortest path from i to j in G . The corresponding Wasserstein balls are called *symmetric edge polytopes*. They are investigated in [36, Section 4].

The following four independence models are used for the case studies in [36, Section 6]. We use the tuple $((m_1)_{d_1}, \dots, (m_k)_{d_k})$ to denote the independence model with $n = \prod_{i=1}^k \binom{m_i+d_i-1}{d_i}$ states where the i th entry $(m_i)_{d_i}$ refers to a multinomial distribution with m_i possible outcomes and d_i trials, which can be interpreted as an unordered set of d_i identically distributed random variables on $[m_i] = \{1, 2, \dots, m_i\}$. The subscript d_i is omitted if $d_i = 1$. For example, $(2_2, 2)$ is the independence model for three binary random variables where the first two are identically distributed. We list the $n = 6$ states in the order 00, 10, 20, 01, 11, 21. These are the vertices of the associated graph G , which is the product of a 3-chain and a 2-chain. This model \mathcal{M} is the image of the map from the square $[0, 1]^2$ into the simplex Δ_5 given by

$$(p, q) \mapsto (p^2 q, 2p(1-p)q, (1-p)^2 q, p^2(1-q), 2p(1-p)(1-q), (1-p)^2(1-q)). \quad (5.12)$$

Example 5.11 We consider four models: the 3-bit model $(2, 2, 2)$ with the L_0 -metric on $[2]^3$, the model $(3, 3)$ for two ternary variables with the L_1 -metric on $[3]^2$, the model (2_6) for six identically distributed binary variables with the discrete metric on $[7]$, and the model $(2_2, 2)$ in (5.12) with the L_1 -metric on $[3] \times [2]$. In Table 5.1, we report the f-vectors of the Wasserstein balls for each of these models.

\mathcal{M}	n	$\dim(\mathcal{M})$	Metric d	f-vector of the $(n-1)$ -polytope P_d^*
$(2, 2, 2)$	8	3	$L_0 = L_1$	(24, 192, 652, 1062, 848, 306, 38)
$(3, 3)$	9	4	L_1	(24, 216, 960, 2298, 3048, 2172, 736, 82)
(2_6)	7	1	discrete	(42, 210, 490, 630, 434, 126)
$(2_2, 2)$	6	2	L_1	(14, 60, 102, 72, 18)

Table 5.1: f-vectors of the Wasserstein balls for the four models in Example 5.11.

Independence models correspond in algebraic geometry to *Segre-Veronese varieties*. They are of considerable current interest in the study of tensor decompositions. We here replace the model, which is a semialgebraic set inside a simplex, by its complex Zariski closure in a projective space. This allows us to compute the algebraic degrees of our optimization problem.

The Segre-Veronese variety $\mathcal{M} = ((m_1)_{d_1}, \dots, (m_k)_{d_k})$ is the embedding of $\mathbb{P}^{m_1-1} \times \cdots \times \mathbb{P}^{m_k-1}$ in the projective space of partially symmetric tensors $\mathbb{P}(\text{Sym}_{d_1} \mathbb{R}^{m_1} \otimes \cdots \otimes \text{Sym}_{d_k} \mathbb{R}^{m_k})$. That projective space

equals \mathbb{P}^{n-1} where $n = \prod_{i=1}^k \binom{m_i+d_i-1}{d_i}$. By definition, the Segre-Veronese variety \mathcal{M} is the set of all tensors of rank one inside this projective space.

Example 5.12 Let $k = 2$. The Segre-Veronese variety $\mathcal{M}((2)_2, (2)_1)$ is an embedding of $\mathbb{P}^1 \times \mathbb{P}^1$ into \mathbb{P}^5 , where it is a quartic surface. Its points are rank one tensors of format $2 \times 2 \times 2$ which are symmetric in the first two indices. This model appears in the last row of Table 5.3.

We identify the projective variety \mathcal{M} with the intersection $\mathcal{M} \cap \Delta_{n-1}$. This is the set of real nonnegative points in \mathcal{M} . Thus, the independence model \mathcal{M} consists of nonnegative rank one tensors whose entries sum to 1. The dimension of \mathcal{M} is denoted $\mathbf{m} := (m_1 - 1) + \dots + (m_k - 1)$. The computation of the polar degrees of \mathcal{M} appears in the doctoral dissertation of Luca Sodomaco [137, Chapter 5]. We here state the result of this computation.

Theorem 5.13 (Sodomaco) *The polar degrees of the Segre-Veronese variety are*

$$\delta_{r-1}(\mathcal{M}) = \sum_{s=0}^{\mathbf{m}-n+1+r} (-1)^s \binom{\mathbf{m}-s+1}{n-r} (\mathbf{m}-s)! \left(\sum_{i_1+\dots+i_k=s} \prod_{l=1}^k \frac{\binom{m_l}{i_l} d_l^{m_l-1-i_l}}{(m_l-1-i_l)!} \right). \quad (5.13)$$

Here r is any integer in the range $n - 1 - \dim(\mathcal{M}) \leq r \leq \dim(\mathcal{M}^*)$.

We next examine this formula for various special cases starting with the binary case.

Corollary 5.14 *Let \mathcal{M} be the k -bit independence model. The formula (5.13) specializes to*

$$\delta_{r-1}(\mathcal{M}) = \sum_{s=0}^{k-2^k+1+r} (-1)^s \binom{k+1-s}{2^k-r} (k-s)! 2^s \binom{k}{s}. \quad (5.14)$$

In algebraic geometry language, our model \mathcal{M} here is the Segre embedding of $(\mathbb{P}^1)^k$ into \mathbb{P}^{2^k-1} . This is the toric variety associated with the k -cube, so its degree is the normalized volume of the cube, which is $k!$. The polar degrees δ_{r-1} in (5.14) are shown for $k \leq 7$ in Table 5.2. The indices r with $\delta_{r-1} \neq 0$ range from $\text{codim}(\mathcal{M}) = 2^k - 1 - k$ to $\dim(\mathcal{M}^*) = 2^k - 1$. For the sake of the table's layout, we shift the indices on each row so that the row labeled 0 contains $\delta_{\text{codim}(\mathcal{M})-1} = \text{degree}(\mathcal{M}) = k!$. The dual variety \mathcal{M}^* is a hypersurface of degree δ_{2^k-2} known as the *hyperdeterminant* of format 2^k . For instance, for $k = 3$, this hypersurface in \mathbb{P}^7 is the $2 \times 2 \times 2$ -hyperdeterminant which has degree four. The entries in the first column ($k = 2$) corresponds to the three scenarios in Figure 5.1, where the algebraic degree equals 2.

$r - \text{codim}(\mathcal{M})$	$k = 2$	$k = 3$	$k = 4$	$k = 5$	$k = 6$	$k = 7$
0	2	6	24	120	720	5040
1	2	12	72	480	3600	30240
2	2	12	96	840	7920	80640
3		4	64	800	9840	124320
4			24	440	7440	120960
5				128	3408	75936
6					880	30016
7						6816

Table 5.2: The polar degrees $\delta_{r-1}(\mathcal{M})$ of the k -bit independence model for $k \leq 7$.

We briefly discuss the independence models (m_1, m_2) for two random variables. These are the classical contingency tables of format $m_1 \times m_2$. Here, $n = m_1 m_2$ and $\mathbf{m} = m_1 + m_2 - 2$. The Segre variety $\mathcal{M} = \mathbb{P}^{m_1-1} \times \mathbb{P}^{m_2-1} \subset \mathbb{P}^{n-1}$ consists of $m_1 \times m_2$ matrices of rank one.

Corollary 5.15 *The Segre variety of $m_1 \times m_2$ matrices of rank one has the polar degrees*

$$\delta_{r-1}(\mathcal{M}) = \sum_{s=0}^{\mathbf{m}-n+1+r} (-1)^s \binom{\mathbf{m}-s+1}{n-r} (\mathbf{m}-s)! \left(\sum_{i+j=s} \frac{\binom{m_1}{i}}{(m_1-1-i)!} \cdot \frac{\binom{m_2}{j}}{(m_2-1-j)!} \right).$$

The polar degrees above serve as upper bounds for any particular Wasserstein distance problem. For a fixed model \mathcal{M} , the equality in Theorem 5.5 holds only when the data (ℓ, L) is generic. However, for the optimization problem in (5.11), the linear space $L = L_F$ and the linear functional $\ell = \ell_F$ are very specific. They depend on the Lipschitz polytope P_d and the type F of the optimal solution v^* . For such specific scenarios, we only get an inequality.

Proposition 5.16 *Consider the problem (5.11) for the independence model $((m_1)_{d_1}, \dots, (m_k)_{d_k})$ with a given face F of the Wasserstein ball $B = P_d^*$. The degree of the optimal solution v^* as an algebraic function of the data μ is bounded above by the polar degree δ_{r-1} in (5.13).*

Proof This follows from Theorem 5.5. The upper bound relies on general principles of algebraic geometry. Namely, the graph of the map $\mu \mapsto v^*(\mu)$ is an irreducible variety, and we seek its degree over μ . The map depends on the parameters (ℓ, L) . When the coordinates of L and ℓ are independent transcendentals then the algebraic degree is the polar degree δ_{r-1} . That algebraic degree can only go down when these coordinates take on special values in the real numbers. That same semi-continuity argument holds for most polynomial optimization problems, including the Euclidean distance optimization in the last lecture. \square

We now examine the drop in algebraic degree for the four models in Example 5.11. In the language of algebraic geometry, they are the Segre threefold $\mathbb{P}^1 \times \mathbb{P}^1 \times \mathbb{P}^1$ in \mathbb{P}^7 , the variety $\mathbb{P}^2 \times \mathbb{P}^2$ of rank one 3×3 matrices in \mathbb{P}^8 , the rational normal curve \mathbb{P}^1 in $\mathbb{P}^6 = \mathbb{P}(\text{Sym}_6(\mathbb{R}^2))$, and the Segre-Veronese surface $\mathbb{P}^1 \times \mathbb{P}^1$ in $\mathbb{P}^5 = \mathbb{P}(\text{Sym}_2(\mathbb{R}^2) \times \text{Sym}_1(\mathbb{R}^2))$. The finite metrics d are specified in the fourth column of Table 5.1. The fifth column in Table 5.1 records the combinatorial complexity of our optimization problem, while the algebraic complexity is recorded in Table 5.3.

\mathcal{M}	Polar degrees	Maximal degree	Average degree
$(2, 2, 2)$	$(0, 0, 0, 6, 12, 12, 4)$	$(0, 0, 0, 4, 12, 6, 0)$	$(0, 0, 0, 2.138, 6.382, 3.8, 0)$
$(3, 3)$	$(0, 0, 0, 6, 12, 12, 6, 3)$	$(0, 0, 0, 2, 8, 6, 6, 0)$	$(0, 0, 0, 1.093, 3.100, 4.471, 6.0, 0)$
(2_6)	$(0, 0, 0, 0, 6, 10)$	$(0, 0, 0, 0, 6, 5)$	$(0, 0, 0, 0, 6, 5)$
$(2_2, 2)$	$(0, 0, 4, 6, 4)$	$(0, 0, 3, 5, 2)$	$(0, 0, 2.293, 3.822, 2.0)$

Table 5.3: The algebraic degrees of the problem (5.8) for the four models in Example 5.11.

The second column in Table 5.3 gives the vector $(\delta_0, \delta_1, \dots, \delta_{n-2})$ of polar degrees. The third and fourth column are the results of a computational experiment. For each model, we take 1000 uniform samples μ with rational coordinates from Δ_{n-1} , and we solve the optimization problem (5.8). The output is an exact representation of the optimal solution v^* . This includes the optimal face F that specifies v^* , along with its maximal ideal over \mathbb{Q} . The algebraic degree of the optimal solution v^* is computed as the number of complex zeros of that maximal ideal. This number is bounded above by the polar degree (cf. Proposition 5.16). The fourth column in Table 5.3 shows the average of the algebraic degrees we found. For example, for the 3-bit model $(2, 2, 2)$ we have $\delta_3 = 6$, corresponding to P_d^* touching \mathcal{M} at a

3-face F . However, the maximum degree we saw in our computations was 4, with an average degree of 2.138. For 4-faces F , we have $\delta_4 = 12$, and this degree was attained in some runs. The average was 6.382.

Such computational experiments are organized naturally into three stages: (1) combinatorial preprocessing, (2) numerical optimization, and (3) algebraic postprocessing. Our object of interest is a model \mathcal{M} in the simplex Δ_{n-1} , typically one of the independence models $((m_1)_{d_1}, \dots, (m_k)_{d_k})$ where $n = \prod_{i=1}^k \binom{m_i+d_i-1}{d_i}$.

The state space $[n]$ is a metric space, with metric given by the matrix $d = (d_{ij})$. This matrix of pairwise distances is part of our input. It defines the Lipschitz polytope P_d and its dual, the Wasserstein ball P_d^* . Our first algorithm computes these combinatorial objects.

Algorithm 1: Combinatorial Preprocessing

- 1 **Input:** An $n \times n$ symmetric matrix $d = (d_{ij})$.
 - 2 **Output:** A description of all facets F of the Wasserstein ball P_d^* .
 - 3 From the inequality presentation in (5.6), find all vertices of the Lipschitz polytope P_d . These vertices are the inner normal vectors ℓ_F to the facets F of P_d^* . Store them.
 - 4 Determine an inequality description of the cone C_F over each facet F .
 - 5 **return** the list of pairs (ℓ_F, C_F) , one for each vertex of the Lipschitz polytope P_d .
-

In the original study [36], the software **Polymake** was used to run Algorithm 1. We next solve the optimization problem in (5.8), by examining each facet F of the Wasserstein ball. The problem is that in (5.11) but with the linear space L_F now replaced by the convex cone C_F that is spanned by F .

Algorithm 2: Numerical Optimization

- 1 **Input:** Model \mathcal{M} and a point μ in the simplex Δ_{n-1} ; complete output from Algorithm 1.
 - 2 **Output:** The optimal solution v^* in (5.8) along with its type G .
 - 3 **for** each facet F of the Wasserstein ball P_d^* **do**
 - 4 Apply global optimization methods to identify a point $v^* \in \mathcal{M}$ that minimizes $\ell_F = \ell_F(v)$ subject to $v \in (\mu + C_F) \cap \mathcal{M}$.
 - 5 Identify the unique face G of F whose span contains v^* in its relative interior.
 - 6 Identify a basis of vectors $e_i - e_j \in C_G$ for the linear space L_G spanned by G .
 - 7 Store the optimal solution v^* and a basis for the linear subspace L_G of \mathbb{R}^n .
 - 8 **end**
 - 9 Among all candidate solutions, identify the solution v^* for which the Wasserstein distance $W_d(\mu, v^*)$ to the given data point μ is smallest. Record its type G .
 - 10 **return** The optimal solution v^* , its associated linear space L_G , and the facet normal ℓ_G .
-

In [36], the software **SCIP** was used to run Algorithm 2. **SCIP** employs sophisticated branch-and-cut strategies to solve constrained polynomial optimization problems via LP relaxation. Algorithm 1 is guaranteed to find the global optimum for our problem (5.8). Moreover, it furnishes an identification of the combinatorial type. This serves as the input to the symbolic computation in Algorithm 3 below.

Algorithm 3 can be carried out with a computer algebra system like **Macaulay2**. Steps 2 and 4 are the result of standard Gröbner basis calculations. The pipeline is illustrated with examples in [36, Section 6].

Algorithm 3: Algebraic Postprocessing

1 **Input:** The optimal solution (ν^*, G) to (5.8) in the form found by Algorithm 2.
 2 **Output:** The maximal ideal in the polynomial ring $\mathbb{Q}[\nu_1, \dots, \nu_n]$ which has the zero ν^* .
 3 Use Lagrange multipliers to give polynomial equations that characterize the critical points of the linear function ℓ_F on the subvariety $(\mu + L_G) \cap \mathcal{M}$ in the affine space \mathbb{R}^n .
 4 Eliminate all variables representing Lagrange multipliers from the ideal in the previous step. This ideal lives in $\mathbb{Q}[\nu_1, \dots, \nu_n]$.
 5 **if** the ideal in step 4 is maximal **then**
 6 | Call the ideal M .
 7 **else**
 8 | Remove extraneous primary components to get the maximal ideal M of ν^* .
 9 **end**
 10 Determine the degree of ν^* , which is the dimension of $\mathbb{Q}[\nu_1, \dots, \nu_n]/M$ over \mathbb{Q} .
 11 **return** the generators for the maximal ideal M along with the degree found in Step 11.

Chapter 6

Curvature

6.1 Plane Curves

In this section, we consider a smooth algebraic curve $C \subset \mathbb{R}^2$ given as the zero set of an irreducible polynomial of degree $d \geq 1$:

$$f(x_1, x_2) \in \mathbb{R}[x_1, x_2]$$

Let $\mathbf{x} = (x_1, x_2)$. Geometrically, the *curvature* of C at a point $\mathbf{x} \in C$ is the rate of change at \mathbf{x} of a unit normal vector traveling along C . To be precise, define

$$N(\mathbf{x}) := \frac{1}{\|\nabla f(\mathbf{x})\|} \nabla f(\mathbf{x}),$$

where $\nabla f(\mathbf{x}) = (\partial f / \partial x_1, \partial f / \partial x_2)$ is the gradient of f . Then, for all $\mathbf{x} \in C$, $N(\mathbf{x})$ returns a normal vector of C at \mathbf{x} ; one calls $N(\mathbf{x})$ a *unit normal field*. Similarly, a *unit tangent field* is given by

$$T(\mathbf{x}) := (N(\mathbf{x})_2, -N(\mathbf{x})_1).$$

The curvature of C at \mathbf{x} is defined as the (signed) magnitude of the derivative of $N(\mathbf{x})$ in tangent direction:

$$c(\mathbf{x}) := \left\langle T(\mathbf{x}), T(\mathbf{x})_1 \cdot \frac{\partial N}{\partial x_1} + T(\mathbf{x})_2 \cdot \frac{\partial N}{\partial x_2} \right\rangle.$$

Example 6.1 Consider the ellipse $f(\mathbf{x}) = x_1^2 + \frac{1}{4}x_2^2 - 1$. The left picture in Figure 6.1 shows the ellipse in green and the normal field $N(\mathbf{x})$ in yellow. The right picture displays the curvature via $c(\mathbf{x}) \cdot T(\mathbf{x})$. The magnitude of a yellow vector attached to a point \mathbf{x} in the right picture gives the curvature at \mathbf{x} . On the top and bottom, where the ellipse is rather flat, the normal vectors don't change much, hence the curvature is small. On the sides, normal vectors change more rapidly, so that the curvature is larger \diamond

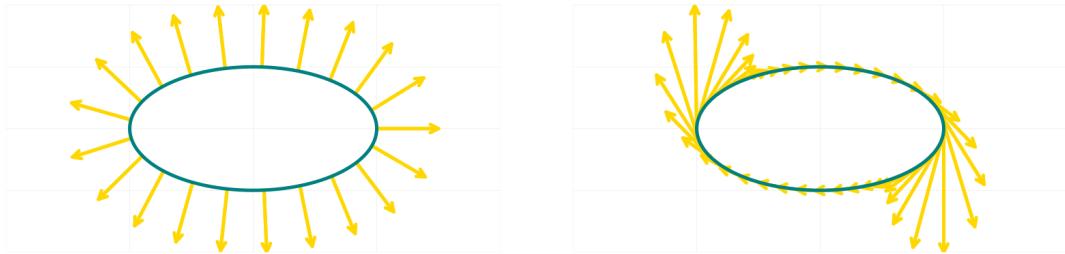


Fig. 6.1: The left picture shows a unit normal field of the ellipse $x_1^2 + \frac{1}{4}x_2^2 - 1 = 0$, and the right picture shows how the normal field changes when travelling along the ellipse.

The inverse of the curvature $R(\mathbf{x}) := c(\mathbf{x})^{-1}$ is called the *radius curvature*. This is because C contains an infinitesimally small arc of a circle with radius $R(\mathbf{x})$ and center $\mathbf{x} - R(\mathbf{x}) \cdot N(\mathbf{x})$. This center is also called a *focal point* of C . The Zariski closure of the set of all focal points is called the *evolute* of C . We will come back to the evolute later in the next chapter. We refer the reader to the book by Salmon [133] or the recent article [121] for a detailed discussion on the algebraic geometry of evolutes of plane curves.

In the remainder of this section we will study two types of points: *inflection points* and *points of critical curvature*. These points exhibit special curvature of C . Inflection points are points where C is locally flat, and critical curvature points are points where the curvature has a local extremum.

Definition 6.2 Let $\mathbf{x} \in C$.

1. We call \mathbf{x} an inflection point, if $c(\mathbf{x}) = 0$.
2. We call \mathbf{x} a critical curvature point, if \mathbf{x} is a critical point of the function $C \rightarrow \mathbb{R}$, $x \mapsto c(x)$.

Example 6.3 We consider the Trott curve $f(\mathbf{x}) = 144(x^4 + y^4) - 225(x^2 + y^2) + 350x^2y^2 + 81$ as we did in Figure 2.1. The Trott curve has degree $d = 4$. Figure 6.2 shows the curve in green. We first compute inflection points using HomotopyContinuation.jl [23] and the formulation in Lemma 6.5.

```
using HomotopyContinuation, LinearAlgebra
@var x y z
v = [x; y; z]
F = 144*(x^4 + y^4) - 225*(x^2 + y^2) + 350*x^2*y^2 + 81*z^4
dF = differentiate(F, v)
H0 = differentiate(dF, v)

f = subs(F, z=>1)
h = subs(-det(H0), z=>1)
inflection_points = solve([f; h])
```

By Theorem 6.6 there are $3d(d - 2) = 24$ complex inflection points. Klein [92] proved that at most $d(d - 2) = 8$ can be real and in this case we find 8 real inflection points. They are the yellow points in Figure 6.2.

Next, we compute critical curvature points using the equations in Lemma 6.7.

```
f1, f2 = dF[1:2]
f11, f12, f21, f22 = H0[1:2,1:2]
hx, hy = differentiate(h,[x; y])

S = f1 * f2 * (f11-f22) + f12 * (f2^2 - f1^2)
c = subs(f2 * hy - f1 * hx - 3 * h * S, z=>1)
crit_curv = solve([f; c])
```

By Theorem 6.8 there are $2d(3d - 5) = 56$ complex critical curvature points. We find that 28 of them are real; out of these 8 are close (but not equal to) to the 8 inflection points, which is why they are not visible in the picture. They are shown as red points in Figure 6.2.

◇

By definition, an inflection point is thus a point where the radius of curvature becomes infinite. Consequently, inflection points correspond to points at infinity on the evolute. Critical curvature points, on the other hand, correspond to cusps on the evolute that are not at infinity. To see this, consider a local parametrization $\gamma(t)$ of C with $\gamma(0) = \mathbf{x}$ and $\dot{\gamma}(0) = T(\mathbf{x})$. Then, $\Gamma(t) = \gamma(t) - R(\gamma(t)) \cdot N(\gamma(t))$ gives a local parametrization of the evolute. We have $\dot{\Gamma}(0) = \langle \dot{R}(\mathbf{x}), \dot{\gamma}(0) \rangle \cdot N(\mathbf{x})$. This shows that the evolute has a cusp ($\dot{\Gamma}(0) = 0$) if and only if $\langle \dot{R}(\mathbf{x}), \dot{\gamma}(0) \rangle = 0$, which is the equation for when $c(\mathbf{x})$ is critical at \mathbf{x} .

We want to count the number of complex inflection and critical curvature points for a curve given by a general polynomial f . For this, let us first understand the curvature $c(\mathbf{x})$ better. In the following, we denote partial derivatives by $f_i := \frac{\partial f}{\partial x_i}$, $f_{i,j} := \frac{\partial^2 f}{\partial x_i \partial x_j}$ and the *Hessian* $H := \begin{bmatrix} f_{1,1} & f_{1,2} \\ f_{1,2} & f_{2,1} \end{bmatrix}$.

Lemma 6.4 $c(\mathbf{x}) = \frac{1}{\|\nabla f(\mathbf{x})\|} \cdot T(\mathbf{x})^T H T(\mathbf{x})$

Proof Recall that $c(\mathbf{x}) = \langle T(\mathbf{x}), T(\mathbf{x})_1 \cdot \frac{\partial N}{\partial x_1} + T(\mathbf{x})_2 \cdot \frac{\partial N}{\partial x_2} \rangle$. By the product rule we have

$$T(\mathbf{x})_1 \cdot \frac{\partial N}{\partial x_1} + T(\mathbf{x})_2 \cdot \frac{\partial N}{\partial x_2} = \|\nabla f(\mathbf{x})\|^{-1} \cdot H T(\mathbf{x}) + a(\mathbf{x}) \cdot \nabla f(\mathbf{x})$$

for some scalar function $a(\mathbf{x})$. Since $\langle T(\mathbf{x}), \nabla f(\mathbf{x}) \rangle = 0$, this gives the asserted formula. □

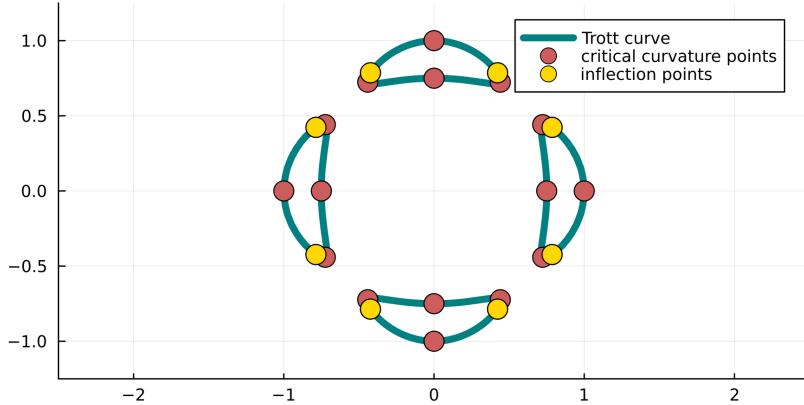


Fig. 6.2: The Trott curve $144(x^4 + y^4) - 225(x^2 + y^2) + 350x^2y^2 + 81 = 0$ in green together with its inflection points (yellow points) and critical curvature points (red points).

We can write the formula from Lemma 6.4 more explicitly as

$$c(\mathbf{x}) = \frac{f_{1,1} \cdot f_2^2 - 2f_{1,2} \cdot f_1 \cdot f_2 + f_{2,2} \cdot f_1^2}{(f_1^2 + f_2^2)^{\frac{3}{2}}}. \quad (6.1)$$

For what follows it will be helpful to embed C into complex projective space. We write

$$F(x_0, x_1, x_2) := x_0^d f\left(\frac{x_1}{x_0}, \frac{x_2}{x_0}\right)$$

for the homogenization of f . Moreover, let

$$H_0 = \begin{pmatrix} F_{0,0} & F_{0,1} & F_{0,2} \\ F_{0,1} & F_{1,1} & F_{1,2} \\ F_{0,2} & F_{1,2} & F_{2,2} \end{pmatrix}.$$

denote the Hessian of F viewed as a polynomial in \mathbf{x} by setting $x_0 = 1$. We can rewrite the curvature of C in terms of F . The next lemma goes back to Salmon [133].

Lemma 6.5 *The curvature can be expressed as*

$$c(\mathbf{x}) = \frac{-\det H_0}{(d-1)^2 \cdot (f_1^2 + f_2^2)^{\frac{3}{2}}}.$$

Proof Homogenizing polynomials in (6.1) we get $c(\mathbf{x}) = \frac{P}{Q}$, where $P = F_{1,1} \cdot F_2^2 - 2F_{1,2} \cdot F_1 \cdot F_2 + F_{2,2} \cdot F_1^2$ and $Q = (F_1^2 + F_2^2)^{\frac{3}{2}}$. By Euler's formula for homogeneous functions we have

$$(d-1) \cdot F_j = x_0 F_{0,j} + x_1 F_{1,j} + x_2 F_{2,j}, \quad 0 \leq j \leq 2.$$

Substituting the F_j in P gives

$$(d-1)^2 \cdot P = (F_{1,1}F_{2,2} - F_{1,2}^2) \cdot (x_1^2F_{1,1} + x_2^2F_{2,2} + 2(x_0x_1F_{0,1} + x_0x_2F_{0,2} + x_1x_2F_{1,2})) \\ + x_0^2(F_{0,1}^2F_{2,2} - 2F_{1,2}F_{0,1}F_{0,2} + F_{1,1}F_{0,2}^2).$$

Furthermore, we have $0 = x_0F_0 + x_1F_1 + x_2F_2$ on C . Therefore,

$$0 = x_0^2F_{0,0} + x_1^2F_{1,1} + x_2^2F_{2,2} + 2(x_0x_1F_{0,1} + x_0x_2F_{0,2} + x_1x_2F_{1,2}).$$

We obtain

$$P = \frac{x_0^2}{(d-1)^2} \cdot (-(F_{1,1}F_{2,2} - F_{1,2}^2)F_{0,0} + F_{0,1}^2F_{2,2} - 2F_{1,2}F_{0,1}F_{0,2} + F_{1,1}F_{0,2}^2) = \frac{-x_0^2 \cdot \det H_0}{(d-1)^2}.$$

Setting $x_0 = 1$ finishes the proof. \square

We can now prove a theorem on inflection points.

Theorem 6.6 *The number of complex inflection points of a curve C defined by a general polynomial f of degree d is $3d(d-2)$.*

This theorem was first proved by Klein [92]. He also proved that the number of real inflection points is at most one third; i.e., $d(d-2)$. Here, we give a short proof for the complex count.

Proof By Lemma 6.5, inflection points on C are given as the zero set of the $f = \det H_0 = 0$, which is a system of two equations in two variables $\mathbf{x} = (x_1, x_2)$. The degree of f is d and the degree of $\det H_0$ is $3(d-2)$. Bézout's theorem implies that the number of inflection points is at most $3d(d-2)$. To show that the number is also at least $3d(d-2)$, we show that there exist polynomials with this number of inflection points.

Consider a univariate polynomial $g(x_1) \in \mathbb{R}[x_1]$ of degree d and let $G(x_0, x_1)$ be its homogenization. Let also $M := \begin{bmatrix} G_{0,1} & G_{0,1} \\ G_{0,1} & G_{1,1} \end{bmatrix}$ the Hessian of G with respect to the variables x_0, x_1 . We assume (1) that g has d regular zeros (2) $\det M = 0$ has only regular zeros, and (3) that $g = \det M = 0$ has no solutions. All three are Zariski open conditions, so almost all polynomials g satisfy this assumption. Define

$$f(x_1, x_2) = x_2^d - g(x_1)$$

Observe that in this case $\det H_0 = x_2^{d-2} \cdot \det M$. Consequently, $\det H_0 = 0$ if and only if either $x_2 = 0$, or x_1 is among the $2(d-2)$ zeros of $\det M$. This means that \mathbf{x} is an inflection point, if either $\mathbf{x} = (x_1, 0)$ and x_1 is a zero of g , or $\mathbf{x} = (x_1, x_2)$ where x_1 is a zero of $\det M$ and $x_2^d = g(x_1)$. In the first case, we find d inflection points and each has multiplicity $d-2$. In the second case we find, since $g(x_1) \neq 0$, we find $2d(d-2)$ many regular inflection points with multiplicity one. Now, if we perturb f slightly, the d points with multiplicity will split into $d(d-2)$ inflection points, while the other $2d(d-2)$ inflection points will remain distinct. In total, this gives $3d(d-2)$ inflection points. \square

Let us now find polynomial equations for critical curvature.

Lemma 6.7 *Critical curvature points are defined by the equations $f(\mathbf{x}) = 0$ and*

$$(f_1^2 + f_2^2) \cdot \left(f_2 \cdot \frac{\partial \det H_0}{\partial x_1} - f_1 \cdot \frac{\partial \det H_0}{\partial x_2} \right) - 3 \det H_0 \cdot S = 0,$$

where $S = f_1f_2 \cdot (f_{1,1} - f_{2,2}) + f_{1,2}(f_2^2 - f_1^2)$.

Proof Critical curvature points on C are defined by the equations $f = 0$ and $f_2 \cdot \frac{\partial c(\mathbf{x})}{\partial x_1} - f_1 \cdot \frac{\partial c(\mathbf{x})}{\partial x_2} = 0$. By Lemma 6.5 and the product rule we have

$$\frac{\partial c(\mathbf{x})}{\partial x_i} = \frac{\partial \det H_0}{\partial x_i} \cdot (f_1^2 + f_2^2) - 3 \det H_0 \cdot (f_1 \cdot f_{1,i} + f_2 \cdot f_{2,i}).$$

This yields the stated polynomial equation. \square

Recall that critical curvature points correspond to finite cusps of the evolute. Piene, Riener and Shapiro prove in [121, Proposition 3.3] that, counting in projective space, the number of cusps on the evolute for a general plane curve C of degree d is $6d^2 - 9d$. Salmon [133] shows that d of these cusps lie at infinity. This yields the following theorem.

Theorem 6.8 *The number of complex critical curvature points of a curve C defined by a general polynomial f of degree d is $2d(3d - 5)$.*

6.2 Surfaces

The curvature of a smooth algebraic surface $S \subset \mathbb{R}^3$ can be studied via the curves on it. At any point $\mathbf{x} \in S$ of the surface, we write $N(\mathbf{x})$ for its normal vector. Now, for any tangent vector T of S at \mathbf{x} , the plane spanned by the normal vector $N(\mathbf{x})$ and the tangent vector T intersects the surface S in a plane curve $C_T(\mathbf{x})$. Ranging over all tangent vectors T at x , we obtain a one-dimensional family of plane curves whose union is the whole surface S . The *principal curvatures* of S at \mathbf{x} are the minimum and maximum of the curvatures of the curves $C_T(\mathbf{x})$ in that family at the point \mathbf{x} .

When the two principal curvatures at \mathbf{x} are equal, the point \mathbf{x} is an *umbilic* of the surface S . Equivalently, at an umbilic \mathbf{x} , all curves $C_T(\mathbf{x})$ have the same curvature. Thus, the best second-order approximation of S at an umbilic is a sphere.

Theorem 6.9 ([134]) *A general surface in \mathbb{R}^3 of degree d has $2d(5d^2 - 14d + 11)$ umbilics.*

6.3 Volumes of Tubular Neighborhoods

Chapter 7

Medial Axis and Reach

The *medial axis* $\text{Med}(X)$ of a subset $X \subset \mathbb{R}^n$ is the set of points $\mathbf{u} \in \mathbb{R}^n$ such that there exist at least two points on X minimizing the distance to \mathbf{u} . The distance from X to $\text{Med}(X)$ is called the *reach* of X and we denote it by $\tau(X)$. In the following, we study the medial axis and related notions in the case when $X \subset \mathbb{R}^n$ is a real variety. In that case, the reach and medial axis are algebraic notions. More concretely, the medial axis is semialgebraic and we can study its complex Zariski closure

$$M_X := \overline{\text{Med}(X)},$$

called the *algebraic medial axis* of X . Moreover, if X is smooth and defined by rational polynomials, then its reach $\tau(X)$ is an algebraic number over \mathbb{Q} [78, Proposition 3.14].

Example 7.1 Consider the parabola $X = V(x_2 - x_1^2 = 0)$. We compute the algebraic medial axis of X . If $\mathbf{x} = (x_1, x_2) \in X$ minimizes the distance to a point $\mathbf{u} = (u_1, u_2) \in \mathbb{R}^2$, we must have $\langle \mathbf{x} - \mathbf{u}, \mathbf{t} \rangle = 0$, where \mathbf{t} spans the tangent space $T_{\mathbf{x}}X$. We use Macaulay2 [67]:

```
R = QQ[x1, x2, y1, y2, u1, u2];
fx = x2 - x1^2; fy = y2 - y1^2;
Jx = matrix {{x1-u1, x2-u2}, {diff(x1, fx), diff(x2, fx)}};
Jy = matrix {{y1-u1, y2-u2}, {diff(y1, fy), diff(y2, fy)}};
distxu = (x1 - u1)^2 + (x2 - u2)^2;
distyu = (y1 - u1)^2 + (y2 - u2)^2;
I = ideal {fx, fy, det(Jx), det(Jy), distxu - distyu};
K = saturate(I, ideal {x1-y1, x2-y2});
eliminate(K, {x1, x2, y1, y2})
```

This returns the ideal $\langle u_1 \rangle$. Indeed, the medial axis is $\text{Med}(X) = \{(0, u_2) \mid u_2 \geq \frac{1}{2}\}$, so that the algebraic medial axis is $M_X = \{u_1 = 0\}$ (see also Figure 7.4 below). The reach is $\tau(X) = \frac{1}{2}$. \diamond

7.1 Bottlenecks

We can characterize the reach of a smooth variety $X \subset \mathbb{R}^n$ in terms of maximal curvature and bottlenecks. Let $\mathbf{x}, \mathbf{y} \in X$ be two distinct points. If $\mathbf{x} - \mathbf{y}$ is normal to $T_{\mathbf{x}}X$ (i.e., for all $\mathbf{t} \in T_{\mathbf{x}}X$ we have $\langle \mathbf{x} + \mathbf{t}, \mathbf{x} - \mathbf{y} \rangle = 0$) and also normal to $T_{\mathbf{y}}X$, then we call (\mathbf{x}, \mathbf{y}) a *bottleneck*. Complex solutions to the corresponding system of polynomial equations are called complex bottleneck. di Rocco, Eklund and Weinstein [48] gave an algorithm for computing the number of complex bottlenecks of a variety in terms of polar classes. The following theorem is their result for planar curves.

Theorem 7.2 *If X is a general curve in the plane of degree d , it has $\frac{1}{2}(d^4 - 5d^2 + 4d)$ complex bottlenecks.*

Example 7.3 We compute bottlenecks of the Trott curve $144(x^4 + y^4) - 225(x^2 + y^2) + 350x^2y^2 + 81 = 0$ using HomotopyContinuation.jl [23].

```
@var x y u v
f = 144*(x^4 + y^4) - 225*(x^2 + y^2) + 350*x^2*y^2 + 81
g = subs(f, x=>u, y=>v)
df = differentiate(f, [x; y])
dg = differentiate(g, [u; v])
N = [x-u; y-v]
bottlenecks = solve([f; g; det([N df]); det([N dg])])
```

By Theorem 7.2 there are $\frac{1}{2}(d^4 - 5d^2 + 4d) = 96$ complex bottlenecks. We compute that 36 of them are real. They are shown in Figure 7.1. \diamond

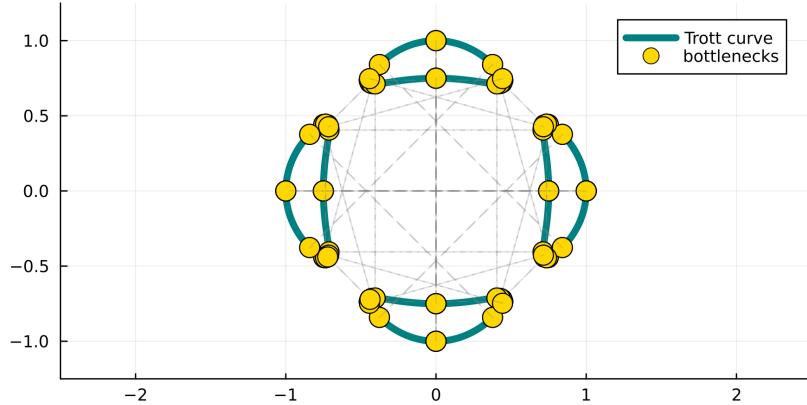


Fig. 7.1: Bottlenecks of the Trott curve $144(x^4 + y^4) - 225(x^2 + y^2) + 350x^2y^2 + 81 = 0$ are displayed as grey normal lines with yellow endpoints.

The *width* of a bottleneck is $b(\mathbf{x}, \mathbf{y}) := \frac{1}{2}\|\mathbf{x} - \mathbf{y}\|$ and we denote the width of the smallest bottleneck of X by

$$B(X) := \min_{(\mathbf{x}, \mathbf{y}) \text{ bottleneck of } X} b(\mathbf{x}, \mathbf{y}).$$

Next, let $\gamma(t)$ be a smooth curve in X such that $\gamma(0) = \mathbf{x}$ and $\|\dot{\gamma}(t)\| = 1$. Then, $\dot{\gamma}(t)$ is a tangent field along $\gamma(t)$. Let also N be a unit normal field of X . Denote $\mathbf{t} := \dot{\gamma}(0) \in T_{\mathbf{x}}X$ and $\mathbf{v} := N(\mathbf{x}) \in N_{\mathbf{x}}X$. The curvature of X at \mathbf{x} in tangent direction \mathbf{t} and normal direction \mathbf{v} is defined to be

$$c(\mathbf{x}, \mathbf{t}, \mathbf{v}) := \left\langle \mathbf{t}, t_1 \cdot \frac{\partial N}{\partial x_1} + \cdots + t_n \cdot \frac{\partial N}{\partial x_n} \right\rangle.$$

The maximal curvature of X is

$$C(X) := \max_{\mathbf{x} \in X, \mathbf{t} \in T_{\mathbf{x}}X, \mathbf{v} \in N_{\mathbf{x}}X} c(\mathbf{x}, \mathbf{t}, \mathbf{v}).$$

Theorem 7.4 If X is smooth,

$$\tau(X) = \min \left\{ B(X), \frac{1}{C(X)} \right\}.$$

Proof For $\mathbf{x} \in X$ denote by $N_{\mathbf{x}}X := \{\mathbf{v} \in \mathbb{R}^n \mid \langle \mathbf{v}, \mathbf{t} \rangle = 0 \text{ for all } \mathbf{t} \in T_{\mathbf{x}}X\}$ the normal space of X at \mathbf{x} and $NX := \{(\mathbf{x}, \mathbf{v}) \in X \times \mathbb{R}^n \mid \mathbf{v} \in N_{\mathbf{x}}X\}$ the normal bundle of X . Furthermore, for $\varepsilon > 0$ let the normal bundle restricted to normal vectors of length at most ε be $N_{\varepsilon}X := \{(\mathbf{x}, \mathbf{v}) \in NX \mid \|\mathbf{v}\| \leq \varepsilon\}$. Let also $\varphi_{\varepsilon} : N_{\varepsilon}X \rightarrow \mathbb{R}^n$, $(\mathbf{x}, \mathbf{v}) \mapsto \mathbf{x} + \mathbf{v}$

Suppose that $\mathbf{u} \notin \text{Med}(X)$. Then, in a Euclidean neighborhood U of \mathbf{u} points have a unique closest point on X . This defines a smooth map $U \rightarrow X, \mathbf{u} \mapsto \mathbf{x}(\mathbf{u})$. The map $U \rightarrow NX, \mathbf{u} \mapsto (\mathbf{x}(\mathbf{u}), \mathbf{x}(\mathbf{u}) - \mathbf{u})$ is then smooth with smooth inverse; i.e., a diffeomorphism onto its image. This implies that the reach can be expressed as $\tau(X) = \sup\{\varepsilon \geq 0 \mid \varphi_{\varepsilon} \text{ is a diffeomorphism}\}$. Recall that φ_{ε} is a diffeomorphism, if and

only if it is (1) injective and (2) an immersion. Let $\varepsilon = \tau(X)$. If φ_ε is not an immersion, then $\varepsilon = C(X)^{-1}$. If φ_ε is an immersion, but not injective, then $\varepsilon = B(X)$. \square

7.2 Offset Hypersurfaces

This section is based on the article [78]. We write $X_{\mathbb{C}}$ for the complex Zariski closure of X . We assume that X (and hence also $X_{\mathbb{C}}$) is irreducible.

The *ED correspondence* \mathcal{E}_X of X is the Zariski closure of the set of tuples (\mathbf{x}, \mathbf{u}) with $\mathbf{x} \in X^{\text{sm}}$ such that \mathbf{x} is an ED-critical point for \mathbf{u} . We recall from Theorem 2.16 that $\mathcal{E}_X = \overline{\{(\mathbf{x}, \mathbf{x} + \mathbf{h}) \mid \mathbf{x} \in X^{\text{sm}}, (\mathbf{x}, \mathbf{h}) \in N_X\}} \subseteq X_{\mathbb{C}} \times \mathbb{C}^n$. The branch locus of the projection $\mathcal{E}_X \rightarrow \mathbb{C}^n$ is called the *ED discriminant* or evolute. For planar curves, it coincides with the definition of the evolute above in Section 1.3. We denote it by $\Sigma_X \subset \mathbb{C}^n$.

For $\varepsilon \in \mathbb{C}$ and $\mathbf{u} \in \mathbb{C}^n$, the ε -sphere around \mathbf{u} is the variety $S(\mathbf{u}, \varepsilon) := V(\|\mathbf{x} - \mathbf{u}\|^2 - \varepsilon^2)$.

Definition 7.5 The *offset correspondence* of X is

$$\text{OC}_X = (\mathcal{E}_X \times \mathbb{C}) \cap \{(\mathbf{x}, \mathbf{u}, \varepsilon) \in \mathbb{C}^n \times \mathbb{C}^n \times \mathbb{C} \mid \mathbf{x} \in S(\mathbf{u}, \varepsilon)\}.$$

That is, OC_X is the complex Zariski closure of the set of tuples $(\mathbf{x}, \mathbf{u}, \varepsilon)$ such that \mathbf{x} is an ED critical point for \mathbf{u} and ε^2 is the squared Euclidean distance (over \mathbb{R}) between \mathbf{x} and \mathbf{u} .

We consider the two coordinate projections $\pi_1 : \text{OC}_X \rightarrow X_{\mathbb{C}}$ and $\pi_2 : \text{OC}_X \rightarrow \mathbb{C}^n \times \mathbb{C}$. Clearly, π_1 is dominant, i.e., $\pi_1(\text{OC}_X) = X_{\mathbb{C}}$. However, the other projection is not:

Definition 7.6 We denote $\text{Off}_X := \overline{\text{OC}_X} \subset \mathbb{C}^n \times \mathbb{C}$ and call it the *offset hypersurface* of X .

The next lemma justifies the name.

Lemma 7.7 $\text{codim } \text{Off}_X = 1$.

Proof The ED correspondence \mathcal{E}_X is the Zariski closure of a vector bundle of rank $\text{codim}(X)$ over X^{sm} , which shows that $\dim \mathcal{E}_X = n$. Since X is irreducible, \mathcal{E}_X is irreducible. The offset correspondence OC_X is the intersection of $\mathcal{E}_X \times \mathbb{C}$, which is also irreducible, with a hypersurface. This implies $\dim \text{OC}_X = n$. Because the Euclidean Distance Degree of X is finite, the projection π_2 has finite fibers generically, which implies $\dim \text{Off}_X = n$. \square

It follows from Lemma 7.7 that Off_X is the zero set of a polynomial that we denote by $g_X(\mathbf{u}, \varepsilon)$; i.e.,

$$\text{Off}_X = V(g_X) \subset \mathbb{C}^n \times \mathbb{C}.$$

We call it the *offset polynomial*. This polynomial is also known as the *ED polynomial*. It is studied in detail in [116].

Example 7.8 Consider the parabola $X = V(x_2 - x_1^2 = 0)$. We compute the offset polynomial of the parabola in Macaulay2 [67].

```
R = QQ[x1, x2, u1, u2, eps];
f = x2 - x1^2; d = (x1-u1)^2 + (x2-u2)^2 - eps^2;
J = matrix {{x1-u1, x2-u2}, {diff(x1, f), diff(x2, f)}};
OC = ideal {f, det(J), d};
O = eliminate(OC, {x1, x2});
g = (gens O)_0_0
```

This gives $g(\mathbf{u}, \varepsilon) = g_0(\mathbf{u}) + g_1(\mathbf{u})\varepsilon^2 + g_2(\mathbf{u})\varepsilon^4 + g_3(\mathbf{u})\varepsilon^6$, where

$$\begin{aligned} g_0(\mathbf{u}) &= (u_1^2 - u_2)^2(16u_1^2 + 16u_2^2 - 8u_2 + 1), & g_2(\mathbf{u}) &= 48u_1^2 + 16u_2^2 + 32u_2 - 8, \\ g_1(\mathbf{u}) &= -48u_1^4 - 32u_1^2u_2^2 + 8u_1^2u_2 - 32u_2^3 - 20u_1^2 - 8u_2^2 + 8u_2 - 1, & g_3(\mathbf{u}) &= -16. \end{aligned}$$

Figure 7.2 shows the offset surface $g(\mathbf{u}, \varepsilon) = 0$ and Figure 7.3 shows the offset surface intersected with the level sets $\varepsilon = 0.5$ and $\varepsilon = 1.25$, respectively. \diamond

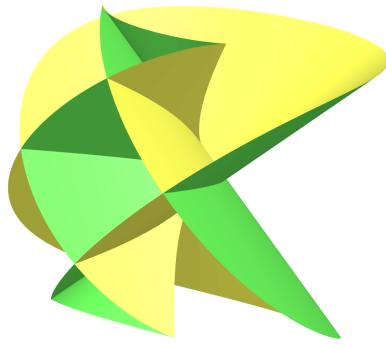


Fig. 7.2: The offset surface Off_X of the parabola. The surface is symmetric along the ε -axis, because only even powers of ε appear in the offset polynomial $g(\mathbf{u}, \varepsilon)$. The parabola itself is visible at level $\varepsilon = 0$. The image was created using [Surfer](#).

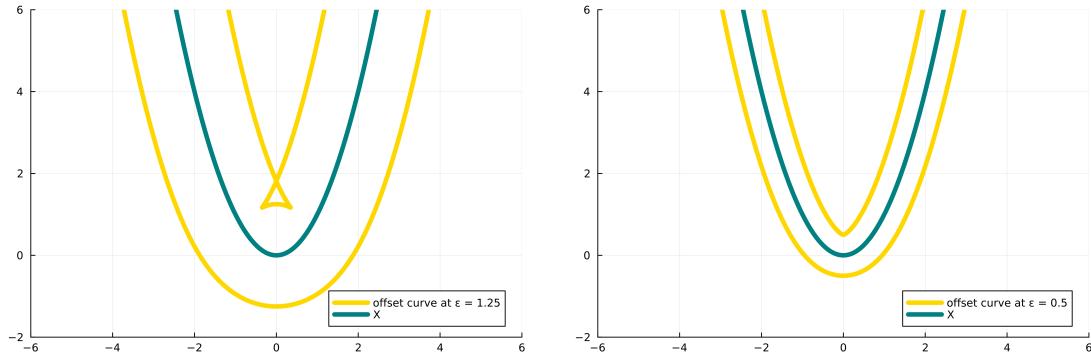


Fig. 7.3: The offset surface Off_X of the parabola intersected with the hypersurface $\varepsilon = 1.25$ and $\varepsilon = 0.5$.

Let us study some properties of the offset polynomial.

Proposition 7.9 1. For a general $\mathbf{u} \in \mathbb{C}^n$, the zeros of $g_X(\mathbf{u}, \varepsilon)$ are precisely $\varepsilon = \pm\sqrt{\|\mathbf{u} - \mathbf{x}\|^2}$, where \mathbf{x} ranges over all ED critical points for \mathbf{u} .

2. The degree of the offset polynomial $g_X(\mathbf{u}, \varepsilon)$ in ε is two times the Euclidean distance degree of X .

Proof First, we observe that the projection $\text{Off}_X \rightarrow \mathbb{C}^n$, $(\mathbf{u}, \varepsilon) \mapsto \mathbf{u}$ is dominant, because general points in \mathbb{C}^n have ED-critical points on $X_{\mathbb{C}}$. Take a general $\mathbf{u} \in \mathbb{C}^n$. Then, $g_X(\mathbf{u}, \varepsilon) = 0$ if and only if there exists $\mathbf{x} \in X_{\mathbb{C}}$ with $(\mathbf{x}, \mathbf{u}) \in \mathcal{E}_X$ and $\varepsilon^2 = \|\mathbf{x} - \mathbf{u}\|^2$. Therefore, $\varepsilon = \pm\sqrt{\|\mathbf{u} - \mathbf{x}\|^2}$, where \mathbf{x} ranges over all ED critical points for \mathbf{u} . In particular, this shows that $g_X(\mathbf{u}, \varepsilon)$ has $2 \cdot \text{EDdeg}(X)$ many zeros for general \mathbf{u} . \square

Example 7.10 In Example 7.8, we see that $g_X(\mathbf{u}, \varepsilon)$ has degree six in ε . This corresponds to the fact that the Euclidean distance degree of the parabola is three. For instance, any point $\mathbf{u} \in \mathbb{R}^2$ in Figure 7.4 that is both above the green curve (the parabola) and the yellow curve (the evolute) has three real ED critical points on the parabola. \diamond

The coefficients of the offset polynomial are studied in [116]. In particular, in that article one can find the following result.

Theorem 7.11 If the variety X is general enough and $g_X(\mathbf{u}, \varepsilon) = c_0(\mathbf{u}) + c_1(\mathbf{u})\varepsilon + \cdots + c_k(\mathbf{u})\varepsilon^k$ is its offset polynomial, then $c_k(\mathbf{u})$ is constant.

Proof See [116, Proposition 4.4]. \square

We now understand that the offset polynomial $g_X(\mathbf{u}, \varepsilon)$ encodes for a fixed $\mathbf{u} \in \mathbb{C}^n$ the distances from \mathbf{u} to its ED-critical points on X . Therefore, if \mathbf{u} is on the medial axis, $g_X(\mathbf{u}, \varepsilon)$ must have a double root in ε . This motivates us to study the discriminant of the offset polynomial in ε .

Definition 7.12 The offset discriminant is the polynomial

$$\delta_X(\mathbf{u}) := \text{Disc}_{\varepsilon} g_X(\mathbf{u}, \varepsilon).$$

Its zero set is denoted $\Delta_X^{\text{Off}} := V(\delta_X) \subset \mathbb{C}^n$.

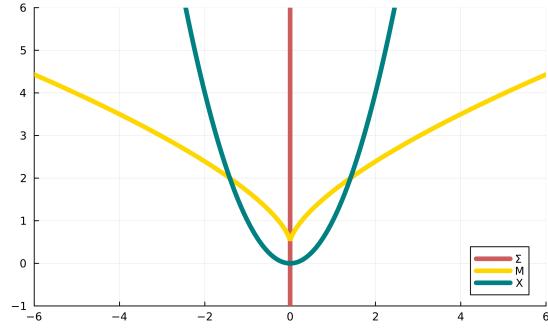


Fig. 7.4: The offset discriminant of the parabola $X = V(x_2 - x_1^2)$ has three real components: the parabola itself (green), the algebraic medial axis M_X (the red vertical line) and the ED-discriminant or evolute Σ_X (the yellow cubic curve).

Example 7.13 Using Macaulay2 [67] we compute the discriminant of the offset polynomial of the parabola from Example 7.8. We get

$$\delta_X(\mathbf{u}) = u_1^4 \cdot (u_1^2 - u_2) \cdot \delta_1(\mathbf{u})^6 \cdot \delta_2(\mathbf{u}),$$

where

$$\delta_1(\mathbf{u}) = -27u_1^2 + 2(2u_2 - 1)^3 \quad \text{and} \quad \delta_2(\mathbf{u}) = 16u_1^2 + (4u_2 - 1)^2.$$

The factor $\delta_2(\mathbf{u})$ has no real zeros, and $u_1^2 - u_2$ is the polynomial of X . The real zero locus of the other factors u_1 and $\delta_1(\mathbf{u})$ are shown in Figure 7.4. The medial axis of the parabola is $\text{Med}(X) = \{(0, u_2) \mid u_2 \geq \frac{1}{2}\}$ and $u_1 = 0$ is the Zariski closure of $\text{Med}(X)$. The variety $\delta_1(\mathbf{u}) = 0$ is the ED-discriminant or evolute of the parabola, also known as the *semicubical parabola*. Above the evolute a point $\mathbf{u} \in \mathbb{R}^2$ has three real ED critical points on X , and below the evolute it has one real and two complex ED critical points. \diamond

The discriminant Δ_X^{Off} in the previous example we observed had three real components: the variety X , its algebraic medial axis and its evolute. We show that this is a general fact, following [78]. For that, we define the *bisector hypersurface* Bis_X of X : Writing $\text{Bl}_X \subset \mathbb{C}^n \times \mathbb{C}$ for the branch locus of the projection $\pi_2 : \text{OC}_X \rightarrow \mathbb{C}^n \times \mathbb{C}$, the bisector hypersurface is the union of the branch points u when varying over all ε :

$$\text{Bis}_X := \bigcup_{(u, \varepsilon) \in \text{Bl}_X} u.$$

Theorem 7.14 *The components of the offset discriminant are*

$$\Delta_X^{\text{Off}} = \text{Bis}_X \cup \Sigma_X \supseteq X_{\mathbb{C}} \cup M_X \cup \Sigma_X.$$

Its real components are the real parts of X , M_X , and Σ_X .

Proof By Proposition 7.9, the offset discriminant is the locus of those \mathbf{u} such that $g_X(\mathbf{u}, \varepsilon)$ has less than $2 \times \text{EDdeg}(X)$ distinct complex solutions. This can happen due to two reasons: \mathbf{u} has either less than $\text{EDdeg}(X)$ distinct ED critical points on X or two distinct ED critical points

$$\mathbf{x}_1 \neq \mathbf{x}_2 \text{ with } \|\mathbf{x}_1 - \mathbf{u}\|^2 = \|\mathbf{x}_2 - \mathbf{u}\|^2. \tag{7.1}$$

The first case is the ED discriminant Σ_X and second case the bisector hypersurface Bis_X . By definition, the medial axis $\text{Med}(X)$ is contained in Bis_X , and thus we also have the inclusion $M_X \subseteq \text{Bis}_X$. Since the ε that come from zeros of $g_X(\mathbf{u}, \varepsilon)$ come in signed pairs (cf. Proposition 7.9), we see that $X \times \{0\}$ is doubly covered by the projection π_2 , meaning that $X \subseteq \text{Bis}_X$. All other components of Bis_X besides $X \cup M_X$ consist of non-real points \mathbf{u} that have ED critical points as in (7.1). \square

Chapter 8

Voronoi Cells

Every real algebraic variety determines a Voronoi decomposition of its ambient Euclidean space. Each Voronoi cell is a convex semialgebraic set in the normal space of the variety at a point. In this chapter we study such Voronoi cells of algebraic varieties, with primary focus on their algebraic boundaries.

8.1 Voronoi Basics

We begin with the familiar case when the given variety X is a finite subset of the Euclidean space \mathbb{R}^n . The *Voronoi cell* of a point $\mathbf{y} \in X$ consists of all points whose closest point in X is \mathbf{y} , i.e.

$$\text{Vor}_X(\mathbf{y}) := \{ \mathbf{u} \in \mathbb{R}^n : \mathbf{y} \in \arg \min_{\mathbf{x} \in X} \|\mathbf{x} - \mathbf{u}\|^2 \}. \quad (8.1)$$

This is a convex polyhedron with at most $|X| - 1$ facets. The study of these cells, and how they depend on the configuration X , is ubiquitous in computational geometry and its numerous applications.

Proposition 8.1 *The Voronoi cell of a point \mathbf{y} in the finite set $X \subset \mathbb{R}^n$ is the polyhedron*

$$\text{Vor}_X(\mathbf{y}) = \{ \mathbf{u} \in \mathbb{R}^n : \mathbf{u} \cdot (\mathbf{x} - \mathbf{y}) \leq \frac{1}{2} (\|\mathbf{x}\|^2 - \|\mathbf{y}\|^2) \text{ for all } \mathbf{x} \in X \setminus \{\mathbf{y}\} \}. \quad (8.2)$$

Proof By definition, $\text{Vor}_X(\mathbf{y})$ consists of all points \mathbf{u} such that $\|\mathbf{x} - \mathbf{u}\|^2 - \|\mathbf{y} - \mathbf{u}\|^2$ is nonnegative for all $\mathbf{x} \in X \setminus \{\mathbf{y}\}$. But, this expression is equal to $\|\mathbf{x}\|^2 - \|\mathbf{y}\|^2 - 2\mathbf{u} \cdot (\mathbf{x} - \mathbf{y})$. The main point is that the quadratic term drops out, so the expression is linear in \mathbf{u} . \square

The collection of all Voronoi cells, as \mathbf{y} ranges over the set X , is known as the *Voronoi diagram* of X . The Voronoi diagram is a polyhedral subdivision of \mathbb{R}^n into finitely many convex cells.

We now shift gears, and we replace the finite set X by a real algebraic variety of positive dimension. As before, the ambient space is \mathbb{R}^n with its standard Euclidean metric. We seek the Voronoi diagram $\{\text{Vor}_X(\mathbf{y})\}_{\mathbf{y} \in X}$ in \mathbb{R}^n where \mathbf{y} runs over all (infinitely many) points in X .

One approach is to take a large but finite sample from X and to consider the Voronoi diagram of that sample. This is a finite approximation to the desired limit object. By taking finer and finer samples, the Voronoi diagram should converge nicely to a subdivision with infinitely many regions. The Voronoi cells in the limit are convex sets. However, for $n \geq 3$, they are generally not polyhedra. This process was studied by Brandt and Weinstein in [20] for the case when $n = 2$ and X is a curve. In [20, Figure 1] we see this for a quartic curve. The authors posted a delightful YouTube video, called *Mathemaddies' Ice Cream Map*. Please do watch that movie! Their curve X is the shoreline that separates the city of Berkeley from the San Francisco Bay. One hopes to find many ice cream shops at the shore.

Let X be a real algebraic variety of codimension c in \mathbb{R}^n , and consider a point $\mathbf{y} \in X$. The Voronoi cell $\text{Vor}_X(\mathbf{y})$ is defined as before. It consists of all points \mathbf{u} in \mathbb{R}^n such that \mathbf{y} is closer or equal to \mathbf{u} than any other point $\mathbf{x} \in X$. The equation (8.2) still holds, and we conclude that $\text{Vor}_X(\mathbf{y})$ is a convex set.

Proposition 8.2 *Suppose that \mathbf{y} is a smooth point of the variety X . Then its Voronoi cell $\text{Vor}_X(\mathbf{y})$ is a convex semialgebraic set of dimension c . This Voronoi cell is contained in the normal space*

$$N_X(\mathbf{y}) = \{ \mathbf{u} \in \mathbb{R}^n : \mathbf{u} - \mathbf{y} \text{ is perpendicular to the tangent space of } X \text{ at } \mathbf{y} \} \simeq \mathbb{R}^c.$$

Proof Fix $\mathbf{u} \in \text{Vor}_X(\mathbf{y})$. Consider any point \mathbf{x} in X that is close to \mathbf{y} , and set $\mathbf{v} = \mathbf{x} - \mathbf{y}$. The inequality in (8.2) implies $\mathbf{u} \cdot \mathbf{v} \leq \frac{1}{2} (\|\mathbf{y} + \mathbf{v}\|^2 - \|\mathbf{y}\|^2) = \mathbf{y} \cdot \mathbf{v} + \frac{1}{2} \|\mathbf{v}\|^2$. For any \mathbf{w} in the tangent space of X at \mathbf{y} , there exists $\mathbf{v} = \epsilon \mathbf{w} + O(\epsilon^2)$ such that $\mathbf{x} = \mathbf{y} + \mathbf{v}$ is in X . The inequality above yields $\mathbf{u} \cdot \mathbf{w} \leq \mathbf{y} \cdot \mathbf{w}$, and the same with $-\mathbf{w}$ instead of \mathbf{w} . Then $(\mathbf{u} - \mathbf{y}) \cdot \mathbf{w} = 0$, and hence \mathbf{u} is in the normal space $N_X(\mathbf{y})$. We already

argued that $\text{Vor}_X(\mathbf{y})$ is convex. It is semialgebraic, by Tarski's Theorem on Quantifier Elimination. This allows us to eliminate \mathbf{x} from the formula (8.2). Finally, the Voronoi cell $\text{Vor}_X(\mathbf{y})$ is full-dimensional in the c -dimensional space $N_X(\mathbf{y})$ because every point \mathbf{u} in an ϵ -neighborhood of \mathbf{y} has a unique closest point in X . If $\mathbf{u} \in N_X(\mathbf{y})$ then that closest point must be \mathbf{y} , by the same inequality as above. \square

The topological boundary of the Voronoi cell $\text{Vor}_X(\mathbf{y})$ in the normal space $N_X(\mathbf{y})$ is denoted by $\partial\text{Vor}_X(\mathbf{y})$. It consists of all points in $N_X(\mathbf{y})$ that have at least two closest points in X , including \mathbf{y} . We are interested in the *algebraic boundary* $\partial_{\text{alg}}\text{Vor}_X(\mathbf{y})$. This is the hypersurface in the complex affine space $N_X(\mathbf{y})_{\mathbb{C}} \simeq \mathbb{C}^c$ obtained as the Zariski closure of $\partial\text{Vor}_X(\mathbf{y})$ over the field of definition of X . The degree of this hypersurface is denoted $\delta_X(\mathbf{y})$ and called the *Voronoi degree* of X at \mathbf{y} . If X is irreducible and \mathbf{y} is a general point on X , then this degree does not depend on the choice of \mathbf{y} .

Example 8.3 (Surfaces in 3-space) Fix a general polynomial $f \in \mathbb{Q}[x_1, x_2, x_3]$ of degree $d \geq 2$ and let $X = V(f)$ be its surface in \mathbb{R}^3 . The normal space at a general point $\mathbf{y} \in X$ is the line $N_X(\mathbf{y}) = \{\mathbf{y} + \lambda(\nabla f)(\mathbf{y}) : \lambda \in \mathbb{R}\}$. The Voronoi cell $\text{Vor}_X(\mathbf{y})$ is a (possibly unbounded) line segment in $N_X(\mathbf{y})$ that contains \mathbf{y} . The boundary $\partial\text{Vor}_X(\mathbf{y})$ consists of at most two points from among the zeros of an irreducible polynomial in $\mathbb{Q}[\lambda]$. We shall see that this univariate polynomial has degree $d^3 + d - 7$. Its complex zeros form the algebraic boundary $\partial_{\text{alg}}\text{Vor}_X(\mathbf{y})$. Thus, the Voronoi degree of the surface X is $d^3 + d - 7$.

Note that, in this example, our hypothesis “over the field of definition” becomes important. The \mathbb{Q} -Zariski closure of one boundary point is the collection of all $d^3 + d - 7$ points in $\partial_{\text{alg}}\text{Vor}_X(\mathbf{y})$.

For a numerical example, we take the degree to be $d = 2$ and we fix $\mathbf{y} = (0, 0, 0)$. Our quadric is $f = x_1^2 + x_2^2 + x_3^2 - 3x_1x_2 - 5x_1x_3 - 7x_2x_3 + x_1 + x_2 + x_3$. Let $r_0 \approx -0.209$, $r_1 \approx -0.107$, $r_2 \approx 0.122$ be the roots of the cubic polynomial $368\lambda^3 + 71\lambda^2 - 6\lambda - 1$. The Voronoi cell $\text{Vor}_X(\mathbf{y})$ is the line segment connecting the points (r_1, r_1, r_1) and (r_2, r_2, r_2) . The topological boundary $\partial\text{Vor}_X(\mathbf{y})$ consists of the two points (r_1, r_1, r_1) and (r_2, r_2, r_2) , whereas the algebraic boundary $\partial_{\text{alg}}\text{Vor}_X(\mathbf{y})$ also contains (r_0, r_0, r_0) .

The cubic polynomial in the unknown λ was found with the algebraic method that is described in the next section. Namely, the Voronoi ideal in (8.3) equals $\text{Vor}_I(0) = \langle u_1 - u_3, u_2 - u_3, 368u_3^3 + 71u_3^2 - 6u_3 - 1 \rangle$. This is a maximal ideal in $\mathbb{Q}[u_1, u_2, u_3]$, and it defines a field extension of degree 3 over \mathbb{Q} .

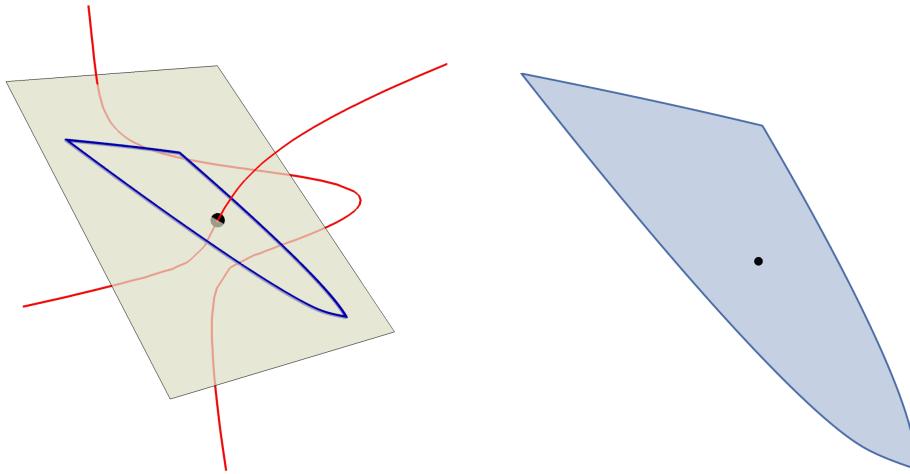


Fig. 8.1: A quartic space curve, shown with the Voronoi cell in one of its normal planes.

Example 8.4 (Curves in 3-space) Let X be a general algebraic curve in \mathbb{R}^3 . For $\mathbf{y} \in X$, the Voronoi cell $\text{Vor}_X(\mathbf{y})$ is a convex set in the normal plane $N_X(\mathbf{y}) \simeq \mathbb{R}^2$. Its algebraic boundary $\partial_{\text{alg}}\text{Vor}_X(\mathbf{y})$ is a plane curve of degree $\delta_X(\mathbf{y})$. This Voronoi degree can be expressed in terms of the degree and genus of X . Specifically, this degree is 12 when X is the intersection of two general quadrics in \mathbb{R}^3 . Figure 8.1 shows one such quartic space curve X together with the normal plane at a point $\mathbf{y} \in X$. The Voronoi cell $\text{Vor}_X(\mathbf{y})$ is the planar convex region highlighted on the right. Its algebraic boundary $\partial_{\text{alg}}\text{Vor}_X(\mathbf{y})$ is a curve of degree $\delta_X(\mathbf{y}) = 12$. The topological boundary $\partial\text{Vor}_X(\mathbf{y})$ is only a very small subset of that algebraic boundary.

8.2 Computing Algebraic Boundaries

Metric algebraic geometry is concerned with properties of real algebraic varieties that depend on a distance metric. Key concepts include the Euclidean distance degree [52], distance function [117], bottlenecks [49, 59], reach, offset hypersurfaces, medial axis [77], and cut locus [41]. Voronoi cells are also an important topic in metric algebraic geometry. We here consider them only for the Euclidean metric, but it also makes much sense to study Voronoi cells with respect to Kullback-Leibler divergence [3] or Wasserstein distance [13].

We study the Voronoi decomposition to answer the question for any point in ambient space, “What point on the variety X am I closest to?” Another question one might ask is, “How far do we have to get away from X before there is more than one answer to the closest point question?” The union of the boundaries of the Voronoi cells is the locus of points in \mathbb{R}^n that have more than one closest point on X . This set is called the *medial axis* (or *cut locus*) of the variety.

The distance from the variety to its medial axis, which is the answer to the “how far” question, is called the *reach* of X . This quantity is of interest, for example, in topological data analysis, as it is the main quantity determining the density of sample points needed to compute the persistent homology of X . We refer to [24, 57] for studies on sampling at the interface of topological data analysis with metric algebraic geometry. The distance from a point \mathbf{y} on X to the variety’s medial axis could be considered the *local reach* of X . Equivalently, this is the distance from \mathbf{y} to the boundary of its Voronoi cell $\text{Vor}_X(\mathbf{y})$.

The material that follows is based on the article [42]. We begin with the exact symbolic computation of the Voronoi boundary at \mathbf{y} from the equations that define X . This uses a Gröbner-based algorithm whose input is \mathbf{y} and the ideal of X and whose output is the ideal defining $\partial_{\text{alg}}\text{Vor}_X(\mathbf{y})$. In the next section we present formulas for the Voronoi degree $\delta_X(\mathbf{y})$ when X and \mathbf{y} are sufficiently general and $\dim(X) \leq 2$. The proofs of these formulas require some intersection theory. Thereafter we study the case when \mathbf{y} is a low rank matrix and X is the variety of these matrices. This relies on the *Eckart-Young Theorem*.

We now describe Gröbner basis methods for finding the Voronoi boundaries of a given variety. We start with an ideal $I = \langle f_1, f_2, \dots, f_m \rangle$ in $\mathbb{Q}[x_1, \dots, x_n]$ whose real variety $X = V(I) \subset \mathbb{R}^n$ is assumed to be nonempty. We assume that I is real radical and prime, so that $X_{\mathbb{C}}$ is an irreducible variety in \mathbb{C}^n whose real points are Zariski dense. Our aim is to compute the Voronoi boundary of a given point $\mathbf{y} \in X$. In our examples, the coordinates of the point \mathbf{y} and the coefficients of the polynomials f_i are rational numbers. Under these assumptions, the following computations can be done in polynomial rings over \mathbb{Q} .

Fix the polynomial ring $R = \mathbb{Q}[x_1, \dots, x_n, u_1, \dots, u_n]$ where $\mathbf{u} = (u_1, \dots, u_n)$ is an auxiliary point with unknown coordinates. The *augmented Jacobian* of X at \mathbf{x} is the following matrix of size $(m+1) \times n$ with entries in R . It contains the n partial derivatives of the m generators of I :

$$J_I(x, u) := \begin{bmatrix} \mathbf{u} - \mathbf{x} \\ (\nabla f_1)(\mathbf{x}) \\ \vdots \\ (\nabla f_m)(\mathbf{x}) \end{bmatrix}$$

Let N_I denote the ideal in R generated by I and the $(c+1) \times (c+1)$ minors of the augmented Jacobian $J_I(\mathbf{x}, \mathbf{u})$, where c is the codimension of the given variety $X \subset \mathbb{R}^n$. The ideal N_I in R defines a subvariety of dimension n in \mathbb{R}^{2n} , namely the *Euclidean normal bundle* of X . Its points are pairs (\mathbf{x}, \mathbf{u}) where \mathbf{x} is a point in the given variety X and \mathbf{u} lies in the normal space of X at \mathbf{x} .

Example 8.5 (Cuspidal cubic) Let $n = 2$ and $I = \langle x_1^3 - x_2^2 \rangle$, so $X = V(I) \subset \mathbb{R}^2$ is a cubic curve with a cusp at the origin. The ideal of the Euclidean normal bundle of X is generated by two polynomials:

$$N_I = \langle x_1^3 - x_2^2, \det \begin{pmatrix} u_1 - x_1 & u_2 - x_2 \\ 3x_1^2 & -2x_2 \end{pmatrix} \rangle \subset R = \mathbb{Q}[x_1, x_2, u_1, u_2]$$

For any $\mathbf{y} \in X$, let $N_I(\mathbf{y})$ denote the linear ideal that is obtained from N_I by replacing the unknown point \mathbf{x} by the specific point \mathbf{y} . For instance, if that point is $\mathbf{y} = (4, 8)$ then $N_I(\mathbf{y}) = \langle u_1 + 3u_2 - 28 \rangle$.

Returning to the general setting, we define the *critical ideal* of the variety X at the point \mathbf{y} as

$$C_I(\mathbf{y}) = N_I + N_I(\mathbf{y}) + \langle \|\mathbf{x} - \mathbf{u}\|^2 - \|\mathbf{y} - \mathbf{u}\|^2 \rangle \subset R.$$

The variety of the ideal $C_I(\mathbf{y})$ consists of pairs (\mathbf{u}, \mathbf{x}) such that \mathbf{x} and \mathbf{y} are equidistant from \mathbf{u} and both are critical points of the distance function from \mathbf{u} to X . The *Voronoi ideal* is the following ideal in $\mathbb{Q}[u_1, \dots, u_n]$. It is obtained from the critical ideal by saturation and elimination:

$$\text{Vor}_I(\mathbf{y}) = (C_I(\mathbf{y}) : \langle \mathbf{x} - \mathbf{y} \rangle^\infty) \cap \mathbb{Q}[u_1, \dots, u_n]. \quad (8.3)$$

The geometric interpretation of each step in our construction implies the following result:

Proposition 8.6 *The affine variety in \mathbb{C}^n defined by the Voronoi ideal $\text{Vor}_I(\mathbf{y})$ contains the algebraic Voronoi boundary $\partial_{\text{alg}} \text{Vor}_X(\mathbf{y})$ of the given real variety X at its point \mathbf{y} .*

Remark 8.7 The verb “contains” sounds weak, but it is much stronger than it may seem. Indeed, in generic situations, the ideal $\text{Vor}_I(\mathbf{y})$ will be prime, and it defines an irreducible hypersurface in the normal space $N_I(\mathbf{y})$. This hypersurface equals the algebraic Voronoi boundary, so containment is an equality. We saw this in Example 8.3. For special data, $\text{Vor}_I(\mathbf{y})$ usually defines a hypersurface in $N_I(\mathbf{y})$, but it can have extraneous components, which are often easy to remove.

Example 8.8 For the point $\mathbf{y} = (4, 8)$ on the cuspidal cubic X in Example 8.5, we have $N_I(\mathbf{y}) = \langle u_1 + 3u_2 - 28 \rangle$. Going through the steps above, we find that the Voronoi ideal is

$$\text{Vor}_I(\mathbf{y}) = \langle u_1 - 28, u_2 \rangle \cap \langle u_1 + 26, u_2 - 18 \rangle \cap \langle u_1 + 3u_2 - 28, 27u_2^2 - 486u_2 + 2197 \rangle.$$

The third component has no real roots and is hence extraneous. The Voronoi boundary consists of two points. Namely, we have $\partial \text{Vor}_X(\mathbf{y}) = \{(28, 0), (-26, 18)\}$. The Voronoi cell $\text{Vor}_X(\mathbf{y})$ is the line segment connecting these points. This segment is shown in green in Figure 8.2. Its right endpoint $(28, 0)$ is equidistant from \mathbf{y} and the point $(4, -8)$. Its left endpoint $(-26, 18)$ is equidistant from \mathbf{y} and the origin $(0, 0)$, whose Voronoi cell will be discussed in Remark 8.9.

The cuspidal cubic X is very special. If we replace X by a general cubic (defined over \mathbb{Q}) in the affine plane, then $\text{Vor}_I(\mathbf{y})$ is generated modulo $N_I(\mathbf{y})$ by an irreducible polynomial of degree eight in $\mathbb{Q}[u_2]$. Thus, the expected Voronoi degree for general (affine) plane cubics is $\delta_X(\mathbf{y}) = 8$.

Remark 8.9 (Singularities) Voronoi cells at singular points can be computed with the same procedure as above. However, these Voronoi cells generally have higher dimensions. For an illustration, consider the cuspidal cubic, and let $\mathbf{y} = (0, 0)$ be the cusp. A Gröbner basis computation yields the Voronoi boundary

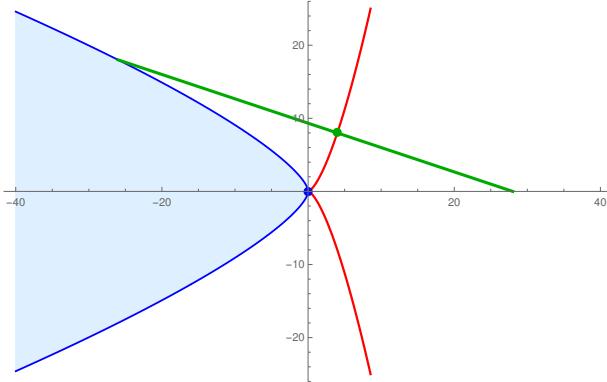


Fig. 8.2: The cuspidal cubic is shown in red. The Voronoi cell of a smooth point is a green line segment. The Voronoi cell of the cusp is the convex region bounded by the blue curve.

$27u_2^4 + 128u_1^3 + 72u_1u_2^2 + 32u_1^2 + u_2^2 + 2u_1$. The Voronoi cell is the two-dimensional convex region bounded by this quartic, shown in blue in Figure 8.2. The Voronoi cell might also be empty at a singularity. This happens for instance for $V(x_1^3 + x_1^2 - x_2^2)$, which has an ordinary double point at $\mathbf{y} = (0, 0)$. In general, the cell dimension depends on both the embedding dimension and the branches of the singularity.

Proposition 8.6 gives an algorithm for computing the Voronoi ideal $\text{Vor}_I(\mathbf{y})$ when \mathbf{y} is a smooth point in $X = V(I)$. Experiments with Macaulay2 [67] are reported in [42]. For small enough instances, the computation terminates and we obtain the defining polynomial of the Voronoi boundary $\partial_{\text{alg}}\text{Vor}_X(\mathbf{y})$. This polynomial is unique modulo the linear ideal of the normal space $N_I(\mathbf{y})$. For larger instances, we can only compute the degree of $\partial_{\text{alg}}\text{Vor}_X(\mathbf{y})$ but not its equation. This is done by working over a finite field and adding $c - 1$ random linear equations in u_1, \dots, u_n in order to get a zero-dimensional polynomial system.

Computations are easiest to set up for the case of hypersurfaces ($c = 1$). One can explore random polynomials f of degree d in $\mathbb{Q}[x_1, \dots, x_n]$, both inhomogeneous and homogeneous. These are chosen among those that vanish at a preselected point \mathbf{y} in \mathbb{Q}^n . In each iteration, the Voronoi ideal $\text{Vor}_I(\mathbf{y})$ from (8.3) was found to be zero-dimensional. In fact, $\text{Vor}_I(\mathbf{y})$ is a maximal ideal in $\mathbb{Q}[u_1, \dots, u_n]$, and the Voronoi degree $\delta_X(\mathbf{y})$ is the degree of the field extension of \mathbb{Q} that is defined by that maximal ideal.

We summarize our results in Tables 8.1 and 8.2, and we extract conjectural formulas.

$n \setminus d$	2	3	4	5	6	7	8	$\delta_X(\mathbf{y}) = \text{degree}(\text{Vor}_{(f)}(\mathbf{y}))$
1	1	2	3	4	5	6	7	$d-1$
2	2	8	16	26	38	52	68	d^2+d-4
3	3	23	61	123	215	343		d^3+d-7
4	4	56	202	520	1112			$d^4-d^3+d^2+d-10$
5	5	125	631					$d^5-2d^4+2d^3+d-13$
6	6	266	1924					$d^6-3d^5+4d^4-2d^3+d^2+d-16$
7	7	551						$d^7-4d^6+7d^5-6d^4+3d^3+d-19$

Table 8.1: The Voronoi degree of an inhomogeneous polynomial f of degree d in \mathbb{R}^n .

Conjecture 8.10 The Voronoi degree of a generic hypersurface of degree d in \mathbb{R}^n equals

$$(d-1)^n + 3(d-1)^{n-1} + \frac{4}{d-2}((d-1)^{n-1} - 1) - 3n.$$

$n \setminus d$	2	3	4	5	6	7	8	$\delta_X(y) = \text{degree}(\text{Vor}_{\langle f \rangle}(y))$
2	2	4	6	8	10	12	14	$2d-2$
3	3	13	27	45	67	93	123	$2d^2-5$
4	4	34	96	202				$2d^3-2d^2+2d-8$
5	5	79	309					$2d^4-4d^3+4d^2-11$
6	6	172						$2d^5-6d^4+8d^3-4d^2+2d-14$
7	7	361						$2d^6-8d^5+14d^4-12d^3+6d^2-17$

Table 8.2: The Voronoi degree of a homogeneous polynomial f of degree d in \mathbb{R}^n .

The Voronoi degree of the cone of a generic homogeneous polynomial of degree d in \mathbb{R}^n is

$$2(d-1)^{n-1} + \frac{4}{d-2}((d-1)^{n-1} - 1) - 3n + 2.$$

Both parts of this conjecture are proved for $n \leq 3$ in [42, Section 4], where the geometric theory of Voronoi degrees of low-dimensional varieties is developed. The case $d = 2$ was analyzed in [41, Proposition 5.8]. In general, for $n \geq 4$ and $d \geq 3$, the problem is open.

8.3 Formulas from Algebraic Geometry

To recap, the algebraic boundary of the Voronoi cell $\text{Vor}_X(\mathbf{y})$ is a hypersurface in the normal space to a variety $X \subset \mathbb{R}^n$ at a point $\mathbf{y} \in X$. We shall present formulas for the degree $\delta_X(\mathbf{y})$ of that hypersurface when X is a curve or a surface. All proofs appear in [42, Section 6]. We identify X and $\partial_{\text{alg}}\text{Vor}_X(\mathbf{y})$ with their Zariski closures in complex projective space \mathbb{P}^n , so there is a natural assigned hyperplane at infinity. We say that X is in *general position* in \mathbb{P}^n if the hyperplane at infinity intersects X transversally, i.e. that the intersection is smooth.

Theorem 8.11 *Let $X \subset \mathbb{P}^n$ be a curve of degree d and geometric genus g with at most ordinary multiple points as singularities. The Voronoi degree at a general point $\mathbf{y} \in X$ equals*

$$\delta_X(\mathbf{y}) = 4d + 2g - 6,$$

provided X is in general position in \mathbb{P}^n .

Example 8.12 If X is a smooth curve of degree d in the plane, then $2g - 2 = d(d - 3)$, so

$$\delta_X(\mathbf{y}) = d^2 + d - 4.$$

This confirms our experimental results in the row $n = 2$ of Table 8.1.

Example 8.13 If X is a rational curve of degree d , then $g = 0$ and hence $\delta_X(\mathbf{y}) = 4d - 6$. If X is an elliptic curve, so the genus is $g = 1$, then we have $\delta_X(\mathbf{y}) = 4d - 4$. A space curve with $d = 4$ and $g = 1$ was studied in Example 8.4. Its Voronoi degree equals $\delta_X(\mathbf{y}) = 12$.

Theorem 8.11 is [42, Theorem 5.1]. The general position assumption is essential. For an example, let X be the twisted cubic curve in \mathbb{P}^3 , with affine parameterization $t \mapsto (t, t^2, t^3)$. Here $g = 0$ and $d = 3$, so the expected Voronoi degree is 6. However, a computation shows that $\delta_X(\mathbf{y}) = 4$. This drop arises because the plane at infinity in \mathbb{P}^3 intersects the curve X in a triple point. After a general linear change of coordinates in \mathbb{P}^3 , which amounts to a linear fractional transformation in \mathbb{R}^3 , we correctly find $\delta_X(\mathbf{y}) = 6$.

We next present a formula for the Voronoi degree of a surface X which is smooth and irreducible in \mathbb{P}^n . Our formula is in terms of its degree d and two further invariants. The first, denoted $\chi(X) := c_2(X)$, is the topological Euler characteristic. This is equal to the degree of the second Chern class of the tangent bundle. The second invariant, denoted $g(X)$, is the genus of the curve obtained by intersecting X with a general smooth quadratic hypersurface in \mathbb{P}^n . Thus, $g(X)$ is the quadratic analogue to the usual sectional genus of the surface X .

Theorem 8.14 (Theorem 5.4 in [42]) *Let $X \subset \mathbb{P}^n$ be a smooth surface of degree d . Then*

$$\delta_X(y) = 3d + \chi(X) + 4g(X) - 11,$$

provided the surface X is in general position in \mathbb{P}^n and y is a general point on X .

Example 8.15 If X is a smooth surface in \mathbb{P}^3 of degree d , then $\chi(X) = d(d^2 - 4d + 6)$, by [62, Ex 3.2.12]. A smooth quadratic hypersurface section of X is an irreducible curve of degree (d, d) in $\mathbb{P}^1 \times \mathbb{P}^1$. The genus of such a curve is $g(X) = (d - 1)^2$. We conclude that

$$\delta_X(y) = 3d + d(d^2 - 4d + 6) + 4(d - 1)^2 - 11 = d^3 + d - 7.$$

This confirms our experimental results in the row $n = 3$ of Table 8.1.

Example 8.16 Let X be the Veronese surface of order e in $\mathbb{P}^{\binom{e+1}{2}-1}$, taken after a general linear change of coordinates in that ambient space. The degree of X equals $d = e^2$. We have $\chi(X) = \chi(\mathbb{P}^2) = 3$, and the general quadratic hypersurface section of X is a curve of genus $g(X) = \binom{2e-1}{2}$. We conclude that the Voronoi degree of X at a general point y equals

$$\delta_X(y) = 3e^2 + 3 + 2(2e-1)(2e-2) - 11 = 11e^2 - 12e - 4.$$

For instance, for the quadratic Veronese surface in \mathbb{P}^5 we have $e = 2$ and hence $\delta_X(y) = 16$. This is smaller than the number 18 found in Example 8.22, since back then we were dealing with the cone over the Veronese surface in \mathbb{R}^6 , and not with the Veronese surface in $\mathbb{R}^5 \subset \mathbb{P}^5$.

We finally consider affine surfaces defined by homogeneous polynomials. Namely, let $X \subset \mathbb{R}^n$ be the affine cone over a general smooth curve of degree d and genus g in \mathbb{P}^{n-1} .

Theorem 8.17 (Theorem 5.7 in [42]) *If $X \subset \mathbb{R}^n$ is the cone over a smooth curve in \mathbb{P}^{n-1} then*

$$\delta_X(y) = 6d + 4g - 9,$$

provided that the curve is in general position and y is a general point.

Example 8.18 If $X \subset \mathbb{R}^3$ is the cone over a smooth curve of degree d in \mathbb{P}^2 , then $2g - 2 = d(d - 3)$, by the degree-genus formula for plane curves. We conclude that the Voronoi degree of X is equal to

$$\delta_X(y) = 2d^2 - 5.$$

This confirms our experimental results in the row $n = 3$ of Table 8.2.

Let us comment on the assumptions made in our theorems. We assumed that the variety X is in general position in \mathbb{P}^n . If this is not satisfied, then the Voronoi degree may drop. The point here is that the Voronoi ideal $\text{Vor}_I(y)$ depends polynomially on the description of X , and the degree of this zero-dimensional ideal can only go down – and not up – when that description specializes. Making this statement precise would require a technical discussion of families in algebraic geometry, a topic best left to the experts on foundations. Nonetheless, the technique introduced in the next section can be adapted to determine the correct value. As an illustration, we consider the affine Veronese surface (Example 8.16).

Example 8.19 Let $X \subset \mathbb{P}^5$ be the Veronese surface with affine parametrization $(s, t) \mapsto (s, t, s^2, st, t^2)$. The hyperplane at infinity intersects X in a double conic, so X is not in general position. In the next section, we will show that the true Voronoi degree is $\delta_X(\mathbf{y}) = 10$. For the Frobenius norm, the Voronoi degree drops further. For this, we shall derive $\delta_X(\mathbf{y}) = 4$.

8.4 Voronoi meets Eckhart-Young

We now turn to the case of great interest in applications. Let X be the variety of real $m \times n$ matrices of rank $\leq r$. We consider two natural norms on the space $\mathbb{R}^{m \times n}$ of real $m \times n$ matrices. Our first matrix norm is the *Frobenius norm* $\|U\|_F := \sqrt{\sum_{ij} U_{ij}^2}$. Our second matrix norm is the *spectral norm* $\|U\|_2 := \max_i \sigma_i(U)$ which extracts the largest singular value of the matrix U .

Fix a rank r matrix V in X . This is a nonsingular point in X . We consider the Voronoi cell $\text{Vor}_X(V)$ with respect to the Frobenius norm. This is consistent with our setting because the Frobenius norm agrees with the Euclidean norm on $\mathbb{R}^{m \times n}$. This identification will no longer be valid when we restrict to the subspace of symmetric matrices.

Fix $U \in \text{Vor}_X(V)$. This means that the closest point to U in the rank r variety X is the matrix V . By the Eckart-Young Theorem, the matrix V is derived from U by computing the singular value decomposition $U = \Sigma_1 D \Sigma_2$. Here Σ_1 and Σ_2 are orthogonal matrices of size $m \times m$ and $n \times n$ respectively, and D is a nonnegative diagonal matrix whose entries are the singular values. Let $D^{[r]}$ be the matrix that is obtained from D by replacing all singular values except for the r largest ones by zero. Then, according to Eckart-Young, we have $V = \Sigma_1 \cdot D^{[r]} \cdot \Sigma_2$.

Remark 8.20 The Eckart-Young Theorem works for both the Frobenius norm and the spectral norm. This means that $\text{Vor}_X(V)$ is also the Voronoi cell for the spectral norm.

The following theorem describes the Voronoi cells for low-rank matrix approximation.

Theorem 8.21 *Let V be an $m \times n$ -matrix of rank r . The Voronoi cell $\text{Vor}_X(V)$ is congruent up to scaling to the unit ball in the spectral norm on the space of $(m - r) \times (n - r)$ -matrices.*

Before we present the proof, let us first see why the statement makes sense. The determinantal variety X has dimension $rm + rn - r^2$ in an ambient space of dimension mn . The dimension of the normal space at a point is the difference of these two numbers, so it equals $(m - r)(n - r)$. Every Voronoi cell is a full-dimensional convex body in the normal space. Next consider the case $m = n$ and restrict to the space of diagonal matrices. Now X is the set of vectors in \mathbb{R}^n having at most r nonzero coordinates. This is a reducible variety with $\binom{n}{r}$ components, each a coordinate subspace. For a general point y in such a subspace, the Voronoi cell $\text{Vor}_X(y)$ is a convex polytope. It is congruent to a regular cube of dimension $n - r$, which is the unit ball in the L^∞ -norm on \mathbb{R}^{n-r} . Theorem 8.21 describes the orbit of this picture under the action of the two orthogonal groups on $\mathbb{R}^{m \times n}$.

For example, consider the special case where $n = 3$ and $r = 1$. In this case, X consists of the three coordinate axes in \mathbb{R}^3 . The Voronoi decomposition of this reducible curve decomposes \mathbb{R}^3 into squares, each normal to a different point on the three lines. The image of this picture under orthogonal transformations is the Voronoi decomposition of $\mathbb{R}^{3 \times 3}$ associated with the affine variety of rank 1 matrices. That variety has dimension 5, and each Voronoi cell is a 4-dimensional convex body in the normal space.

Proof (of Theorem 8.21) The Voronoi cell is invariant under orthogonal transformations. We may therefore assume that the matrix $V = (v_{ij})$ satisfies $v_{11} \geq v_{22} \geq \dots \geq v_{rr} = u > 0$ and $v_{ij} = 0$ for all other entries. The Voronoi cell of the diagonal matrix V consists of matrices U whose block-decomposition into $r + (m - r)$ rows and $r + (n - r)$ columns satisfies

$$\begin{pmatrix} I & 0 \\ 0 & T_1 \end{pmatrix} \cdot \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix} \cdot \begin{pmatrix} I & 0 \\ 0 & T_2 \end{pmatrix} = \begin{pmatrix} V_{11} & 0 \\ 0 & V_{22} \end{pmatrix}.$$

Here $V_{11} = \text{diag}(v_{11}, \dots, v_{rr})$ agrees with the upper $r \times r$ -block of V , and V_{22} is a diagonal matrix whose entries are bounded above by u in absolute value. This implies that $U_{11} = V_{11}$, $U_{12} = 0$ and $U_{21} = 0$. Moreover, U_{22} is an arbitrary $(m-r) \times (n-r)$ matrix with spectral norm at most u . Hence the Voronoi cell of the given diagonal matrix V is congruent to the set of all such matrices U_{22} . This convex body equals u times the unit ball in $\mathbb{R}^{(m-r) \times (n-r)}$ under the spectral norm. \square

Our problem becomes even more interesting when we restrict to matrices in a linear subspace. To see this, let X denote the variety of symmetric $n \times n$ matrices of rank $\leq r$. We can regard X either as a variety in the ambient matrix space $\mathbb{R}^{n \times n}$, or in the space $\mathbb{R}^{\binom{n+1}{2}}$ whose coordinates are the upper triangular entries of a symmetric matrix. On the latter space we have both the *Euclidean norm* and the *Frobenius norm*. These are now different!

The Frobenius norm on $\mathbb{R}^{\binom{n+1}{2}}$ is the restriction of the Frobenius norm on $\mathbb{R}^{n \times n}$ to the subspace of symmetric matrices. For instance, if $n = 2$, we identify the vector (a, b, c) with the symmetric matrix $\begin{pmatrix} a & b \\ b & c \end{pmatrix}$. The Frobenius norm of this matrix is $\sqrt{a^2 + 2b^2 + c^2}$, whereas the Euclidean norm is $\sqrt{a^2 + b^2 + c^2}$. The two norms have dramatically different properties with respect to low rank approximation. The Eckart-Young Theorem remains valid for the Frobenius norm on $\mathbb{R}^{\binom{n+1}{2}}$, but it is not valid for the Euclidean norm. The implications of this are explained in [52, Example 3.2].

In what follows we elucidate this point by comparing the Voronoi cells with respect to the two norms.

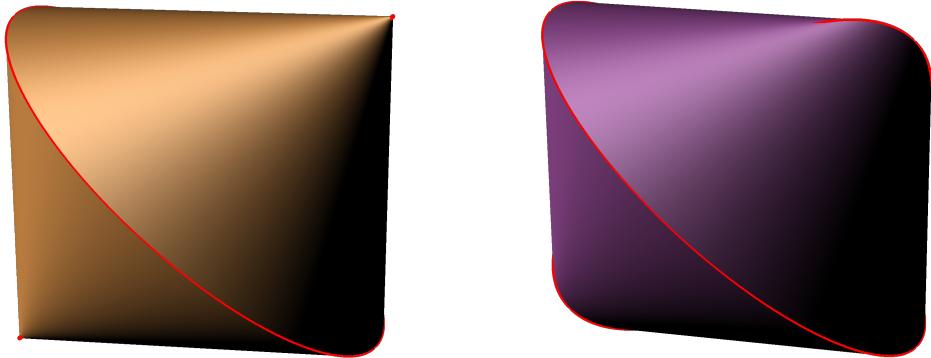


Fig. 8.3: The Voronoi cell of a symmetric 3×3 matrix of rank 1 is a convex body of dimension 3. It is shown for the Frobenius norm (left) and for the Euclidean norm (right).

Example 8.22 Let X be the variety of symmetric 3×3 matrices of rank ≤ 1 . For the Euclidean metric, X lives in \mathbb{R}^6 . For the Frobenius metric, X lives in a 6-dimensional subspace of $\mathbb{R}^{3 \times 3}$. Let V be a smooth point in X , i.e. a symmetric 3×3 matrix of rank 1. The normal space to X at V has dimension 3. Hence, in either norm, the Voronoi cell $\text{Vor}_X(V)$ is a 3-dimensional convex body. Figure 8.3 illustrates these two bodies.

For the Frobenius metric, the Voronoi cell is congruent to the set of matrices $\begin{pmatrix} a & b \\ b & c \end{pmatrix}$ with eigenvalues between -1 and 1 . This semialgebraic set is bounded by the surfaces defined by the singular quadrics $\det \begin{pmatrix} a+1 & b \\ b & c+1 \end{pmatrix}$ and $\det \begin{pmatrix} a-1 & b \\ b & c-1 \end{pmatrix}$. The Voronoi ideal is of degree 4, defined by the product of these two determinants (modulo the normal space). The Voronoi cell is shown on the left in Figure 8.3. It is the intersection of two quadratic cones. The cell is the convex hull of the circle in which the two quadrics meet, together with the two vertices.

For the Euclidean metric, the Voronoi boundary at a generic point V in X is defined by an irreducible polynomial of degree 18 in a, b, c . In some cases, the Voronoi degree can drop. For instance, consider the special rank 1 matrix $V = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$. For this point, the degree of the Voronoi boundary is only 12. This particular Voronoi cell is shown on the right in Figure 8.3. This cell is the convex hull of two ellipses, which are shown in red in the diagram.

Chapter 9

Condition Numbers

9.1 Errors in Numerical Computations

Input data for numerical algorithms can have errors, caused, for instance, by measurements errors. Consequently, the output of the computation also has errors.

Example 9.1 (Exact algorithm) Given a matrix $A \in \mathbb{R}^{2 \times 2}$ with $\det(A) \neq 0$ we want to compute its inverse. We consider two instances of this problem. We measure distances by the Euclidean norm.

1. First, let $A = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$. We consider this matrix to be the true input data without errors. A small measurement error gives the new input data $\tilde{A} = \begin{pmatrix} 1 & 1 \\ -1+\varepsilon & 1 \end{pmatrix}$, where $0 < \varepsilon \ll 1$. The *exact* solutions A^{-1} and \tilde{A}^{-1} are then

$$A^{-1} = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \quad \text{and} \quad \tilde{A}^{-1} = \frac{1}{2-\varepsilon} \begin{pmatrix} 1 & -1 \\ 1-\varepsilon & 1 \end{pmatrix} = A^{-1} + \frac{\varepsilon}{2(2-\varepsilon)} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

Comparing the errors we find $\|A^{-1} - \tilde{A}^{-1}\| \approx \|A - \tilde{A}\|$; i.e., the error in the input $\|A - \tilde{A}\|$ is the error in the output $\|A^{-1} - \tilde{A}^{-1}\|$ are roughly the same.

2. The true input in the second example is the matrix $B = \begin{pmatrix} 1 & 1 \\ 1 & 1+\delta \end{pmatrix}$, where $|\delta| \neq 0$ is small, and we consider as perturbed input $\tilde{B} = \begin{pmatrix} 1 & 1 \\ 1+\varepsilon & 1+\delta \end{pmatrix}$. Their matrix inverses are

$$B^{-1} = \frac{1}{\delta} \begin{pmatrix} 1+\delta & -1 \\ -1 & 1 \end{pmatrix} \quad \text{and} \quad \tilde{B}^{-1} = \frac{1}{\delta-\varepsilon} \begin{pmatrix} 1+\delta & -1 \\ -1-\varepsilon & 1 \end{pmatrix} = B^{-1} + \frac{\varepsilon}{\delta(\varepsilon-\delta)} \begin{pmatrix} 1+\delta & -1 \\ -(1+\delta) & 1 \end{pmatrix}.$$

This implies $\|B^{-1} - \tilde{B}^{-1}\| \approx \frac{1}{\delta(\varepsilon-\delta)} \cdot \|B - \tilde{B}\|$. If $\varepsilon < \delta$, then we have an amplification of the error by a factor of roughly δ^{-2} , which is large.

Even though we applied an exact algorithm to the problem we got different quantities in the output. In the first example, the output for the perturbed data \tilde{A}^{-1} was close the true output A^{-1} , while in the second example \tilde{B}^{-1} was far from B^{-1} . \diamond

The previous example shows that, even if we can compute the *exact* solution of a problem, small errors in the data may be amplified tremendously in the output. The theory of *condition numbers* helps us to understand when and why this happens. In simple terms, a condition number is a quantity associated to a *computational problem*, and it measures the sensitivity of the output to small errors in the input data.

Definition 9.2 A *computational problem* is a function $f : X \rightarrow Y$ from a space of inputs X to a space of outputs Y .

Example 9.3 In Example 9.1 the input space is $X = \{A \in \mathbb{R}^{2 \times 2} \mid \det(A) \neq 0\}$, the output space is $Y = X$, and $f(A) = A^{-1}$. \diamond

The following definition is due to Rice [128].

Definition 9.4 Let (X, d_X) and (Y, d_Y) be metric spaces. The (absolute) condition number of f at the input datum $\mathbf{x} \in X$ is

$$\kappa[f](\mathbf{x}) := \lim_{\varepsilon \rightarrow 0} \sup_{\mathbf{y} \in X: d_X(\mathbf{x}, \mathbf{y}) \leq \varepsilon} \frac{d_Y(f(\mathbf{x}), f(\mathbf{y}))}{d_X(\mathbf{x}, \mathbf{y})}.$$

The motivation for the definition of a condition number is that for small $d_X(\mathbf{x}, \mathbf{y})$ we have

$$d_Y(f(\mathbf{x}), f(\mathbf{y})) \leq \kappa[f](\mathbf{x}) \cdot d_X(\mathbf{x}, \mathbf{y}) + o(d_X(\mathbf{x}, \mathbf{y})).$$

In other words, a small error $\varepsilon = d_X(\mathbf{x}, \mathbf{y})$ in the input data causes an error of roughly $\kappa[f](\mathbf{x}) \cdot \varepsilon$ in the output data – regardless of the algorithm used to compute $f(\mathbf{x})$!

Remark 9.5 Suppose that $X = \mathbb{R}^n$ and $Y = \mathbb{R}^m$ are Euclidean spaces. What does “small error” mean in this case? If $\|\mathbf{x}\| = 10^4$, is an error of size $\|\mathbf{x} - \mathbf{y}\| = 10^2$ small or large? This ambiguity motivates the definition of *relative error* $\text{RelError}(\mathbf{x}, \mathbf{y}) = \frac{\|\mathbf{x} - \mathbf{y}\|_1}{\|\mathbf{x}\|_2}$ in numerical analysis, where $\|\cdot\|_1$, $\|\cdot\|_2$ are two norms (not necessarily equal). The relative condition number is then

$$\kappa_{\text{REL}}[f](\mathbf{x}) := \lim_{\varepsilon \rightarrow 0} \sup_{\text{RelError}(\mathbf{x}, \mathbf{y}) \leq \varepsilon} \frac{\text{RelError}(f(\mathbf{x}), f(\mathbf{y}))}{\text{RelError}(\mathbf{x}, \mathbf{y})} = \kappa[f](\mathbf{x}) \cdot \frac{\|\mathbf{x}\|_2}{\|f(\mathbf{x})\|_2}.$$

In fact, relative errors are more significant in numerical analysis, because *floating point* arithmetic introduces relative errors (see, e.g., [149, p. 91] or [74]) and modern architecture is optimized for computing with floating point numbers. Recall that a floating point number system $\mathcal{F} \subseteq \mathbb{R}$ is defined by four integers $\beta, t, e_{\min}, e_{\max}$, where $s\beta$ is called *base*, t is called *precision*, and $[e_{\min}, e_{\max}]$ is called exponential range. Then, $\mathcal{F} = \{\pm \beta^e \sum_{i=1}^t \frac{d_i}{\beta^i} \mid 0 \leq d_i \leq \beta - 1, e_{\min} \leq e \leq e_{\max}\}$. The number $u = \frac{1}{2}\beta^{1-t}$ is called *relative precision*. The key property of such a floating point number system is that the rounding function $\text{fl} : \mathbb{R} \rightarrow \mathcal{F}, x \mapsto \operatorname{argmin}_{y \in \mathcal{F}} |x - y|$ satisfies $\text{fl}(x) = x(1 + \delta) \in \mathcal{F}$ for all $x \in \mathcal{G}$, where $|\delta| \leq u$ and $\mathcal{G} := \{x \in \mathbb{R} \mid \beta^{e_{\min}-1} \leq |x| \leq \beta^{e_{\max}}(1 - \beta^{-1})\} \supseteq \mathcal{F}$ is the *range* of \mathcal{F} . In other words, every number in \mathcal{G} can be approximated by an element of \mathcal{F} with relative precision u :

$$\text{RelError}(x, \text{fl}(x)) = \|\delta\| \leq u \quad \text{for all } x \in \mathcal{G}.$$

The IEEE 754 standard defines a floating point arithmetic system with

	β	t	e_{\min}	e_{\max}	u
half (16 bit)	2	11	-14	$16 = 2^4$	$\approx 5 \cdot 10^{-4}$
single (32 bit)	2	24	-125	$128 = 2^7$	$\approx 6 \cdot 10^{-8}$
double (64 bit)	2	53	-1021	$1024 = 2^{10}$	$\approx 10^{-16}$

and operations $\text{fl}(x \circ y) = (x \circ y)(1 + \delta)$, $|\delta| \leq u$ where $\circ \in \{e+, -, \times, /, \sqrt{\cdot}\}$. For instance, 64-bit floating point number system can approximate any real number within its range with a relative error of at most $u \approx 10^{-16}$.

The following theorem is also due to Rice [128].

Theorem 9.6 *If X and Y are Riemannian manifolds and $f : X \rightarrow Y$ is differentiable, then for $\mathbf{x} \in X$:*

$$\kappa[f](\mathbf{x}) = \max_{\mathbf{v} \in T_{\mathbf{x}}X: \|\mathbf{v}\|=1} \|D_{\mathbf{x}}f(\mathbf{v})\|.$$

Inspired by this theorem we define the *operator norm* of a matrix $A \in \mathbb{R}^{m \times n}$ by

$$\|A\|_{\text{op}} := \max_{\|\mathbf{x}\|=1} \|\mathbf{Ax}\|.$$

The usual Euclidean norm, on the other hand, is given by $\|A\|^2 = \sum_{i,j} a_{ij}^2 = \text{Trace}(AA^T)$. If U and V are orthogonal matrices, we have $\|UAV^T\|_{\text{op}} = \|A\|_{\text{op}}$ and $\|UAV^T\| = \|A\|$. This property is called *orthogonal invariance*. Suppose $n \leq m$. Let $A = U\Sigma V^T$ be the singular value decomposition of A , where $U \in \mathbb{R}^{m \times m}$ and $V \in \mathbb{R}^{n \times n}$ are orthogonal matrices and $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_n)$ with $\sigma \geq \dots \geq \sigma_n \geq 0$ is the $m \times n$ diagonal matrix of singular values. Orthogonal invariance implies $\|A\|_{\text{op}} = \sigma_1$ and $\|A\| = \sqrt{\sigma_1^2 + \dots + \sigma_n^2}$. If $n = m$ and $\sigma_1 \neq 0$, we have $A^{-1} = V\Sigma^{-1}U^T$ and so $\|A^{-1}\|_{\text{op}} = \sigma_1^{-1}$.

9.2 Matrix Inversion

We study the condition number of the problem of matrix inversion. This corresponds to the map

$$\text{inv} : \mathcal{D} \rightarrow \mathcal{D}, A \mapsto A^{-1},$$

where $\mathcal{D} = \{A \in \mathbb{R}^{n \times n} \mid \det(A) \neq 0\}$. The main goal of this section is to prove the following characterization of the condition number of matrix inversion.

Theorem 9.7 *The condition number of matrix inversion at $A \in \mathcal{D}$ is*

$$\kappa[\text{inv}](A) = \|A^{-1}\|_{\text{op}}^2.$$

In particular, if $\sigma_n > 0$ is the smallest singular value of A we have $\kappa[\text{inv}](A) = \sigma_n^{-2}$.

Before we prove this theorem, let us briefly bring it in context with Remark 9.5. In numerical analysis, a popular choice for measuring the relative error is using the operator norm. In this case, by Theorem 9.7 the relative condition number can be expressed as the ratio of the largest and smallest singular value of A

$$\kappa_{\text{REL}}[\text{inv}](A) = \kappa[\text{inv}](A) \cdot \frac{\|A\|_{\text{op}}}{\|A^{-1}\|_{\text{op}}} = \frac{\sigma_1}{\sigma_n}$$

This formulation of the condition number is known as *Turing's condition number* and goes back to the work of Turing [150].

Proof (of Theorem 9.7) Let $\text{adj}(A)$ denote the adjoint matrix of A . Since $\text{inv}(A) = A^{-1} = \frac{1}{\det(A)} \cdot \text{adj}(A)$, the map inv is a rational polynomial function on \mathcal{D} . This implies inv is differentiable on \mathcal{D} . By Theorem 9.6 the condition number is $\kappa[\text{inv}](A) = \|D_A \text{inv}\|_{\text{op}}$. We compute the derivative of inv . Taking the derivative of $AB = 1_n$ we have $\dot{A}B + A\dot{B} = 0$ and knowing that $B = A^{-1}$ we obtain $\dot{B} = -A^{-1}\dot{A}A^{-1}$. For a tangent vector $\dot{A} = R \in \mathbb{R}^{n \times n}$ we therefore have

$$D_A \text{inv}(R) = A^{-1}RA^{-1}.$$

Let $A = U\Sigma V^T$ be the singular value decomposition of A . Then, $A^{-1} = V\Sigma^{-1}U^T$ and by orthogonal invariance of the Euclidean norm we have

$$\max_{\|R\|=1} \|A^{-1}RA^{-1}\|^2 = \max_{\|\dot{A}\|=1} \|\Sigma^{-1}R\Sigma^{-1}\|^2 = \max_{\sum_{i,j} r_{i,j}^2=1} \sum_{i,j} \frac{r_{i,j}^2}{\sigma_i^2 \sigma_j^2}.$$

The last expression is maximized for $r_{n,n} = 1$. We get $\kappa[\text{inv}](A) = \frac{1}{\sigma_n^2} = \|A^{-1}\|_{\text{op}}^2$. \square

Example 9.8 Let us come back to Example 9.1. The two matrices were $A = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$ and $B = \begin{pmatrix} 1 & 1 \\ 1 & 1+\delta \end{pmatrix}$. For the purpose of being concrete let us consider $\delta = 10^{-8}$. Since $A^T A = 2 \cdot 1_2$, we have $\|A^{-1}\mathbf{x}\| = \frac{1}{2}\|\mathbf{x}\|$ for all $\mathbf{x} \in \mathbb{R}^2$. By Theorem 9.7,

$$\kappa[\text{inv}](A) = \|A^{-1}\|_{\text{op}}^2 = \frac{1}{4}.$$

On the other hand, and $\|B^{-1}\|_{\text{op}} \geq \|B^{-1}\mathbf{e}_1\| \geq 10^8$, so that

$$\kappa[\text{inv}](B) = \|B^{-1}\|_{\text{op}}^2 \geq 10^{16}.$$

This explains the different behaviors of the outputs with respect to errors in the input in Example 9.1. \diamond

The Eckhart-Young Theorem (Theorem 2.6) yields another metric interpretation of Turing's condition number $\kappa[\text{inv}](A)$ from Theorem 9.7. Let σ_n be the smallest singular value of A . By the Eckhart-Young Theorem, σ_n is also the Euclidean distance of A to the variety of singular matrices. Let us denote this variety by $\Sigma := \{A \in \mathbb{R}^{n \times n} \mid \det(A) = 0\}$. Then, what we have just observed is

$$\kappa[\text{inv}](A) = \frac{1}{\text{dist}(A, \Sigma)^2} \quad \text{and} \quad \kappa_{\text{REL}}[\text{inv}](A) = \frac{\|A\|_{\text{op}}}{\text{dist}(A, \Sigma)}; \quad (9.1)$$

i.e., Turing's condition number of the matrix A is the inverse distance (squared) to the variety of singular matrices, also called *ill-posed inputs*. Such a relation is called a *condition number theorem* in the literature. Condition number theorems are a central theme in numerical analysis and give us the metric geometric interpretation that the numerical difficulty of an input to a problem is directly related to the distance of this input to the locus of ill-posed inputs. Condition number theorems were, for instance, also derived for computing zeros of polynomials [79] or computing eigenvalues of matrices [151]. See also [47].

Example 9.9 Consider the determinant hypersurface for 2×2 -matrices $\Sigma = V(\det) \subset \mathbb{R}^{2 \times 2}$. Following the discussion above, the Zariski closure of those matrices $A \in \mathbb{R}^{2 \times 2}$, for which $\kappa[\text{inv}](A) = \varepsilon^{-1}$, is given by the offset hypersurface of Σ at level $\sqrt{\varepsilon}$. We can compute the offset hypersurface as in Example 7.8. In this example let us instead consider the surface defined by $\kappa_{\text{REL}}[\text{inv}](A) = \varepsilon^{-1}$ for $\varepsilon > 0$. To make the formula in (9.1) algebraic, we replace $\|A\|_{\text{op}}$ by $\|A\|$. We proceed as in Section 7.2 to compute a polynomial equation for $\text{dist}(A, \Sigma) = \varepsilon \cdot \|A\|$ in terms of A and ε , but for $B \in \Sigma$ we replace the affine sphere $\|A - B\| = \varepsilon$ by the homogeneous sphere $\|A - B\| = \varepsilon \cdot \|A\|$. We use Macaulay2 [67]:

```
R = QQ[a_0..a_3, b_0..b_3, eps];
f = b_0*b_3 - b_1*b_2;
normAsq = a_0^2 + a_1^2 + a_2^2 + a_3^2;
d = (a_0-b_0)^2 + (a_1-b_1)^2 + (a_2-b_2)^2 + (a_3-b_3)^2 - eps^2 * normAsq;
J1 = {diff(b_0, f), diff(b_1, f), diff(b_2, f), diff(b_3, f)};
J2 = {diff(b_0, d), diff(b_1, d), diff(b_2, d), diff(b_3, d)};
J = matrix {J1, J2};
OC = ideal {f, minors(2, J), d};
O = eliminate(OC, {b_0, b_1, b_2, b_3});
g = (gens O)_0_0
```

The result is the polynomial $g(\mathbf{a}, \varepsilon) = (a_0^2 + a_1^2 + a_2^2 + a_3^2)^2 \cdot (g_0(\mathbf{a}) + g_1(\mathbf{a})\varepsilon^2 + g_2(\mathbf{a})\varepsilon^4 + g_3(\mathbf{a})\varepsilon^6 + g_4(\mathbf{a})\varepsilon^8)$, where the coefficients of the second factor are

$$\begin{aligned} g_4(\mathbf{a}) &= (a_0^2 + a_1^2 + a_2^2 + a_3^2)^2 \\ g_3(\mathbf{a}) &= -3(a_0^2 + a_1^2 + a_2^2 + a_3^2)^2 \\ g_2(\mathbf{a}) &= 3a_0^4 + 6a_0^2a_1^2 + 3a_1^4 + 6a_0^2a_2^2 + 7a_1^2a_2^2 + 3a_2^4 - 2a_0a_1a_2a_3 + 7a_0^2a_3^2 + 6a_1^2a_3^2 + 6a_2^2a_3^2 + 3a_3^4 \\ g_1(\mathbf{a}) &= -(a_0^4 + 2a_0^2a_1^2 + a_1^4 + 2a_0^2a_2^2 + 4a_1^2a_2^2 + a_2^4 - 4a_0a_1a_2a_3 + 4a_0^2a_3^2 + 2a_1^2a_3^2 + 2a_2^2a_3^2 + a_3^4) \\ g_0(\mathbf{a}) &= (a_1a_2 - a_0a_3)^2. \end{aligned}$$

Figure 9.1 shows the zero set of $g(\mathbf{a}, \varepsilon)$ at level $\varepsilon = 0.5$ in the affine patch $a_0 = 1$. We remark that, if $\text{dist}(A, \Sigma) = \varepsilon \cdot \|A\|$, then $\varepsilon = \sin \alpha$, where α is the minimal angle between the line $\mathbb{R} \cdot A$ and a line $\mathbb{R} \cdot B$ with $B \in \Sigma$. In this case, ε^{-1} is also called a *conic condition number* (see [29, Chapters 20 & 21]). \diamond

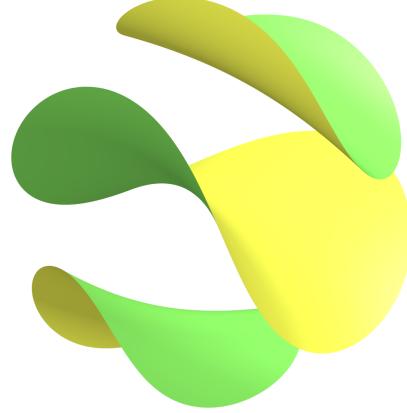


Fig. 9.1: The picture shows the determinantal hypersurface $\Sigma = \{\det(A) = 0\} \subset \mathbb{R}^{2 \times 2}$ (the surface in the middle) together with the hypersurface defined by $\text{dist}(A, \Sigma) = \varepsilon \cdot \|A\|$ with $\varepsilon = 0.5$ (the union of the two surfaces on the outside) in the affine patch where the upper left entry of A is fixed to be one. The image was created using [Surfer](#).

9.3 Proof of the Eckart-Young Theorem

The goal of this section is now to give a short proof of the Eckart-Young theorem. For this we return now to rectangular matrices and denote by $X_r := \{A \in \mathbb{R}^{m \times n} \mid \text{rank}(A) \leq r\}$ the variety of real matrices of rank at most r . We first compute the normal space of X_r at a smooth point.

Lemma 9.10 *Let $A \in X_r$ be a smooth point (i.e., $\text{rank}(A) = r$). Suppose that $A = RS^T$, where $R \in \mathbb{R}^{m \times r}$ and $S \in \mathbb{R}^{n \times r}$ have rank r . Then*

$$N_A X_r = \text{span} \{ \mathbf{u}\mathbf{v}^T \mid \mathbf{u}^T R = 0 \text{ and } S^T \mathbf{v} = 0 \}.$$

Proof Let $R(t) \in \mathbb{R}^{m \times r}$ and $S(t) \in \mathbb{R}^{n \times r}$ be smooth curves with $R(0) = R$ and $S(0) = S$. Then, $\gamma(t) := R(t)S(t)^T$ is a smooth curve with $\gamma(0) = A$. The product rule gives

$$\frac{\partial}{\partial t} \gamma(t) \Big|_{t=0} = R \left(\frac{\partial}{\partial t} S(t) \Big|_{t=0} \right)^T + \left(\frac{\partial}{\partial t} R(t) \Big|_{t=0} \right) S^T. \quad (9.2)$$

Let $\mathcal{V} := \{RP^T \mid P \in \mathbb{R}^{n \times r}\}$ and $\mathcal{W} := \{QS^T \mid Q \in \mathbb{R}^{m \times r}\}$. Then, $T_A X_r = \mathcal{V} + \mathcal{W}$ by (9.2). On the other hand, \mathcal{V} consists of all those matrices $L \in \mathbb{R}^{m \times n}$ such that $\mathbf{u}^T L \mathbf{x} = 0$ for all \mathbf{u} with $\mathbf{u}^T R = 0$ and $\mathbf{x} \in \mathbb{R}^n$ arbitrary. Since $\mathbf{u}^T L \mathbf{x} = \text{Trace}(L^T \mathbf{u} \mathbf{x}^T)$, this shows that the normal space of \mathcal{V} is spanned by matrices of the form $\mathbf{u} \mathbf{x}^T$. Similarly, the normal space of \mathcal{W} is spanned by $\mathbf{y} \mathbf{v}^T$, where $S^T \mathbf{v} = 0$ and $\mathbf{y} \in \mathbb{R}^m$ arbitrary. Therefore, the normal space of $T_A X_r = \mathcal{V} + \mathcal{W}$ is spanned by all $\mathbf{u} \mathbf{v}^T$ with \mathbf{u} and \mathbf{v} as above. \square

Corollary 9.11 $\dim X_r = nm - (m-r)(n-r) = r(m+n-r)$.

We use Lemma 9.10 to prove the Eckart-Young Theorem.

Proof (of Theorem 2.6) Let $B \in X_r$ be a matrix of rank r and $B = U\Sigma V^T$ be a singular value decomposition of B , where $U \in \mathbb{R}^{m \times r}$, $V \in \mathbb{R}^{r \times n}$ are matrices with orthonormal columns and $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_r)$ with $\sigma_1, \dots, \sigma_r > 0$ (not necessarily ordered). We prove Theorem 2.6 by showing that the singular value decomposition of all matrices $A \in \mathbb{R}^{m \times n}$, such that B is an ED-critical point for A , is of the form $A = [U' U'] \begin{pmatrix} \Sigma & 0 \\ 0 & \Sigma' \end{pmatrix} [V' V']^T$, where $\Sigma' = \text{diag}(\sigma_{r+1}, \dots, \sigma_n)$.

By orthogonal invariance, we can assume that $B = \begin{pmatrix} \Sigma & 0 \\ 0 & 0 \end{pmatrix}$. Let $A \in B + N_B X_r$ be a matrix in the normal space of B . By Lemma 9.10, we have $A = B + \sum_{i=r+1}^m \sum_{j=r+1}^n a_{i,j} \mathbf{e}_i \mathbf{e}_j^T$ for some coefficients $a_{i,j} \in \mathbb{R}$; i.e.,

$$A = \begin{pmatrix} \Sigma & 0 \\ 0 & A' \end{pmatrix}, \quad \text{where } A' = (a_{i,j}) \in \mathbb{R}^{(m-r) \times (n-r)}.$$

Let now $A' = U' \Sigma' V'$ be the singular value decomposition of A' . Then,

$$A = [1_r \ U'] \begin{pmatrix} \Sigma & 0 \\ 0 & \Sigma' \end{pmatrix} [1_r \ V']^T. \quad (9.3)$$

Since the singular value decomposition of a matrix is unique up to ordering the singular values, (9.3) must be the singular value decomposition of A . \square

Remark 9.12 The proof of the Eckart-Young theorem also implies that the rank- r matrix that minimizes the distance to a symmetric matrix is also symmetric.

9.4 Distance to the Polynomial Discriminant

Let \mathcal{H}_d be the vector space of homogeneous polynomials in $n+1$ many variables $\mathbf{x} = (x_0, \dots, x_n)$ of degree d . For $m \leq n$ and a tuple $\mathbf{d} = (d_1, \dots, d_m)$ we write $\mathcal{H}_{\mathbf{d}} := \mathcal{H}_{d_1} \times \dots \times \mathcal{H}_{d_m}$.

The goal of this section is to use the Eckart-Young theorem for computing the distance of a polynomial system $F \in \mathcal{H}_{\mathbf{d}}$ to the real polynomial discriminant

$$\Omega := \{F \in \mathcal{H}_{\mathbf{d}} \mid \text{there is } \mathbf{x} \in \mathbb{P}_{\mathbb{R}}^n \text{ s.t. } F(\mathbf{x}) = 0 \text{ and } \text{rank } JF(\mathbf{x}) < m\}, \quad (9.4)$$

where $JF(\mathbf{x}) = \left(\frac{\partial f_i}{\partial x_j}(\mathbf{x}) \right) \in \mathbb{R}^{m \times (n+1)}$ is the Jacobian matrix of F at \mathbf{x} . For this, we first need to introduce a distance on \mathcal{H}_d . We use the so-called *Bombieri-Weyl distance*.

Write $I := \{\alpha \in \mathbb{N}^{n+1} \mid \alpha_0 + \dots + \alpha_n = d\}$. The *Bombieri-Weyl inner product* between two polynomials $f = \sum_{\alpha \in I} f_{\alpha} \mathbf{x}^{\alpha} \in \mathcal{H}_d$ and $g = \sum_{\alpha \in I} g_{\alpha} \mathbf{x}^{\alpha} \in \mathcal{H}_d$ is defined by

$$\langle f, g \rangle_{\text{BW}} := \sum_{\alpha \in I} \frac{\alpha_0! \cdots \alpha_n!}{d!} f_{\alpha} \cdot g_{\alpha}.$$

Notice that for $d = 1$ this is the usual Euclidean inner product in \mathbb{R}^{n+1} . The motivation for the multinomial coefficients in the definition of $\langle \cdot, \cdot \rangle_{\text{BW}}$ is that the Bombieri-Weyl inner product – like the Euclidean inner product in \mathbb{R}^{n+1} – is invariant under orthogonal change of variables. More specifically, if $U \in O(n+1)$ is an orthogonal matrix, then

$$\langle f \circ U, g \circ U \rangle_{\text{BW}} = \langle f, g \rangle_{\text{BW}}.$$

As before, we call this property *orthogonal invariance*. Kostlan [95, 96] classified all orthogonally invariant inner products on \mathcal{H}_d and he showed that the Bombieri-Weyl inner product is the unique orthogonally invariant inner product (up to scaling) such that monomials are pairwise orthogonal.

The Bombieri-Weyl inner product extends to $\mathcal{H}_{\mathbf{d}}$. For $F = (f_1, \dots, f_m)$ and $G = (g_1, \dots, g_m)$ we have

$$\langle F, G \rangle_{\text{BW}} := \langle f_1, g_1 \rangle_{\text{BW}} + \dots + \langle f_m, g_m \rangle_{\text{BW}}.$$

The Bombieri-Weyl norm is $\|F\|_{\text{BW}} := \sqrt{\langle F, F \rangle_{\text{BW}}}$ and the distance corresponding to this norm is given by $\text{dist}_{\text{BW}}(F, G) := \|F - G\|_{\text{BW}}$ for $F, G \in \mathcal{H}_{\mathbf{d}}$.

Example 9.13 Let $n = 1, d = 2$. Consider two quadrics in two variables $f(x_0, x_1) = ax_0^2 + bx_0x_1 + cx_1^2$ and $g(x_0, x_1) = \alpha x_0^2 + \beta x_0x_1 + \gamma x_1^2$. The inner product between them is

$$\langle f, g \rangle_{\text{BW}} = \frac{2! \cdot 0!}{2!} a\alpha + \frac{1! \cdot 1!}{2!} b\beta + \frac{2! \cdot 0!}{2!} c\gamma = a\alpha + \frac{1}{2} b\beta + c\gamma.$$

We can also write $f(\mathbf{x}) = \mathbf{x}^T A \mathbf{x}$ and $g(\mathbf{x}) = \mathbf{x}^T B \mathbf{x}$, where $\mathbf{x} = (x_0, x_1)^T$, with

$$A = \begin{pmatrix} a & b/2 \\ b/2 & c \end{pmatrix}, \quad B = \begin{pmatrix} \alpha & \beta/2 \\ \beta/2 & \gamma \end{pmatrix}.$$

Then, $\langle f, g \rangle_{\text{BW}} = a\alpha + \frac{1}{2} b\beta + c\gamma = \text{Trace}(A^T B)$. The same holds true for quadrics in more than 2 variables, so the Bombieri-Weyl products for quadrics is the usual Euclidean inner products for matrices. In this sense, the Bombieri-Weyl product is a generation of the Euclidean inner product for symmetric matrices to homogeneous polynomials of any degree. \diamond

The next theorem was proved by Rafalli [127] for the case $m = 1$. The book by Bürgisser and Cucker [29] covers the case $m = n$.

Theorem 9.14 Let $m \leq n$ and $\mathbf{d} = (d_1, \dots, d_m)$ be a tuple of degrees. Let $F \in \mathcal{H}_{\mathbf{d}}$. Then,

$$\text{dist}_{\text{BW}}(F, \Omega) = \min_{\mathbf{x} \in \mathbb{S}^n} \sqrt{\|F(\mathbf{x})\|^2 + \sigma_m(D^{-1/2} JF(\mathbf{x}) P_{\mathbf{x}})^2},$$

where $D = \text{diag}(d_1, \dots, d_m)$ and $P_{\mathbf{x}} := \mathbf{1}_{n+1} - \mathbf{x}\mathbf{x}^T$ is the projection onto the tangent space $T_{\mathbf{x}}\mathbb{S}^n$.

Proof Since we are considering homogeneous polynomials, we can replace real projective space $\mathbb{P}_{\mathbb{R}}^n$ by the sphere \mathbb{S}^n in the definition of Ω from (9.4). Let $\Omega(\mathbf{x}) := \{F \in \mathcal{H}_{\mathbf{d}} \mid F(\mathbf{x}) = 0 \text{ and } \text{rank } JF(\mathbf{x}) < m\}$ for $\mathbf{x} \in \mathbb{S}^n$. By definition, we have $\Omega = \bigcup_{\mathbf{x} \in \mathbb{S}^n} \Omega(\mathbf{x})$, so that

$$\text{dist}_{\text{BW}}(F, \Omega) = \min_{\mathbf{x} \in \mathbb{S}^n} \text{dist}_{\text{BW}}(F, \Omega(\mathbf{x})) \tag{9.5}$$

(the minimum is obtained, because \mathbb{S}^n is compact). Fix $\mathbf{x} \in \mathbb{S}^n$, let $U \in O(n+1)$ be an orthogonal matrix with $U\mathbf{e}_1 = \mathbf{x}$ and denote $F_0 := F \circ U$. By orthogonal invariance we have

$$\text{dist}_{\text{BW}}(F, \Omega(\mathbf{x})) = \text{dist}_{\text{BW}}(F_0, \Omega(\mathbf{e}_1)),$$

We compute the latter. For this let us write

$$F_0(\mathbf{x}) = x_0^d \cdot a + x_0^{d-1} \cdot A (x_1, \dots, x_n)^T + h(\mathbf{x}),$$

where $a \in \mathbb{R}^m$, $A \in \mathbb{R}^{m \times n}$ and h involves only powers of x_0 of degree less than $d-1$. Then,

$$a = F_0(\mathbf{e}_1) = F(\mathbf{x}) \quad \text{and} \quad A = JF_0(\mathbf{e}_1) P_{\mathbf{e}_1} = JF(\mathbf{x}) P_{\mathbf{x}} U^T.$$

Recall that $G = (g_1, \dots, g_m) \in \Omega(\mathbf{e}_1)$, if and only if $G(\mathbf{e}_1) = 0$ and the Jacobian $JG(\mathbf{x})$ has rank at most $m-1$. This means that the distance from $\Omega(\mathbf{e}_1)$ to F_0 is minimized at a polynomial of the form $G_0(\mathbf{x}) = x_0^{d-1} \cdot B (x_1, \dots, x_n)^T \in \Omega(\mathbf{e}_1)$, where B has rank at most $m-1$. We have

$$\|F_0 - G_0\|_{\text{BW}}^2 = \|a\|^2 + \|D^{-1/2} (A - B)\|^2.$$

The Eckhart-Young theorem implies that the distance of $D^{-1}A$ to the variety of matrices of rank at most $m-1$ is precisely $\sigma_m(D^{-1/2}A)$. Since the singular values of a matrix are invariant under multiplication

with orthogonal matrices, we have $\sigma_m(D^{-1/2}A) = \sigma_m(D^{-1/2}JF(\mathbf{x})P_{\mathbf{x}})$. Consequently,

$$\text{dist}_{\text{BW}}(F, \Omega(\mathbf{x})) = \sqrt{\|a\|^2 + \sigma_m(D^{-1}A)^2} = \sqrt{\|F(\mathbf{x})\|^2 + \sigma_m(D^{-1/2}JF(\mathbf{x})P_{\mathbf{x}})^2}.$$

Combining this with (9.5) proves the statement. \square

Remark 9.15 The statement of Theorem 9.14 can be generalized as follows. Fix $1 \leq k < m$. The distance of $F \in \mathcal{H}_{\mathbf{d}}$ to the space of systems of polynomials $F \in \mathcal{H}_{\mathbf{d}}$, such that there exists $\mathbf{x} \in \mathbb{P}_{\mathbb{R}}^n$ with $F(\mathbf{x}) = 0$ and $\text{rank } JF(\mathbf{x}) < k$ is given by

$$\min_{\mathbf{x} \in \mathbb{S}^n} \sqrt{\|F(\mathbf{x})\|^2 + \sum_{i=k+1}^m \sigma_i(D^{-1}JF(\mathbf{x})P_{\mathbf{x}})^2},$$

where $\sigma_{k+1}(\cdot), \dots, \sigma_m(\cdot)$ denote the $m - k$ smallest singular values. This is because the distance of a matrix $A \in \mathbb{R}^{m \times n}$ to the nearest matrix of rank at most $k - 1$ is $\sqrt{\sum_{i=k+1}^m \sigma_i(A)^2}$ by the Eckart-Young theorem.

Remark 9.16 In the case $m = 1$, where we have only one polynomial $f \in \mathcal{H}_{\mathbf{d}}$, Theorem 9.14 yields $\text{dist}_{\text{BW}}(f, \Omega) = \min_{\mathbf{x} \in \mathbb{S}^n} \sqrt{f(\mathbf{x})^2 + \frac{1}{d} \|P_{\mathbf{x}} \nabla f(\mathbf{x})\|^2}$, where $\nabla f(\mathbf{x}) = (\frac{\partial f}{\partial x_1}(\mathbf{x}), \dots, \frac{\partial f}{\partial x_n}(\mathbf{x}))^T$ is the gradient of f at \mathbf{x} (the gradient is a column vector, so we have to multiply it by $P_{\mathbf{x}}$ from the left). By Euler's formula for homogeneous functions, $\mathbf{x}^T \nabla f(\mathbf{x}) = d \cdot f(\mathbf{x})$, so $P_{\mathbf{x}} \nabla f(\mathbf{x}) = \nabla f(\mathbf{x}) - (d \cdot f(\mathbf{x})) \mathbf{x}$. We get

$$\text{dist}_{\text{BW}}(f, \Omega) = \min_{\mathbf{x} \in \mathbb{S}^n} \sqrt{f(\mathbf{x})^2 + \frac{1}{d} \|\nabla f(\mathbf{x}) - (d \cdot f(\mathbf{x})) \mathbf{x}\|^2}. \quad (9.6)$$

Example 9.17 We use the formula (9.6) for computing the distance of the Fermat cubic $f(\mathbf{x}) = x_0^3 + x_1^3 + x_2^3$ to the real polynomial discriminant Ω . Let $h(\mathbf{x}) = (x_0^3 + x_1^3 + x_2^3)^2 + 3 \sum_{i=0}^2 (x_i^2 - (x_0^3 + x_1^3 + x_2^3) x_i)^2$. Then $\text{dist}_{\text{BW}}(f, \Omega) = \min_{\mathbf{x} \in \mathbb{S}^n} \sqrt{h(\mathbf{x})}$. The polynomial function $h : \mathbb{S}^2 \rightarrow \mathbb{R}$ is minimized at the point $\mathbf{x}_0 = \frac{1}{\sqrt{3}}(1, 1, 1)$, which gives

$$\text{dist}_{\text{BW}}(f, \Omega) = \sqrt{h(\mathbf{x}_0)} = \frac{1}{\sqrt{3}}.$$

The norm of the Fermat Cubic is also $\|f\|_{\text{BW}} = \sqrt{3}$. Since Ω is a cone, the minimal angle (measured in the Bombieri-Weyl metric) between f and a polynomial in Ω therefore is $\arcsin(1) = \frac{\pi}{2}$. \diamond

We interpret Theorem 9.14 from the perspective of condition numbers. Consider the problem of computing the regular zeros of a square system of polynomial equations $F \in \mathcal{H}_{\mathbf{d}}$, where $\mathbf{d} = (d_1, \dots, d_n)$, in $n + 1$ variables $\mathbf{x} = (x_1, \dots, x_n)$. We can compute the zeros in projective space $\mathbb{P}_{\mathbb{R}}^n$ or in the sphere \mathbb{S}^n . We use the metric structure of the latter to establish a condition number for this problem.

Suppose that $\mathbf{x} \in \mathbb{S}^n$ is a regular zero of $F \in \mathcal{H}_{\mathbf{d}}$. The implicit function theorem implies that there exists a neighborhood $\mathcal{U} \subset \mathcal{H}_{\mathbf{d}}$ of F and a smooth map $s : \mathcal{U} \rightarrow \mathbb{S}^n$ such that $F(s(F)) = 0$ for all $F \in \mathcal{U}$. One can show that the operator norm of $D_F s$ is the operator norm of $(JF(\mathbf{x})P_{\mathbf{x}})^{-1}$. By Rice's theorem (Theorem 9.6), the condition number of solving $F(\mathbf{x}) = 0$ therefore is

$$\kappa[s](F) = \|JF(\mathbf{x})^{-1}\|_{\text{op}} = \frac{1}{\sigma_n(JF(\mathbf{x})P_{\mathbf{x}})}.$$

By contrast, in the proof of Theorem 9.14 we have shown that $\sigma_n(D^{-1/2}JF(\mathbf{x})P_{\mathbf{x}}) = \text{dist}_{\text{BW}}(f, \Omega(\mathbf{x}))$. This means that for the problem of solving systems of polynomial equations we have an “almost” condition number theorem (up to the additional factor $D^{-1/2}$).

Chapter 10

Machine Learning

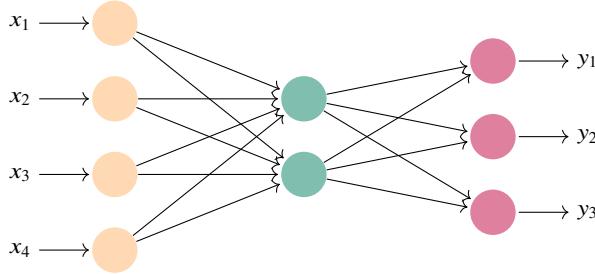


Fig. 10.1: A fully-connected feedforward neural network with two layers $f_{1,\theta} : \mathbb{R}^4 \rightarrow \mathbb{R}^2$ and $f_{2,\theta} : \mathbb{R}^2 \rightarrow \mathbb{R}^3$.

A *feedforward neural network* is a family of functions that is parametrized by the network's parametrization map

$$\begin{aligned}\mu : \mathbb{R}^N &\longrightarrow \mathcal{M}, \\ \theta &\longmapsto f_{L,\theta} \circ \dots \circ f_{2,\theta} \circ f_{1,\theta};\end{aligned}\tag{10.1}$$

see Figure 10.1. Each parameter tuple θ determines a function $f_{i,\theta}$ in each layer of the network whose composition is the end-to-end function $\mu(\theta)$. The map μ depends on the network's architecture, including the number L of layers, the width of each layer (i.e., the dimension of the domain of each $f_{i,\theta}$), and the type of each layer function $f_{i,\theta}$. Most commonly, the layer functions are compositions

$$f_{i,\theta} = \sigma_i \circ \alpha_{i,\theta}\tag{10.2}$$

of an affine map $\alpha_{i,\theta} : \mathbb{R}^{k_{i-1}} \rightarrow \mathbb{R}^{k_i}$ with a (typically non-linear) map $\sigma_i : \mathbb{R}^{k_i} \rightarrow \mathbb{R}^{k_i}$ that applies the same *activation function* $\tilde{\sigma}_i : \mathbb{R} \rightarrow \mathbb{R}$ to each component, i.e., $\sigma_i(x) = (\tilde{\sigma}_i(x_1), \dots, \tilde{\sigma}_i(x_{k_i}))$. The image \mathcal{M} of the network's parametrization map μ is called the *function space* or *neuromanifold* of the neural network architecture (although \mathcal{M} is typically not a smooth manifold).

A neural network is typically trained by minimizing a loss function of the form

$$\mathcal{L} : \mathbb{R}^N \xrightarrow{\mu} \mathcal{M} \xrightarrow{\ell_{\mathcal{D}}} \mathbb{R},\tag{10.3}$$

where the functional $\ell_{\mathcal{D}}$ depends on training data \mathcal{D} . Many geometric questions arise in the theoretical study of this optimization problem, e.g.,

1. How does the network architecture affect the geometry of the function space \mathcal{M} ?
2. How does the geometry of the function space impact the training of the network?

We discuss these questions in the following two sections for network architectures that can be studied with techniques from nonlinear algebra, i.e., where the activation function is the identity, polynomial, or ReLU. In Section 10.3, we give a brief account of the practical usage of machine learning for algebro-geometric computations. This chapter is not intended as a complete survey of the mathematical theory of machine learning with neural networks. We refer the interested reader to the book *Mathematical Aspects of Deep Learning* [69] and the references therein. In the following, we only highlight some algebro-geometric concepts in neural-network theory.

10.1 Expressivity

The study of which functions a given neural network can express or approximate is commonly referred to as expressivity.

Linear and Fully Connected.

The simplest class of networks are *linear fully-connected neural networks* where the activation function $\tilde{\sigma}_i$ in each layer i is the identity and the layer functions $f_{i,\theta}$ are arbitrary linear maps. In that case, the parameters θ are the entries of the matrices representing the linear layer functions. In other words, the network parametrization map (10.1) specializes to

$$\begin{aligned} \mu : \mathbb{R}^{k_1 \times k_0} \times \mathbb{R}^{k_2 \times k_1} \times \dots \times \mathbb{R}^{k_L \times k_{L-1}} &\longrightarrow \mathbb{R}^{k_L \times k_0}, \\ (W_1, W_2, \dots, W_L) &\longmapsto W_L \cdots W_2 W_1. \end{aligned} \tag{10.4}$$

Its image is the determinantal variety $\mathcal{M} = \{W \in \mathbb{R}^{k_L \times k_0} \mid \text{rank}(W) \leq \min(k_0, k_1, \dots, k_L)\}$. If the input or output dimension is one of the minimal widths (i.e., $\min(k_0, k_1, \dots, k_L) = \min(k_0, k_L)$), the function space is the whole ambient vector space: $\mathcal{M} = \mathbb{R}^{k_L \times k_0}$. Otherwise, the function space \mathcal{M} is a lower-dimensional Zariski closed subset whose singular locus is parametrized by a smaller network architecture: $\text{Sing}(\mathcal{M}) = \{W \in \mathbb{R}^{k_L \times k_0} \mid \text{rank}(W) \leq \min(k_0, k_1, \dots, k_L) - 1\}$.

Linear and Convolutional.

Many neural networks that are used in practice have *convolutional layers* (instead of fully-connected ones) where the affine map $\alpha_{i,\theta}$ in (10.2) is a convolution. A convolution on one-dimensional signals depends on a *filter* $w \in \mathbb{R}^r$ and a stride $s \in \mathbb{N}$. It computes the inner product of the filter w with parts of a given input vector v , and traverses the whole vector v by moving the filter w through it with stride s ; in formulas,

$$\begin{aligned} \alpha_{w,s} : \mathbb{R}^{s(k-1)+r} &\longrightarrow \mathbb{R}^k, \\ v &\longmapsto \left(\sum_{j=0}^{r-1} w_j \cdot v_{is+j} \right)_{i=0}^{k-1}. \end{aligned}$$

A *linear convolutional neural network* is the composition of L such convolutions with filter sizes (r_1, r_2, \dots, r_L) and strides (s_1, s_2, \dots, s_L) . The resulting end-to-end function is also a convolution with filter size $r := \sum_{i=1}^L (r_i - 1)S_i + 1$, where $S_i := \prod_{j=1}^{i-1} s_j$ (and $S_1 := 1$), and stride S_{L+1} . Hence, the network parametrization map (10.1) becomes

$$\mu : \mathbb{R}^{r_1} \times \mathbb{R}^{r_2} \times \dots \times \mathbb{R}^{r_L} \longrightarrow \mathbb{R}^r,$$

sending the filters of each layer to the filter of the end-to-end convolution. Equivalently, the end-to-end filter can be computed via polynomial multiplication as follows: For positive integers S and r , we write $\mathbb{R}[x^S, y^S]_{r-1}$ for the vector space of all polynomials that are homogeneous of degree $r - 1$ in the pair (x^S, y^S) . We then identify any filter of size r with the coefficient vector of such a polynomial via

$$\begin{aligned}\pi_{S,r} : \mathbb{R}^r &\longrightarrow \mathbb{R}[x^S, y^S]_{r-1}, \\ w &\longmapsto w_0 x^{S(r-1)} + w_1 x^{S(r-2)} y^S + \dots + w_{r-2} x^S y^{S(r-2)} + w_{r-1} y^{S(r-1)}.\end{aligned}$$

Then, the end-to-end filter corresponds to a polynomial with a sparse factorization given by the filters in the L layers:

$$\pi_{1,r}(\mu(w_1, \dots, w_L)) = \pi_{S_L, r_L}(w_L) \cdots \pi_{S_2, r_2}(w_2) \cdot \pi_{S_1, r_1}(w_1).$$

In other words, we can reinterpret the network parametrization map as polynomial multiplication:

$$\begin{aligned}\mu : \mathbb{R}[x^{S_1}, y^{S_1}]_{r_1-1} \times \mathbb{R}[x^{S_2}, y^{S_2}]_{r_2-1} \times \dots \times \mathbb{R}[x^{S_L}, y^{S_L}]_{r_L-1} &\longrightarrow \mathbb{R}[x, y]_{r-1}, \\ (P_1, P_2, \dots, P_L) &\longmapsto P_L \cdots P_2 P_1.\end{aligned}\tag{10.5}$$

Hence, the function space $\mathcal{M}_{r,s} = \text{im}(\mu)$ of a linear convolutional network is a semialgebraic set of polynomials with a sparse factorization given by the network's filter sizes $r = (r_1, \dots, r_L)$ and strides $s = (s_1, \dots, s_L)$. It is closed in the Euclidean topology, and describing its Euclidean relative boundary is a challenging problem [94]. As in the case of fully-connected linear networks, its singular locus is parametrized by smaller network architectures. To see this, we successively merge all neighboring layers $i - 1$ and i in (10.5) with $S_{i-1} = S_i$ to eventually obtain a *reduced architecture* (\tilde{r}, \tilde{s}) such that $1 = \tilde{S}_1 < \tilde{S}_2 < \tilde{S}_3 < \dots$ (where $\tilde{S}_i := \prod_{j=1}^{i-1} \tilde{s}_j$). This process can enlarge the function space, i.e., $\mathcal{M}_{r,s} \subseteq \mathcal{M}_{\tilde{r},\tilde{s}}$, but does not change its Zariski closure in $\mathbb{R}[x, y]_{r-1}$, i.e., $\overline{\mathcal{M}}_{r,s} = \overline{\mathcal{M}}_{\tilde{r},\tilde{s}}$ [94, Lemma 3.5]. Hence, to determine the singular locus of the Zariski closure of the function space, it is sufficient to assume that its architecture is reduced. If the reduced architecture has a single layer, the Zariski closure of the function space is the whole ambient vector space: $\overline{\mathcal{M}}_{r,s} = \mathbb{R}[x, y]_{r-1}$. Otherwise, it is a lower-dimensional subvariety whose singular locus is a union of lower-dimensional function spaces with the same reduced stride sequence:

Theorem 10.1 ([94, Theorem 2.8]) *Let (r, s) be a reduced architecture with $L > 1$ layers of a linear convolutional network. Then,*

$$\text{Sing}(\overline{\mathcal{M}}_{r,s}) = \{0\} \cup \bigcup_{r' \in R} \overline{\mathcal{M}}_{r',s} = \{0\} \cup \bigcup_{r' \in R} \mathcal{M}_{r',s},$$

where $R := \{r' \in \mathbb{Z}_{\geq 0}^L \mid \overline{\mathcal{M}}_{r',s} \subsetneq \overline{\mathcal{M}}_{r,s}\}$.

Remark 10.2 The discussion above is restricted to convolutions on one-dimensional signals. Many practical neural networks use convolutions on two-dimensional signals, e.g., when the input data is pictures. Higher-dimensional convolutions move a *filter tensor* w through an *input tensor* v of the same dimension. The composition of such convolutions corresponds to the multiplication of multivariate polynomials (cf. [93, Section 4.3]).

Non-Linear.

The theoretical study of neural networks becomes a lot more challenging if the activation function is non-linear. A first algebro-geometric study for polynomial activation functions is pursued in [90]. For fully-connected neural networks with an activation function that takes the n -th power (i.e., $\tilde{\sigma}_i : x \mapsto x^n$), the authors provide bounds on the dimension of the semi-algebraic function space, with equality in some cases, and conditions for when the (Zariski closure) of the function space is a vector space.

A common activation function in practice is *rectified linear unit (ReLU)*, i.e., $\tilde{\sigma}_i : x \mapsto \max(0, x)$. The end-to-end function of a ReLU neural network is piecewise affine-linear. In fact, every piecewise linear functions with finitely many pieces can be obtained from a fully-connected ReLU network [5]. Although ReLU end-to-end functions are not algebraic, it was explained in [155] that they can be interpreted as tropical rational functions. That perspective was developed further in [112] to provide sharp bounds on the number of linear regions of the end-to-end functions. The local dimension of ReLU function spaces was investigated in [68].

10.2 Optimization

The theoretical works on the optimization problem of training neural networks can be roughly grouped into *static* and *dynamic* studies. Static investigations concern the loss landscape [105] and the critical points of (10.3), while dynamic studies depend on the choice of a training algorithm, e.g., investigating its convergence.

10.2.1 Static Properties

One of the big mysteries in machine learning theory is why training neural networks (i.e., minimizing the loss function (14.5)) results in “nice” minima. The concrete meaning of the adjective nice varies in the literature (see also the algebro-geometric article [108] clarifying the various uses of “flat” minima).

Training a neural network minimizes the loss function $\mathcal{L} = \ell_{\mathcal{D}} \circ \mu$ in (10.3) on the parameter space. The meaningful critical points of that minimization problem are those that actually come from critical points of $\ell_{\mathcal{D}}$ on the function space. Formally, such *pure critical points* θ of \mathcal{L} satisfy that $\mu(\theta)$ is a smooth point of the function space \mathcal{M} and a critical point of the functional $\ell_{\mathcal{D}}$ restricted to smooth locus $\text{Reg}(\mathcal{M})$. The network parametrization map μ can induce additional *spurious critical points* of \mathcal{L} .

Linear and Fully-Connected.

For linear fully-connected networks, the pure and spurious critical points were characterized in [28]. Recall that in that case the function space \mathcal{M} is the determinantal variety consisting of all matrices whose rank is bounded from above by a constant determined by the network’s architecture. The critical points θ of \mathcal{L} such that $\mu(\theta)$ is a matrix of maximal possible rank are pure [28, Proposition 6]. In other words, all spurious critical points θ correspond to lower-rank matrices $\mu(\theta)$ (i.e., they map to the singular locus of the function space \mathcal{M} if the latter is a proper subvariety of the ambient vector space). Moreover, spurious critical points are essentially always saddles [28, Proposition 9]. More concretely, if $\ell_{\mathcal{D}}$ is a smooth and convex function, then all non-global local minima of \mathcal{L} (often called “bad” minima in the literature) are pure critical points [28, Proposition 10]. It is a common, but false, belief that linear fully-connected networks generally do not have “bad” minima. In fact, the previous cited result implies the following:

Theorem 10.3 ([28, Proposition 10]) *Consider a linear fully-connected network and a smooth and convex function $\ell_{\mathcal{D}}$. Then, $\mathcal{L} = \ell_{\mathcal{D}} \circ \mu$ has non-global local minima if and only if $\ell_{\mathcal{D}}|_{\text{Reg}(\mathcal{M})}$ has non-global local minima.*

Two well-known results from machine learning theory are immediate consequences of this theorem. First, if \mathcal{M} is equal to the ambient vector space (i.e., the input or output dimension of the network is one of

its minimal widths), then any convex function $\ell_{\mathcal{D}}$ has exactly one minimum on \mathcal{M} (namely, its global minimum), and hence \mathcal{L} does not have any non-global minima. This is the main result from [102]. The second well-known result applies to the squared-error loss $\ell_{\mathcal{D}}$

$$\begin{aligned}\ell_{\mathcal{D}} : \mathbb{R}^{k_L \times k_0} &\longrightarrow \mathbb{R}, \\ W &\longmapsto \sum_{i=1}^d \|Wx_i - y_i\|^2,\end{aligned}\tag{10.6}$$

where the training data \mathcal{D} consists of pairs of input and output vectors $(x_i, y_i) \in \mathbb{R}^{k_0} \times \mathbb{R}^{k_L}$. Writing $X \in \mathbb{R}^{k_0 \times d}$ and $Y \in \mathbb{R}^{k_L \times d}$ for the data matrices whose i -th columns are x_i and y_i , respectively, the squared-error loss becomes the squared Frobenius norm $\ell_{\mathcal{D}}(W) = \|WX - Y\|^2$. If XX^\top is a full-rank matrix, minimizing this squared Frobenius norm over all $W \in \text{Reg}(\mathcal{M})$ is equivalent to minimizing the squared Euclidean distance

$$\|W - U\|^2, \quad \text{where } U := YX^\top((XX^\top)^{\frac{1}{2}})^{-1},\tag{10.7}$$

over all $W \in \text{Reg}(\mathcal{M})$; see [28, Section 3.3]. Now, the Eckart-Young Theorem tells us that the latter optimization problem has a unique local and global minimum if the singular values of U are pairwise distinct and positive. Hence, if there are sufficiently many and sufficiently generic data pairs (x_i, y_i) , the squared-error loss $\ell_{\mathcal{D}}$ has no non-global minima on $\text{Reg}(\mathcal{M})$ and so Theorem 10.3 shows that the squared-error loss \mathcal{L} on the parameter space has no “bad” minima. The latter is a celebrated result in the machine learning community, often attributed to [8] or [88]. However, the settings where the function space \mathcal{M} is a vector space or the loss function is the squared-error loss, are rather special, and Theorem 10.3 suggests that we should expect the existence of non-global local minima for other loss functions and architectures where \mathcal{M} is a proper determinantal variety; see also [28, Example 13].

Linear and Convolutional.

For linear convolutional networks where all strides are one, the associated reduced network architecture has a single layer and so the function space \mathcal{M} is a Euclidean closed, full-dimensional semialgebraic subset of the ambient vector space $\mathbb{R}[x, y]_{r-1}$. Therefore, critical points of the loss \mathcal{L} often correspond to points $\mu(\theta)$ on the Euclidean boundary of \mathcal{M} , and in particular have to be critical points of the network parametrization map μ . This is in sharp contrast to linear convolutional networks where all strides are strictly larger one (i.e., reduced architectures):

Theorem 10.4 ([94, Theorem 2.11]) *Let (r, s) be a reduced architecture with L layers of a linear convolutional network. Moreover, let $d \geq r := \sum_{i=1}^L (r_i - 1)S_i + 1$, where $S_i := \prod_{j=1}^{i-1} s_j$. For almost all d -tuples \mathcal{D} of training data, every critical point θ of the squared-error loss $\mathcal{L} = \ell_{\mathcal{D}} \circ \mu$ satisfies one of the following:*

1. θ is a regular point of μ and $\mu(\theta)$ is a smooth point in the Euclidean relative interior of \mathcal{M} (in particular, θ is a pure critical point), or
2. $\mu(\theta) = 0$.

Here, the squared-error loss is the same as in (10.6) where the W are the matrices representing the end-to-end convolutions.

We summarize the discussion so far for training linear networks with the squared-error loss. For fully-connected networks, the function space \mathcal{M} is a determinantal variety. In particular, its Euclidean relative boundary is empty. Nevertheless, spurious critical points commonly appear; namely, they correspond to

singular points of \mathcal{M} . For convolutional networks of stride one, the function space is a semialgebraic, Euclidean closed, full-dimensional subset. So its singular locus (formally, the singular locus of its Zariski closure) is empty, but often critical points are on its Euclidean boundary and are thus critical points of μ . Finally, for convolutional networks with all strides strictly larger one, the function space \mathcal{M} is a semialgebraic, Euclidean closed, lower-dimensional subset. Hence, it typically has a non-trivial Euclidean relative boundary and a non-trivial singular locus (of its Zariski closure). Nevertheless, these loci are not relevant for training the network when using a sufficient amount of generic data, because all critical points – except those where a filter in one of the layers is zero – are pure (even stronger, regular points of μ) and correspond to interior smooth points of \mathcal{M} .

10.2.2 Dynamic Properties

The most common optimization algorithms in the training of neural networks are variations of gradient descent. After picking initial parameters θ , gradient descent adapts the parameters successively with the goal to minimize the loss $\mathcal{L}(\theta)$.

Linear and Fully-Connected.

When training linear fully-connected networks using the squared-error loss such that the data matrix XX^\top in (10.7) has full rank, gradient descent converges for almost all initializations (under reasonable assumptions on its step sizes) to a critical point θ of the loss \mathcal{L} [114, Theorem 2.4]. Moreover, the matrix $\mu(\theta) \in \mathcal{M}$ is a global minimum of ℓ_D restricted to the smooth manifold of all matrices of the same format and same rank [114, Theorem 2.6]. The authors of [114] conjecture that the matrix $\mu(\theta)$ has in fact the maximal possible rank in \mathcal{M} (in other words, that $\mu(\theta)$ is a smooth point of the function space \mathcal{M}), but their proof techniques cannot exclude that the critical point θ computed by gradient descent is a *non-strict saddle point* of the loss \mathcal{L} and those saddle points may correspond to lower-rank matrices $\mu(\theta)$.

An essential ingredient in the convergence analysis of [114] are the *algebraic invariants* of gradient flow. The curve in parameter space traced by gradient flow is typically transcendental, but it does satisfy some algebraic relations. In other words, its Zariski closure is not the whole ambient parameter space.

Proposition 10.5 ([6]) *Consider a linear fully-connected neural network with parametrization map (10.4). Let $\theta(t) = (W_1(t), W_2(t), \dots, W_L(t))$ for $t \geq 0$ be the curve traced by gradient flow initialized at $t = 0$. Then the quantities*

$$W_i^\top(t)W_i(t) - W_{i-1}(t)W_{i-1}^\top(t) \quad \text{for } i = 2, 3, \dots, L$$

remain constant for all $t \geq 0$.

This result also has practical consequences: A parameter tuple $\theta = (W_1, \dots, W_L)$ is called *balanced* if $W_i^\top W_i = W_{i-1}^\top W_{i-1}$ for all $i \in \{2, \dots, L\}$. In particular, all matrices in a balanced tuple need to have the same Frobenius norm, i.e., $\|W_i\| = \|W_1\|$ for all $i \in \{2, \dots, L\}$. If a linear network is initialized at a balanced parameter tuple $\theta(0)$, then it follows from Proposition 10.5 that every parameter tuple $\theta(t)$ along the gradient flow curve is balanced. Since all matrices in the balanced tuple $\theta(t)$ need to have the same Frobenius norm, it can in particular not happen that one of the matrices converges to zero while another matrix in the tuple has entries that converge to infinity. In fact, if one matrix in a balanced tuple converges to zero, the whole tuple converges to zero.

Algebraic invariants of gradient flow have also been computed for linear convolutional networks [93, Proposition 5.13] and ReLU networks [152, Lemma 3]; see also [54, Theorems 2.1–2.2].

Nonlinear Autoencoders.

Invariants also play a crucial role in the study of attractors of autoencoders. An *autoencoder* is a composition of two feedforward neural networks: an encoder and a decoder network, such that the input dimension of the encoder equals the output dimension of the decoder. It is typically trained using the *autoencoding loss*

$$\arg \min_{f \in \mathcal{M}} \sum_{i=1}^d \|f(x_i) - x_i\|^2,$$

where \mathcal{M} is the function space of the composed autoencoder network and the x_1, \dots, x_d are training data. It is shown in [126] that an autoencoder trained with gradient descent on a single training example x (i.e., $d = 1$) memorizes that example x as an attractor (under suitable assumptions on the activation function and initialization). An *attractor* x of the learned function $f \in \mathcal{M}$ is a fixed point such that in an open neighborhood O of x , for any $y \in O$, the sequence $(f^i(y))_{i \in \mathbb{N}}$ converges to x as $i \rightarrow \infty$.

10.3 Machine Learning in Algebraic Geometry

Several works have explored how machine learning can be helpful in algebraic geometry research, some of which we outline shortly below. However, it is not clear yet what type of information can be learned and which type of tasks can be solved by training neural networks. Despite its massive success for classification tasks (e.g., “is there a cat on this picture?”), machine learning with neural networks has not improved explicitly geometric tasks such as solving systems of polynomial equations. For instance, the structure-from-motion problem in computer vision (see Chapter 13) is essentially equivalent to solving certain polynomial equation systems. The attempts to solve that problem with machine learning methods have not been as successful as traditional computer vision techniques that are based on symbolic computations with Gröbner bases or resultants [135, 156].

The works that have used machine learning techniques to answer questions in algebraic geometry come roughly in two flavors. On the one hand, several machine learning techniques have been implemented to directly compute geometric properties, e.g. of Hilbert series [9], of irreducible representations [39], or numerical Calabi-Yau (Ricci flat Kähler) metrics [51]. Those approaches trade off the reliability of the computed solutions with performance, which can yield insights into problem instances that lie outside of the scope of traditional computation techniques.

On the other hand, many algebro-geometric algorithms depend on a heuristic that has to be chosen by the user and that might heavily influence their performance. For instance, to obtain a Gröbner basis of a polynomial equation system, we need to choose a monomial ordering. Machine learning has been successful at predicting such a heuristic for a given problem instance which then speeds up the computation using traditional algorithms. In that way the performance can be enhanced without compromising the reliability of the final output. This approach has been used to speed up both Buchberger’s algorithm by learning S-pair selection strategies [120] and Cylindrical Algebraic Decomposition by learning a variable ordering and whether Gröbner basis preconditioning is beneficial [82]. In a similar spirit, the authors of [72] improve the computation of periods of hypersurfaces. Their strategy considers pencils of hypersurfaces and uses neural networks to predict the complexity of the Gauss-Manin connection which governs the change of the period matrix along the pencil. Based on that prediction, they explore the space of smooth quartic surface in \mathbb{P}^3 that are defined by a sum of five monomials and guess for which of those their periods are computable by non-learning algorithms. This leads them to determine the periods of 96% of those surfaces.

Although neural networks have not shown a great potential for explicitly solving systems of polynomial equations, they can be trained to predict their number of real solutions [14, 25]. Such a prediction can be potentially used by real homotopy methods that only track real solutions instead of all complex solutions if one has pre-computed a starting system for each possible number of real solutions (in best case, even for each chamber in the complement of the real discriminant). That would yield a reliable numerical computation that requires less computation time since it tracks fewer paths. A more drastic approach has been taken in [81] where the authors learn a *single* starting solution for a real homotopy that has good chances to reach a good solution of the desired target system. That way of computing produces a less reliable solution, but since they propose their method as part of a random sample consensus (RANSAC) scheme, bad solutions can be detected and disregarded. Since tracking a single solution can be very fast, they can simply repeat their approach for each bad solution.

Chapter 11

Maximum Likelihood

This book started out with the problem of minimizing the Euclidean distance from a data point \mathbf{u} to a model X that is given by polynomial equations. We studied the analogous problem in the setting of algebraic statistics [144], where the model X represents a family of probability distributions, and we used the Wasserstein metric to measure the distances from \mathbf{u} to X . In this chapter we stay with statistical models but we now use Kullback-Leibler divergence and likelihood inference instead of Wasserstein distance.

11.1 Kullback-Leibler Divergence

The two scenarios of most interest for statisticians are Gaussian models and discrete models. We start with discrete models, where we take the state space is the finite set $\{0, 1, \dots, n\}$. The simplex of all probability distributions on this state space equals

$$\Delta_n = \{\mathbf{p} = (p_0, p_1, \dots, p_n) \in \mathbb{R}^{n+1} : p_0 + p_1 + \dots + p_n = 1 \text{ and } p_0, p_1, \dots, p_n > 0\}. \quad (11.1)$$

Given two probability distributions \mathbf{q} and \mathbf{p} in Δ_n , their *Kullback-Leibler (KL) divergence* is defined as

$$D_{\text{KL}}(\mathbf{q} \parallel \mathbf{p}) = \sum_{i=0}^n q_i \cdot \log(q_i/p_i). \quad (11.2)$$

This function is not symmetric in its two arguments, i.e. we have $D_{\text{KL}}(\mathbf{q} \parallel \mathbf{p}) \neq D_{\text{KL}}(\mathbf{p} \parallel \mathbf{q})$ in general. Nevertheless, we interpret KL divergence as a kind of metric on the open simplex Δ_n .

Lemma 11.1 *The KL divergence is nonnegative and it is zero if and only if the two distributions agree. In symbols, $D_{\text{KL}}(\mathbf{q} \parallel \mathbf{p}) \geq 0$ for all $\mathbf{p}, \mathbf{q} \in \Delta_n$, and equality holds if and only if $\mathbf{p} = \mathbf{q}$.*

Proof We use the calculus fact that the function $x \mapsto (x - 1) - \log(x)$ is nonnegative for $x \in \mathbb{R}_{>0}$ and its only zero occurs at $x = 1$. Hence sum in (11.2) is bounded below as follows:

$$D_{\text{KL}}(\mathbf{q} \parallel \mathbf{p}) = - \sum_{i=0}^n q_i \cdot \log(p_i/q_i) \geq - \sum_{i=0}^n q_i \cdot (p_i/q_i - 1) = \sum_{i=0}^n p_i - \sum_{i=0}^n q_i = 1 - 1 = 0.$$

Moreover, equality holds if and only if $p_i/q_i = 1$ for all indices i . \square

Our model is a subset X of Δ_n defined by homogeneous polynomial equations. As before, for venturing beyond linear algebra, we identify X with its Zariski closure in complex projective space \mathbb{P}^n .

We shall present the algebraic approach to maximum likelihood estimation (MLE). Our sources include [34, 55, 75, 85, 86, 144] and references therein. Suppose we are given N i.i.d. samples. These are summarized in the *data vector* $\mathbf{u} = (u_0, u_1, \dots, u_n)$ where u_i is the number of samples that were in state i . Thus the sample size is $N = u_0 + u_1 + \dots + u_n$. The associated log-likelihood function equals

$$\ell_{\mathbf{u}} : \Delta_n \rightarrow \mathbb{R}, \mathbf{p} \mapsto u_0 \cdot \log(p_0) + u_1 \cdot \log(p_1) + \dots + u_n \cdot \log(p_n).$$

Performing MLE for the model X means solving the following optimization problem:

$$\text{Maximize } \ell_{\mathbf{u}}(\mathbf{p}) \text{ subject to } \mathbf{p} \in X. \quad (11.3)$$

Viewed through the lens of metric algebraic geometry, this problem amounts to minimizing a certain distance, namely KL divergence, to the variety X . Namely, given a data vector \mathbf{u} with $u_i > 0$ for all i , we write $\mathbf{q} = \frac{1}{N}\mathbf{u}$ for the corresponding empirical distribution in Δ_n .

Remark 11.2 The maximum likelihood estimation problem (11.3) is equivalent to:

$$\text{Minimize } D_{\text{KL}}(\mathbf{q} \parallel \mathbf{p}) \text{ subject to } \mathbf{p} \in X. \quad (11.4)$$

This holds because the KL divergence can be rewritten as the entropy of the empirical distribution \mathbf{q} minus the log-likelihood function: $D_{\text{KL}}(\mathbf{q} \parallel \mathbf{p}) = \sum_{i=0}^n q_i \log(q_i) - \frac{1}{N} \ell_{\mathbf{u}}(\mathbf{p})$.

As before, we identify the model X with a projective variety in \mathbb{P}^n . The objective function in the optimization problem (11.3) involves logarithms and it is not an algebraic function. However, each of its partial derivatives is a rational function, and therefore we can study this problem using algebraic geometry.

11.2 Maximum Likelihood Degree

We fix a real projective variety X in \mathbb{P}^n , and we consider the the optimization problem in (11.3) or (11.4). The *maximum likelihood degree (ML degree)* of X is defined to be the number of complex critical points of this optimization problem for generic data \mathbf{u} . For arbitrary fixed data \mathbf{u} , the optimal solution is denoted $\hat{\mathbf{p}}$ and called the *maximum likelihood estimate* of the model X for the data \mathbf{u} . Thus ML degree is the analogue to ED degree, when now KL divergence replaces Euclidean distance.

The critical equations for (11.3) are similar to those of ED problem. Let $I_X = \langle f_1, \dots, f_k \rangle$ be the homogeneous ideal of the model X . In addition, we consider the inhomogeneous linear polynomial $f_0 := p_0 + p_1 + \dots + p_n - 1$. Let $\mathcal{J} = (\partial f_i / \partial p_j)$ denote the Jacobian matrix of size $(k+1) \times (n+1)$ for these polynomials, and set $c = \text{codim}(X)$. The *augmented Jacobian* \mathcal{AJ} is obtained from \mathcal{J} by prepending one more row, namely the gradient of the objective function

$$\nabla \ell_{\mathbf{u}} = (u_0/p_0, u_1/p_1, \dots, u_n/p_n).$$

To obtain the critical equations, enlarge I_X by the $(c+2) \times (c+2)$ minors of the $(k+2) \times (n+1)$ matrix \mathcal{AJ} , then clear denominators, and remove extraneous components by saturation.

Example 11.3 (Space curves) Let $n = 3$ and X the curve in Δ_3 defined by two general polynomials f_1 and f_2 of degrees d_1 and d_2 in p_0, p_1, p_2, p_3 . The augmented Jacobian matrix is

$$\mathcal{AJ} = \begin{pmatrix} u_0/p_0 & u_1/p_1 & u_2/p_2 & u_3/p_3 \\ 1 & 1 & 1 & 1 \\ \partial f_1 / \partial p_0 & \partial f_1 / \partial p_1 & \partial f_1 / \partial p_2 & \partial f_1 / \partial p_3 \\ \partial f_2 / \partial p_0 & \partial f_2 / \partial p_1 & \partial f_2 / \partial p_2 & \partial f_2 / \partial p_3 \end{pmatrix}. \quad (11.5)$$

Clearing denominators amounts to multiplying the i th column by p_i , so the determinant contributes a polynomial of degree $d_1 + d_2 + 1$ to the critical equations. Since the codimension of X equals $c = 2$, we need to take the 4×4 minors of \mathcal{AJ} . The generators of I_X have degrees d_1 and d_2 respectively. We therefore conclude that the ML degree of X equals $d_1 d_2 (d_1 + d_2 + 1)$.

The following general upper bound on the ML degree is established in [75, Theorem 5].

Proposition 11.4 Let X be a model of codimension c in the probability simplex Δ_n whose ideal I_X is generated by polynomials $f_1, f_2, \dots, f_c, \dots, f_k$ of degrees $d_1 \geq d_2 \geq \dots \geq d_c \geq \dots \geq d_k$. Then

$$\text{MLdegree}(X) \leq d_1 d_2 \cdots d_c \cdot \sum_{i_1+i_2+\dots+i_c \leq n-c} d_1^{i_1} d_2^{i_2} \cdots d_c^{i_c}. \quad (11.6)$$

Equality holds when X is a generic complete intersection of codimension c (hence $c = k$).

We next present a more precise formula. For the ED degree, the polar degrees in \mathbb{P}^n were used to give such a formula. For the ML degree, we shall use the Euler characteristic instead.

Given our variety X in the complex projective space \mathbb{P}^n , and let X° be the open subset of X that is obtained by removing the hyperplane arrangement $\{p_0 p_1 \cdots p_n (\sum_{i=0}^n p_i) = 0\}$. We recall from [84, 85] that a *very affine variety* is a closed subvariety of an algebraic torus $(\mathbb{C}^*)^r$. In our setting, the open set X° is a very affine variety, with $r = n + 2$. The following formula works for any very affine variety.

Theorem 11.5 Suppose that the very affine variety X° is non-singular. The ML degree of the model X equals the signed Euler characteristic $(-1)^{\dim(X)} \cdot \chi(X^\circ)$ of the manifold X° .

Proof (and Discussion) This was proved under additional assumptions in [34, Theorem 19], and in full generality in [84, Theorem 1]. If the very affine variety X° is singular, then the Euler characteristic can be replaced by the Chern-Schwartz-MacPherson class, as shown in [84, Theorem'2]. \square

The optimal solution to our optimization problem (11.3)-(11.4) in the statistical model $X^\circ \cap \Delta_n = X \cap \Delta_n$ is denoted $\hat{\mathbf{p}}$. This point is called the *maximum likelihood estimate (MLE)* for the given data \mathbf{u} and the model X . The ML degree measures the algebraic complexity of the MLE. Theorem 11.5 says that the ML degree is a topological invariant. Varieties X for which the ML degree is equal to one are of special interest, both statistically and geometrically. For a model X to have ML degree one means that the MLE $\hat{\mathbf{p}}$ is a rational function of the data \mathbf{u} . Here are two natural examples where this happens.

Example 11.6 ($n = 3$) The independence model for two binary random variables is a quadratic surface X in the tetrahedron Δ_3 . This model is described by the constraints

$$\det \begin{bmatrix} p_0 & p_1 \\ p_2 & p_3 \end{bmatrix} = 0 \quad \text{and} \quad p_0 + p_1 + p_2 + p_3 = 1 \quad \text{and} \quad p_0, p_1, p_2, p_3 > 0.$$

Consider data $\mathbf{u} = \begin{bmatrix} u_0 & u_1 \\ u_2 & u_3 \end{bmatrix}$ of sample size $|u| = u_0 + u_1 + u_2 + u_3$. The ML degree of the surface X equals one because the MLE $\hat{\mathbf{p}}$ is a rational function of the data. To be precise, the coordinates of the MLE $\hat{\mathbf{p}}$ are

$$\begin{aligned} \hat{p}_0 &= |u|^{-2}(u_0+u_1)(u_0+u_2), & \hat{p}_1 &= |u|^{-2}(u_0+u_1)(u_1+u_3), \\ \hat{p}_2 &= |u|^{-2}(u_2+u_3)(u_0+u_2), & \hat{p}_3 &= |u|^{-2}(u_2+u_3)(u_1+u_3). \end{aligned} \tag{11.7}$$

In words, we multiply the row sums with the column sums in the empirical distribution $\frac{1}{|u|}\mathbf{u}$.

Here is another simple model where the MLE is a rational function in the data.

Example 11.7 ($n = 2$) Given a biased coin, we perform the following experiment: *Flip a biased coin. If it shows heads, flip it again.* The outcome of this experiment is the number of heads: 0, 1 or 2.

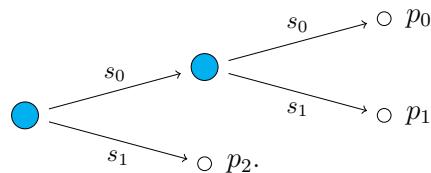


Fig. 11.1: Probability tree that describes the coin toss model in Example 11.7.

If s denotes the bias of our coin, then the model is the parametric curve X given by

$$(0, 1) \rightarrow X \subset \Delta_2, \quad s \mapsto (s^2, s(1-s), 1-s).$$

This model is the conic $X = V(p_0 p_2 - (p_0 + p_1) p_1) \subset \mathbb{P}^2$. Its MLE is given by the formula

$$(\hat{p}_0, \hat{p}_1, \hat{p}_2) = \left(\frac{(2u_0 + u_1)^2}{(2u_0 + 2u_1 + u_2)^2}, \frac{(2u_0 + u_1)(u_1 + u_2)}{(2u_0 + 2u_1 + u_2)^2}, \frac{u_1 + u_2}{2u_0 + 2u_1 + u_2} \right). \quad (11.8)$$

Since the coordinates of \hat{p} are rational functions, the ML degree of X is equal to one.

The following theorem explains what we saw in equations (11.7) and (11.8):

Theorem 11.8 *If $X \subset \Delta_n$ is a model of ML degree one, so that $\hat{\mathbf{p}}$ is a rational function of \mathbf{u} , then each coordinate \hat{p}_i is an alternating product of linear forms with positive coefficients.*

Proof (and Discussion) This was proved in the setting of arbitrary complex very affine varieties by Huh in [85]. It was adapted to real algebraic geometry and hence to statistical models in [55]. These two articles offer precise statements via Horn uniformization for A -discriminants [65], i.e. hypersurfaces dual to toric varieties. For additional information we refer to [86, Corollary 3.12]. \square

Models given by rank constraints on matrices and tensors are particularly important in applications, since these represent conditional independence. Consider two random variables, having n_1 and n_2 states respectively, which are conditionally independent, given a hidden random variable with r states. In algebraic geometry, this model is the variety X_r in $\mathbb{P}^{n_1 n_2 - 1}$ that is defined by the $(r+1) \times (r+1)$ minors of an $n_1 \times n_2$ matrix (p_{ij}) . The ML degree of this rank r model was first studied by Hauenstein, Rodriguez and Sturmfels in [71], who obtained the following results using methods from numerical algebraic geometry.

Proposition 11.9 *For small values of n_1 and n_2 , the ML degrees of low rank models X_r are*

	$(n_1, n_2) = (3, 3) (3, 4) (3, 5) (4, 4) (4, 5) (4, 6) (5, 5)$						
$r = 1$	1	1	1	1	1	1	1
$r = 2$	10	26	58	191	843	3119	6776
$r = 3$	1	1	1	191	843	3119	61326
$r = 4$				1	1	1	6776
$r = 5$							1

Every entry in the $r = 1$ row is 1 because the MLE for the independence model is a rational function in the data (u_{ij}) . One finds $\hat{\mathbf{p}} = (\hat{p}_{ij})$ by multiplying the column vector of row sums of \mathbf{u} with the row vector of column sums of \mathbf{u} , and then dividing by $|\mathbf{u}|^2$, as shown in (11.7). The other entries are more interesting, and they give precise information on the algebraic complexity of minimizing the Kullback-Leibler distance from a given data matrix \mathbf{u} to the conditional independence model X_r . Here is an example taken from [71].

Example 11.10 ($n_1 = n_2 = 5$) Following [71, Example 7], we consider the data

$$\mathbf{u} = \begin{pmatrix} 2864 & 6 & 6 & 3 & 3 \\ 2 & 7577 & 2 & 2 & 5 \\ 4 & 1 & 7543 & 2 & 4 \\ 5 & 1 & 2 & 3809 & 4 \\ 6 & 2 & 6 & 3 & 5685 \end{pmatrix}.$$

For $r = 2$ and $r = 4$, this instance of our MLE problem has the expected number of 6776 distinct complex critical points. In both cases, 1774 of these are real and 90 of these are real and positive. This illustrates the last statement in Theorem 11.11 below. The number of local maxima for $r = 2$ equals 15, and the number of local maxima for $r = 4$ equals 6. For $r = 3$, we have 61326 critical points, of which 15450 are real. Of these, 362 are positive and 25 are local maxima. We invite our readers to critically check these claims, by running software for solving polynomial equations, such as `HomotopyContinuation.jl`.

The columns of the table in (11.9) exhibit an obvious symmetry. This was conjectured in [71], and it was proved by Draisma and Rodriguez in their article [53] on maximum likelihood duality. We now state their result. Given an $n_1 \times n_2$ matrix \mathbf{u} , we write $\Omega_{\mathbf{u}}$ for the matrix whose (i, j) entry equals

$$\frac{u_{ij}u_{i+j}}{(u_{++})^3}.$$

In the following theorem, the symbol \star denotes the Hadamard product (or entrywise product) of two matrices. All matrices \mathbf{p}_i and \mathbf{q}_i have format $n_1 \times n_2$ and they have complex entries.

Theorem 11.11 *Fix $n_1 \leq n_2$ and \mathbf{u} an $n_1 \times n_2$ -matrix with strictly positive integer entries. There exists a bijection between the complex critical points $\mathbf{p}_1, \mathbf{p}_2, \dots, \mathbf{p}_s$ of the likelihood function for \mathbf{u} on X_r and the complex critical points $\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_s$ on X_{n_1-r+1} such that*

$$\mathbf{p}_1 \star \mathbf{q}_1 = \mathbf{p}_2 \star \mathbf{q}_2 = \cdots = \mathbf{p}_s \star \mathbf{q}_s = \Omega_{\mathbf{u}}. \quad (11.10)$$

In particular, this bijection preserves reality, positivity, and rationality of the critical points.

This result represents a multiplicative version of the duality we encountered in our study of ED degrees. Recall that the ED degree of any projective variety X , when viewed as a cone in affine space, equals that of its dual variety X^\vee . Under some genericity assumption, this common ED degree is the sum of the polar degrees, which arises from the conormal variety $N_X = N_{X^\vee}$. By “multiplicative” we mean that $\mathbf{u}_i/\mathbf{p}_i$ instead of $\mathbf{u}_i - \mathbf{p}_i$ appears in the first row of the augmented Jacobian matrix.

It is a challenge in intersection theory and singularity theory to find general formulas for the ML degrees in Proposition 11.9. This problem was solved for $r = 2$ by Rodriguez and Wang in [131]. They give a recursive formula in [131, Theorem 4.1], and they present impressive values in [131, Table 1]. They unravel the recursion, and they obtain the explicit formulas for the ML degree of conditional independence in many cases. In particular, they obtain the following result which had been stated as a conjecture in [71].

Theorem 11.12 (Rodriguez-Wang [131]) *Consider the variety $X_2 \subset \mathbb{P}^{3n-1}$ whose points are the $3 \times n$ matrices of rank ≤ 2 . The ML degree of this variety equals $2^{n+1} - 6$.*

11.3 Scattering Equations

We now turn to a connection between algebraic statistics and particle physics that was developed in [142]. The context is scattering amplitudes, where the critical equations for (11.3)-(11.4) are known as *scattering equations*. We consider the *CEGM model*, due to Cachazo and his collaborators [30, 31]. The role of the data vector \mathbf{u} is played in physics by the *Mandelstam invariants*. This theory rests on the space X^o of m labeled points in general position in \mathbb{P}^{k-1} , up to projective transformations. Consider the Grassmannian $\text{Gr}(k, m)$ in its Plücker embedding into $\mathbb{P}^{\binom{m}{k}-1}$. The torus $(\mathbb{C}^*)^m$ acts on $\text{Gr}(k, m)$ by scaling the columns of $k \times m$ matrices representing subspaces. Let $\text{Gr}(k, m)^o$ be the open Grassmannian where all Plücker coordinates are nonzero. The CEGM model is the $(k-1)(m-k-1)$ -dimensional manifold

$$X^o = \text{Gr}(k, m)^o / (\mathbb{C}^*)^m. \quad (11.11)$$

Example 11.13 ($k = 2$) For $k = 2$, the very affine variety in (11.11) has dimension $m - 3$, and it is the moduli space of m distinct labeled points on the complex projective line \mathbb{P}^1 . This space is ubiquitous in algebraic geometry where it is known as $\mathcal{M}_{0,m}$. The punchline of our discussion here is that we interpret the moduli space $\mathcal{M}_{0,m}$ as a statistical model. And, we then argue that its ML degree is equal to $(m-3)!$.

For instance, if $m = 4$ then $X^o = \mathcal{M}_{0,4}$ is the Riemann sphere \mathbb{P}^1 with three points removed. The signed Euler characteristic of this surface is one, and Theorem 11.8 applies.

Proposition 11.14 *The configuration space X^o in (11.11) is a very affine variety, with coordinates given by the $k \times k$ minors of the following $k \times m$ matrix, which we denote by $M_{k,m}$:*

$$\begin{bmatrix} 0 & 0 & 0 & \cdots & 0 & (-1)^k & 1 & 1 & 1 & \cdots & 1 \\ 0 & 0 & 0 & \cdots & (-1)^{k-1} & 0 & 1 & x_{1,1} & x_{1,2} & \cdots & x_{1,m-k-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & -1 & \cdots & 0 & 0 & 1 & x_{k-3,1} & x_{k-3,2} & \cdots & x_{k-3,m-k-1} \\ 0 & 1 & 0 & \cdots & 0 & 0 & 1 & x_{k-2,1} & x_{k-2,2} & \cdots & x_{k-2,m-k-1} \\ -1 & 0 & 0 & \cdots & 0 & 0 & 1 & x_{k-1,1} & x_{k-1,2} & \cdots & x_{k-1,m-k-1} \end{bmatrix}.$$

To be precise, the coordinates on $X^o \subset (\mathbb{C}^*)^{m \choose k}$ are the non-constant minors $p_{i_1 i_2 \dots i_k}$ of the matrix M_k .

Following [2, equation (4)], the antidiagonal matrix in the left $k \times k$ block of $M_{k,m}$ is chosen so that each unknown $x_{i,j}$ is precisely equal to $p_{i_1 i_2 \dots i_k}$ for some $i_1 < i_2 < \dots < i_k$. No signs are needed. The scattering potential for the CEGM model is the following multivalued function on X^o :

$$\ell_u = \sum_{i_1 i_2 \dots i_k} u_{i_1 i_2 \dots i_k} \cdot \log(p_{i_1 i_2 \dots i_k}). \quad (11.12)$$

The critical point equations, known as *scattering equations* [2, equation (7)], are given by

$$\frac{\partial \ell_u}{\partial x_{i,j}} = 0 \quad \text{for } 1 \leq i \leq k-1 \text{ and } 1 \leq j \leq m-k-1. \quad (11.13)$$

These are equations of rational functions. Solving these equations is the agenda in [30, 31, 142].

Corollary 11.15 *The number of complex solutions to (11.13) is the ML degree of the CEGM model X^o . This number equals the signed Euler characteristic $(-1)^{(k-1)(m-k-1)} \cdot \chi(X^o)$.*

Example 11.16 ($k = 2, m = 6$) The very affine threefold $X^o = \mathcal{M}_{0,6}$ is embedded in $(\mathbb{C}^*)^9$ via

$$\begin{aligned} p_{24} &= x_1, p_{25} = x_2, p_{26} = x_3, p_{34} = x_1 - 1, p_{35} = x_2 - 1, \\ p_{36} &= x_3 - 1, p_{45} = x_2 - x_1, p_{46} = x_3 - x_1, p_{56} = x_3 - x_2. \end{aligned}$$

These nine coordinates on $X^o \subset (\mathbb{C}^*)^9$ are the non-constant 2×2 minors of our matrix

$$M_{2,6} = \begin{bmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ -1 & 0 & 1 & x_1 & x_2 & x_3 \end{bmatrix}.$$

The scattering potential is the analogue to the log-likelihood function in statistics:

$$\ell_u = u_{24} \log(p_{24}) + u_{25} \log(p_{25}) + \dots + u_{56} \log(p_{56}).$$

This function has six critical points in X^o . Hence $\text{MLdegree}(X^o) = -\chi(X^o) = 6$.

We now examine the number of critical points of the scattering potential (11.12).

Theorem 11.17 *The known values of the ML degree for the CEGM model (11.11) are as follows. For $k = 2$, the ML degree equals $(m-3)!$ for all $m \geq 4$. For $k = 3$, the ML degree equals 2, 26, 1272, 188112, 74570400 when the number of points is $m = 5, 6, 7, 8, 9$. For $k = 4, m = 8$, the ML degree equals 5211816.*

Proof We refer to [2, Example 2.2], [2, Theorem 5.1] and [2, Theorem 6.1] for $k = 2, 3, 4$. \square

Knowing these ML degrees helps in solving the scattering equations reliably. It was demonstrated in [2, 142] how this can be done in practice, namely with the software `HomotopyContinuation.jl` [26, 27]. For instance, we see in [142, Table 1] that the $10! = 3628800$ critical points for $k = 2, m = 13$ are found in under one hour. See [2, Section 6] for the solution in the challenging case $k = 4, m = 8$.

11.4 Gaussian Models

We now change topic by turning to models for Gaussian random variables. Let PD_n denote the set of positive-definite symmetric $n \times n$ matrices, i.e. matrices all of whose eigenvalues are positive. This is an open convex cone in a real vector space in the matrix space $\text{Sym}_2(\mathbb{R}^n)$, which has dimension $\binom{n+1}{2}$. This cone now plays the role which was played by the simplex Δ_n when we discussed discrete models.

Given a mean vector $\mu \in \mathbb{R}^n$ and a covariance matrix $\Sigma \in \text{PD}_n$, the associated *Gaussian distribution* is supported on \mathbb{R}^n . Its density has the familiar “bell shape”; it is the function

$$f_{\mu, \Sigma}(x) := \frac{1}{\sqrt{(2\pi)^n \det \Sigma}} \cdot \exp\left(-\frac{1}{2}(x - \mu)^T \Sigma^{-1}(x - \mu)\right).$$

We fix a model $Y \subset \mathbb{R}^n \times \text{PD}_n$ that is defined by polynomial equations in (μ, Σ) . Suppose we are given N samples $U^{(1)}, \dots, U^{(N)}$. These samples are vectors in \mathbb{R}^n . They are summarized in the *sample mean* $\bar{U} = \frac{1}{N} \sum_{i=1}^N U^{(i)}$ and in the *sample covariance matrix* $S = \frac{1}{N} \sum_{i=1}^N (U^{(i)} - \bar{U})(U^{(i)} - \bar{U})^T$. Given this representation of the data, the log-likelihood is the following function in the unknowns (μ, Σ) :

$$\ell(\mu, \Sigma) = -\frac{N}{2} \cdot \left[\log \det \Sigma + \text{trace}(S \Sigma^{-1}) + (\bar{U} - \mu)^T \Sigma^{-1}(\bar{U} - \mu) \right]. \quad (11.14)$$

The task of likelihood inference is to minimize this function subject to $(\mu, \Sigma) \in Y$.

There are two extreme cases. First, consider a model where Σ is fixed to be the identity matrix Id_n . Then $Y = X \times \{\text{Id}_n\}$ and we are supposed to minimize the Euclidean distance from the sample mean \bar{U} to the variety X in \mathbb{R}^n . This is precisely the earlier ED problem.

We instead focus on the second case, the family of *centered Gaussians*, where the mean vector μ is fixed to be zero. The model has the form $\{0\} \times X$, where X is a variety in the space $\text{Sym}_2(\mathbb{R}^n)$ of symmetric $n \times n$ matrices. Following [144, Proposition 7.1.10], our task is now as follows:

$$\text{Minimize the function } \Sigma \mapsto \log \det \Sigma + \text{trace}(S \Sigma^{-1}) \text{ subject to } \Sigma \in X. \quad (11.15)$$

Using the concentration matrix $K = \Sigma^{-1}$, we can write this equivalently as follows:

$$\text{Maximize the function } K \mapsto \log \det K - \text{trace}(SK) \text{ subject to } K \in X^{-1}. \quad (11.16)$$

Here the variety X^{-1} is the Zariski closure of the set of inverses of all matrices in X .

Remark 11.18 The optimization problem (11.15)-(11.16) has a metric interpretation as in (11.4). Namely, we can define the KL divergence between two probability distributions on \mathbb{R}^n by replacing the sum in (11.2) with the corresponding integral over \mathbb{R}^n . For two Gaussians we obtain a certain kind of distance between the unknown Σ and the sample covariance matrix S .

The critical equations of the optimization problem (11.15)-(11.16) can be written as polynomials, since the partial derivatives of the logarithm are rational functions. These equations have finitely many complex solutions. Their number is the *ML degree* of the Gaussian statistical model X^{-1} .

In the remainder of this section we focus on Gaussian models that are described by linear constraints on either the covariance matrix or its inverse, which is the concentration matrix. Let $\mathcal{L} \subset \text{Sym}_2(\mathbb{R}^n)$ be a linear space of symmetric matrices (LSSM), whose general element is assumed to be invertible. We are interested in the models $X^{-1} = \mathcal{L}$ and $X = \mathcal{L}$. It is convenient to use primal-dual coordinates (Σ, K) to write the respective critical equations.

Proposition 11.19 Fix an LSSM \mathcal{L} and its orthogonal complement \mathcal{L}^\perp for the inner product $\langle X, Y \rangle = \text{trace}(XY)$. The critical equations for the linear concentration model $X^{-1} = \mathcal{L}$ are

$$K \in \mathcal{L} \text{ and } K\Sigma = \text{Id}_n \text{ and } \Sigma - S \in \mathcal{L}^\perp. \quad (11.17)$$

The critical equations for the linear covariance model $X = \mathcal{L}$ are

$$\Sigma \in \mathcal{L} \text{ and } K\Sigma = \text{Id}_n \text{ and } KSK - K \in \mathcal{L}^\perp. \quad (11.18)$$

Proof This is well-known in statistics. For proofs see [143, Propositions 3.1 and 3.3]. \square

The system (11.17) is linear in the unknown matrix K , whereas the last group of equations in (11.18) is quadratic in K . The numbers of complex solutions are the *ML degree* of \mathcal{L} and the *reciprocal ML degree* of \mathcal{L} . The former is smaller than the latter, and (11.17) is easier to solve than (11.18).

Example 11.20 Let $n = 4$ and \mathcal{L} a generic LSSM of dimension k . Our degrees are as follows:

$k = \dim(\mathcal{L}) :$	2	3	4	5	6	7	8	9
ML degree :	3	9	17	21	21	17	9	3
reciprocal ML degree :	5	19	45	71	81	63	29	7

These numbers and many more appear in [143, Table 1].

ML degrees and reciprocal ML degrees of linear spaces of symmetric matrices have been studied intensively in the recent literature, both for generic and special spaces \mathcal{L} . See [4, 18, 60] and the references therein. We now present an important result due to Manivel, Michalek, Monin, Seynnaeve, Vodička and Wiśniewski. Theorem 11.21 paraphrases highlights from their articles [106, 110].

Theorem 11.21 The ML degree of a generic linear subspace \mathcal{L} of dimension k in $\text{Sym}_2(\mathbb{R}^n)$ is the number of quadrics in \mathbb{P}^{n-1} that pass through $\binom{n+1}{2} - k$ general points and are tangent to $k - 1$ general hyperplanes. For fixed k , this number is a polynomial in n of degree $k - 1$.

Proof The first statement is [110, Corollary 2.6 (4)], here interpreted classically in terms of Schubert calculus. For a detailed discussion see the introduction of [106]. The second statement appears in [106, Theorem 1.3 and Corollary 4.13]. \square

Example 11.22 ($n = 4$) Fix $10 - k$ points and $k - 1$ planes in \mathbb{P}^3 . We are interested in all quadratic surfaces that contain the points and are tangent to the planes. This points and planes impose 9 constraints on $\mathbb{P}(\text{Sym}_2(\mathbb{C}^4)) \simeq \mathbb{P}^9$. Passing through a point is a linear equation. Being tangent to a plane is a cubic constraint on \mathbb{P}^9 . Bézout's Theorem suggests that there could be 3^{k-1} solutions. This is correct for $k \leq 3$ but it overcounts for $k \geq 4$. Indeed, in Example 11.20 we see 17, 21, 21, ... instead of 27, 81, 243, ...

The intersection theory approach in [106, 110] leads to formulas for the ML degrees of linear Gaussian models. From this we obtain provably correct numerical methods for maximum likelihood estimation. Namely, after computing critical points as in [143], we can certify them as in [26]. Since the ML degree is known, one can then be sure that all solutions have been found.

Chapter 12

Tensors

Tensors are a generalization of matrices and can be viewed as tables of higher dimensions: A 2×2 -matrix is a table that contains 4 numbers aligned in two directions and each direction has dimension 2; a $2 \times 2 \times 2$ tensor is a table with 8 numbers aligned in three directions where each direction has dimension 2.

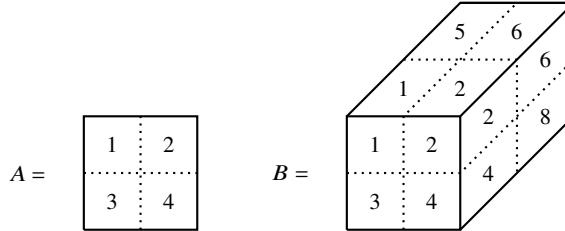


Fig. 12.1: A 2×2 matrix A and a $2 \times 2 \times 2$ tensor B .

For positive integers n_1, \dots, n_d the vector space of real $n_1 \times \dots \times n_d$ -tensors is denoted

$$\mathbb{R}^{n_1 \times \dots \times n_d} := \left\{ A = (a_{i_1, \dots, i_d})_{1 \leq i_1 \leq n_1, \dots, 1 \leq i_d \leq n_d} \mid a_{i_1, \dots, i_d} \in \mathbb{R} \right\}.$$

In the literature, elements in $\mathbb{R}^{n_1 \times \dots \times n_d}$ are also sometimes called *hypermatrices* or *Cartesian tensors*, because our definition of a tensor as a multidimensional array relies on a choice of basis. The dimension of $\mathbb{R}^{n_1 \times \dots \times n_d}$ is $n_1 \cdots n_d$. The number d is called the *order* or *power* of the tensor. Tensors of order 2 are matrices. We can also consider the space of complex tensors $\mathbb{C}^{n_1 \times \dots \times n_d}$.

A common notation for order-3 tensors is by writing them as a pencil of matrices.

Example 12.1 The tensor $B = (b_{i,j,k})_{1 \leq i,j,k \leq 2}$ from Figure 12.1 is denoted

$$B = \left(\begin{array}{cc|cc} 1 & 2 & 5 & 6 \\ 3 & 4 & 7 & 8 \end{array} \right) \in \mathbb{R}^{2 \times 2 \times 2}.$$

The left matrix contains the entries $b_{i,j,1}$ and the matrix on the right contains the entries $b_{i,j,2}$. ◊

As in the previous chapters, the Euclidean inner product is

$$\langle A, B \rangle := \sum_{i_1=1}^{n_1} \cdots \sum_{i_d=1}^{n_d} a_{i_1, \dots, i_d} \cdot b_{i_1, \dots, i_d}$$

for $A = (a_{i_1, \dots, i_d})$ and $B = (b_{i_1, \dots, i_d})$. The induced norm is $\|A\| = \sqrt{\langle A, A \rangle}$.

Given d vectors $\mathbf{v}_i \in \mathbb{R}^{n_i}$, $1 \leq i \leq d$ their *outer product* is the following tensor:

$$\mathbf{v}_1 \otimes \cdots \otimes \mathbf{v}_d := ((\mathbf{v}_1)_{i_1} \cdots (\mathbf{v}_d)_{i_d})_{1 \leq i_1 \leq n_1, \dots, 1 \leq i_d \leq n_d}.$$

That is, the entries of $\mathbf{v}_1 \otimes \cdots \otimes \mathbf{v}_d$ are all possible products between the entries of the \mathbf{v}_i . In fact, we have that $(a_{i_1, \dots, i_d}) = \sum_{i_1=1}^{n_1} \cdots \sum_{i_d=1}^{n_d} a_{i_1, \dots, i_d} \mathbf{e}_{i_1} \otimes \cdots \otimes \mathbf{e}_{i_d}$.

If $n := n_1 = \cdots = n_d$ are all equal, we write the space of order- d tensors as

$$(\mathbb{R}^n)^{\otimes d} := \mathbb{R}^{n \times \cdots \times n}.$$

The action of the symmetric group \mathfrak{S}_d on $(\mathbb{R}^n)^{\otimes d}$ is defined to be the linear extension of the action $\pi(\mathbf{v}_1 \otimes \cdots \otimes \mathbf{v}_d) = \mathbf{v}_{\pi(1)} \otimes \cdots \otimes \mathbf{v}_{\pi(d)}$. This is the generalization of matrix transposition.

Definition 12.2 We say $A \in (\mathbb{R}^n)^{\otimes d}$ is *symmetric* if $\pi(A) = A$ for all $\pi \in \mathfrak{S}_d$. The space of symmetric tensors in $(\mathbb{R}^n)^{\otimes d}$ is denoted

$$S^d(\mathbb{R}^n) := \{A \in (\mathbb{R}^n)^{\otimes d} \mid A \text{ is symmetric}\}.$$

Since $S^d(\mathbb{R}^n)$ is the image of the linear map $A \mapsto \sum_{\pi \in \mathfrak{S}_d} \pi(A)$, it is a linear subspace. The dimension of the space of symmetric tensors is $\binom{n+d-1}{d}$. For $\mathbf{v} \in \mathbb{R}^n$ we denote

$$\mathbf{v}^{\otimes d} := \mathbf{v} \otimes \cdots \otimes \mathbf{v} \in S^d(\mathbb{R}^n).$$

Furthermore, for $A \in S^d(\mathbb{R}^n)$

$$F_A(\mathbf{x}) := \sum_{i_1=1}^n \cdots \sum_{i_d}^n a_{i_1, \dots, i_d} x_{i_1} \cdots x_{i_d} \quad (12.1)$$

is a homogeneous polynomial of degree d in n variables. The map $A \rightarrow F_A$ is a linear isomorphism between $S^d(\mathbb{R}^n)$ and the vector space of homogeneous polynomials of degree d in n variables. We can write the polynomial F_A from (12.1) as

$$F_A(\mathbf{x}) = \langle A, \mathbf{x}^{\otimes d} \rangle.$$

For $A \in S^d(\mathbb{R}^n)$ we have $\|A\| = \|F_A\|_{\text{BW}}$, where the latter is the Bombieri-Weyl metric from Chapter 9.

Example 12.3 Consider the symmetric matrix $A = \begin{pmatrix} 1 & 2 \\ 2 & 0 \end{pmatrix} \in S^2(\mathbb{R}^2)$. The associated polynomial is

$$F_A(\mathbf{x}) = \mathbf{x}^T A \mathbf{x} = x_1^2 + 4x_1 \cdot x_2.$$

The polynomial associated to the symmetric order-3 tensor $B = \begin{pmatrix} 1 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 2 \end{pmatrix} \in S^3(\mathbb{R}^2)$ is

$$F_B(\mathbf{x}) = x_1^3 - 3x_1^2 x_2 + 2x_2^3.$$

◊

A central topic of this lecture are *rank-one tensors*. Let $A \in \mathbb{R}^{n_1 \times \cdots \times n_d}$ be a tensor. We say that A is a rank-one tensor or that it has rank-one, if there exist vectors $\mathbf{v}_i \in \mathbb{R}^{n_i}$, $1 \leq i \leq d$, such that $A = \mathbf{v}_1 \otimes \cdots \otimes \mathbf{v}_d$.

Definition 12.4 The (real) *Segre variety* is defined as

$$\mathcal{S} := \{\mathbf{v}_1 \otimes \cdots \otimes \mathbf{v}_d \mid \mathbf{v}_i \in \mathbb{R}^{n_i}, 1 \leq i \leq d\}.$$

Example 12.5 Take $\mathbf{v} = (v_1, v_2) \in \mathbb{R}^2$ and $\mathbf{w} = (w_1, w_2, w_3) \in \mathbb{R}^3$. Then,

$$\mathbf{v} \otimes \mathbf{w} = \begin{pmatrix} v_1 \cdot w_1 & v_1 \cdot w_2 & v_1 \cdot w_3 \\ v_2 \cdot w_1 & v_2 \cdot w_2 & v_2 \cdot w_3 \end{pmatrix}$$

is the rank one matrix with column space $\mathbb{R} \cdot \mathbf{v}$ and row space $\mathbb{R} \cdot \mathbf{w}$. Another common notation is $\mathbf{v}\mathbf{w}^T$. ◊

The most immediate way to see that \mathcal{S} is an algebraic variety goes as follows. We can always *flatten* a tensor $A \in \mathbb{R}^{n_1 \times \cdots \times n_d}$ into d matrices F_1, \dots, F_d , where $F_i \in \mathbb{R}^{n_i \times (\prod_{j \neq i} n_j)}$. Then, we have $A \in \mathcal{S}$ if and only if the column span of F_i has dimension at most 1 for $1 \leq i \leq d$. This is equivalent to say that the F_i are all of rank at most 1; i.e., their 2×2 -minors vanish. The dimension of the Segre variety is

$$\dim \mathcal{S} = n_1 + \cdots + n_d + 1 - d.$$

Given a d -tuple of matrices $(M_1, \dots, M_d) \in \mathbb{R}^{k_1 \times n_1} \times \dots \times \mathbb{R}^{k_d \times n_d}$ we define

$$(M_1, \dots, M_d).(\mathbf{v}_1 \otimes \dots \otimes \mathbf{v}_d) := (M_1 \mathbf{v}_1) \otimes \dots \otimes (M_d \mathbf{v}_d), \quad (12.2)$$

and we extend this action linearly to all of $\mathbb{R}^{n_1 \times \dots \times n_d}$. The action (12.2) is called *multilinear multiplication*. It induces a representation of $\mathrm{GL}(n_1) \times \dots \times \mathrm{GL}(n_d)$ into the general linear group of $\mathbb{R}^{n_1 \times \dots \times n_d}$.

Example 12.6 Let $A \in \mathbb{R}^{n_1 \times n_2}$ and $(M_1, M_2) \in \mathbb{R}^{k_1 \times n_1} \times \mathbb{R}^{k_2 \times n_2}$. Then, $(M_1, M_2).A = M_1 A M_2^T$. Thus, multilinear multiplication is a generalization of simultaneous left-right multiplication for matrices. \diamond

The symmetric analogue of the Segre variety is the Veronese variety.

Definition 12.7 The *Veronese variety* is the variety of symmetric rank-one tensors

$$\mathcal{V} := \{\mathbf{v}^{\otimes d} \mid \mathbf{v} \in \mathbb{R}^n\}.$$

Example 12.8 Let $\mathbf{v} = (x, y) \in \mathbb{R}^2$. Then,

$$\mathbf{v}^{\otimes 3} = \left(\begin{array}{cc|cc} x^3 & x^2y & x^2y & xy^2 \\ x^2y & xy^2 & xy^2 & y^3 \end{array} \right).$$

The four independent coordinates of this symmetric tensor give all monomials of degree 3 in x and y . In general, $\mathbf{v}^{\otimes d}$ is given by all monomials of degree d in the entries of \mathbf{v} . \diamond

Since \mathcal{V} is the intersection of \mathcal{S} with a linear subspace, it is an algebraic variety. Its dimension is

$$\dim \mathcal{V} = n.$$

The inner product between rank-one tensors is

$$\langle \mathbf{v}_1 \otimes \dots \otimes \mathbf{v}_d, \mathbf{w}_1 \otimes \dots \otimes \mathbf{w}_d \rangle = \langle \mathbf{v}_1, \mathbf{w}_1 \rangle \cdots \langle \mathbf{v}_d, \mathbf{w}_d \rangle.$$

12.1 Tensor Rank

The Segre variety induces a notion of rank for tensors.

$$\mathrm{rank}(A) := \min \{r \geq 0 \mid \text{there exists } A_1, \dots, A_r \in \mathcal{S} \text{ with } A = A_1 + \dots + A_r\}.$$

For matrices ($d = 2$) this coincides with the usual matrix rank. We denote tensors of rank at most r by

$$\Sigma_r := \{A \in \mathbb{R}^{n_1 \times \dots \times n_d} \mid \mathrm{rank}(A) \leq r\}.$$

A tensor of order 3 and rank r can be visualized as follows:

In the case of matrices Σ_r is a variety for every r , defined by $(r+1) \times (r+1)$ -minors. For $d \geq 3$ and $r \geq 2$, however, Σ_r is not necessarily a variety anymore. This is implied by the following result going back to the work by da Silva and Lim [46].

Proposition 12.9 For $d \geq 3$ the set of rank at most 2-tensors Σ_2 is not closed in the Euclidean topology.

Proof First consider the case $d = 3$. Let $\mathbf{x}_1, \mathbf{x}_2 \in \mathbb{R}^{n_1}$, $\mathbf{y}_1, \mathbf{y}_2 \in \mathbb{R}^{n_2}$ and $\mathbf{z}_1, \mathbf{z}_2 \in \mathbb{R}^{n_3}$ be three pairs of linearly independent vectors. Define for $\varepsilon > 0$ the tensor $A_\varepsilon \in \Sigma_2$ by

$$A_\varepsilon := \varepsilon \left(\mathbf{x}_1 + \varepsilon^{-1} \mathbf{x}_2 \right) \otimes \left(\mathbf{y}_1 + \varepsilon^{-1} \mathbf{y}_2 \right) \otimes \left(\mathbf{z}_1 + \varepsilon^{-1} \mathbf{z}_2 \right) - \varepsilon \mathbf{x}_1 \otimes \mathbf{y}_1 \otimes \mathbf{z}_1.$$

Then, $A := \lim_{\varepsilon \rightarrow 0} A_\varepsilon = \mathbf{x}_1 \otimes \mathbf{y}_1 \otimes \mathbf{z}_2 + \mathbf{x}_1 \otimes \mathbf{y}_2 \otimes \mathbf{z}_1 + \mathbf{x}_2 \otimes \mathbf{y}_1 \otimes \mathbf{z}_1$. To see that this tensor is of rank 3, we first observe that $A = (P_x, P_y, P_z).A$, where P_x is the projection onto the plane spanned by \mathbf{x}_1 and \mathbf{x}_2 , and similar for P_y and P_z . Therefore, we can assume $n_1 = n_2 = n_3 = 2$. Let us consider multilinear multiplication by $X := (\mathbf{1}_2, \mathbf{1}_2, \mathbf{h}^T)$, where $\mathbf{h} \in \mathbb{R}^2$:

$$X.A = \langle \mathbf{h}, \mathbf{z}_2 \rangle \cdot \mathbf{x}_1 \otimes \mathbf{y}_1 + \langle \mathbf{h}, \mathbf{z}_1 \rangle \cdot \mathbf{x}_1 \otimes \mathbf{y}_2 + \langle \mathbf{h}, \mathbf{z}_1 \rangle \cdot \mathbf{x}_2 \otimes \mathbf{y}_1 \quad (12.3)$$

Choosing \mathbf{h} with $\langle \mathbf{h}, \mathbf{z}_1 \rangle \neq 0$ yields a matrix of rank 2, which shows that A has rank at least two. Suppose now $A = \mathbf{u}_1 \otimes \mathbf{v}_1 \otimes \mathbf{w}_1 + \mathbf{u}_2 \otimes \mathbf{v}_2 \otimes \mathbf{w}_2$ has rank two. Among the three pairs of vectors there must be at least one that is linearly independent. We assume without restriction that $\mathbf{w}_1, \mathbf{w}_2$ are independent. We have

$$X.A = \langle \mathbf{h}, \mathbf{w}_1 \rangle \cdot \mathbf{u}_1 \otimes \mathbf{v}_1 + \langle \mathbf{h}, \mathbf{w}_2 \rangle \cdot \mathbf{u}_2 \otimes \mathbf{v}_2. \quad (12.4)$$

Let us now pick \mathbf{h} such that $\langle \mathbf{h}, \mathbf{z}_1 \rangle = 0$. By (12.3) $X.A$ has rank 1 and we must have $\langle \mathbf{h}, \mathbf{w}_1 \rangle = 0$ or $\langle \mathbf{h}, \mathbf{w}_2 \rangle = 0$ by (12.4). Without restriction we assume $\langle \mathbf{h}, \mathbf{w}_1 \rangle = 0$. This implies that \mathbf{z}_1 is a multiple of \mathbf{w}_1 , since they both satisfy the linear equation imposed by \mathbf{h} . Next, we consider \mathbf{h} with $\langle \mathbf{h}, \mathbf{w}_1 \rangle \neq 0$ but $\langle \mathbf{h}, \mathbf{w}_2 \rangle = 0$. Then, $\langle \mathbf{h}, \mathbf{z}_1 \rangle \neq 0$ and so $X.A$ has rank two by (12.3) and it has rank one by (12.4). This is a contradiction, so A can't have rank two.

For the case $d \geq 3$ we tensor A with as many factors as needed. \square

A decomposition of the form $A = A_1 + \dots + A_r$, where the $A_i \in \mathcal{S}$, is *rank decomposition*. In the signal processing literature it is also called *canonical polyadic decompositions*. One appealing property of higher order tensors is *identifiability*. That is, many tensor decompositions are actually unique (rank decompositions of matrices are never unique). The following is [40, Theorem 1.1] and [125, Lemma 28].

Theorem 12.10 Let $n_1 \geq \dots \geq n_d$ with $\prod_{i=1}^d n_i \leq 15000$ and

$$r_0 = \left\lceil \frac{\dim \mathbb{R}^{n_1 \times \dots \times n_d}}{\dim \mathcal{S}} \right\rceil = \left\lceil \frac{n_1 \cdots n_d}{1 + \sum_{i=1}^d (n_i - 1)} \right\rceil.$$

Suppose that $r < r_0$ and (n_1, \dots, n_d, r) is not one of the following cases

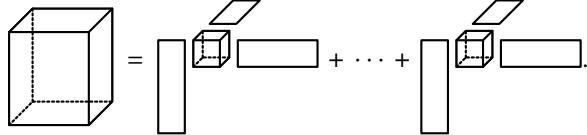
(n_1, \dots, n_d)	r
(4, 4, 3)	5
(4, 4, 4)	6
(6, 6, 3)	8
$(n, n, 2, 2)$	$2n - 1$
(2, 2, 2, 2, 2)	5
$n_1 > \prod_{i=2}^d n_i - \sum_{i=2}^d (n_i - 1)$	$r \geq \prod_{i=2}^d n_i - \sum_{i=2}^d (n_i - 1)$

Then, a general tensor in Σ_r has a unique rank- r decomposition.

Remark 12.11 Another important decomposition is the so-called *block term decomposition*. This is a decomposition of the form $A = A_1 + \dots + A_r$, where the A_i are low-multilinear rank tensors. A block term decomposition models it a mixture of distributions which allow correlations between the variables,

other than the rank decomposition, which models a mixture of independence models. An example, where this is relevant, is detecting epileptic seizures [87]. The interaction between the variables in this case is extremely complex, so that a mixture of independence models is not the appropriate model.

The definition of the block term decomposition is as follows: Let $k = (k_1, \dots, k_d)$ be a vector of integers with $1 \leq k_i \leq n_i$. Let $A \in \mathbb{R}^{n_1 \times \dots \times n_d}$ and F_1, \dots, F_d be the flattenings of A . Then, we say that A has multilinear-rank (at most) k , if $\text{rank}(F_j) \leq k_j$ for $1 \leq j \leq d$. Note that the rank decomposition above is the special case $k = (1, \dots, 1)$. For order-3 tensors a block term decomposition can be visualized as follows:



Identifiability of block term decompositions is less well-studied than for rank- r decompositions. Results exist for the decomposition of tensors into tensors of multilinear rank $(1, k_1, k_2)$ [153], $(1, k, k)$ [45, 50], $(k_1, k_2, 1)$ [139], and (k_1, k_2, k_3) [101]. \diamond

12.2 Singular Vectors and Eigenvectors

We study Euclidean Distance Degree of the Segre- and of the Veronese variety. A key property of both the Segre and Veronese variety is that they are *unirational*. One can see that each of them is the image of a polynomial map:

$$\psi : \mathbb{R}^{n_1} \times \dots \times \mathbb{R}^{n_d} \rightarrow \mathcal{S}, (\mathbf{v}_1, \dots, \mathbf{v}_d) \mapsto \mathbf{v}_1 \otimes \dots \otimes \mathbf{v}_d, \quad (12.5)$$

and

$$\nu : \mathbb{R}^n \rightarrow \mathcal{V}, \mathbf{v} \mapsto \mathbf{v}^{\otimes d}. \quad (12.6)$$

These maps are called the Segre- and Veronese-map, respectively.

Remark 12.12 Proposition 12.9 implies that for tensors of order $d \geq 3$ the problem of computing $\min_{B \in \Sigma_r} \|A - B\|$ for a tensor A can be ill-posed (the minimizer does not need to exist). In fact, da Silva and Lim [46] prove that there is full-dimensional open subset of tensors such that this problem is ill-posed. This is different for matrices, where the Eckart-Young Theorem (Theorem 2.6) provides an explicit algorithm for computing the minimizer. By contrast, the Segre- and the Veronese-variety are closed (both in the Euclidean and Zariski topology).

We first study the Euclidean Distance Degree of the Segre variety \mathcal{S} . For this, we consider a tensor $A \in \mathbb{R}^{n_1 \times \dots \times n_d}$ and the optimization problem

$$\min_{B \in \mathcal{S}} \|A - B\| = \min_{\mathbf{v}_i \in \mathbb{R}^{n_i}} \|A - \psi(\mathbf{v}_1, \dots, \mathbf{v}_d)\|.$$

The polynomial map ψ is a smooth map of constant rank, which implies that these critical values of the distance function $\mathcal{S} \rightarrow \mathbb{R}, B \mapsto \|A - B\|$ are in one-to-one correspondence to the critical values of $\|A - \psi(\mathbf{v}_1, \dots, \mathbf{v}_d)\|$ up to scaling $(\mathbf{v}_1, \dots, \mathbf{v}_d) \mapsto (t_1 \mathbf{v}_1, \dots, t_1 \mathbf{v}_d)$. Let us write

$$\|A - \psi\|^2 = \|A\|^2 - 2\langle A, \psi \rangle + \|\psi\|^2.$$

By (12.3) we have $\|\psi\|^2 = \|\mathbf{v}_1\|^2 \cdots \|\mathbf{v}_d\|^2$. We use this to get the critical equation

$$\begin{aligned}
0 &= \frac{d}{d\mathbf{v}_i} \|A - \psi\|^2 = -2 \frac{d}{d\mathbf{v}_i} \langle A, \psi \rangle + \frac{d}{d\mathbf{v}_i} (\|\mathbf{v}_1\|^2 \cdots \|\mathbf{v}_d\|^2) \\
&= \begin{pmatrix} \langle A, \mathbf{v}_1 \otimes \cdots \otimes \mathbf{v}_{i-1} \otimes \mathbf{e}_1 \otimes \mathbf{v}_{i+1} \otimes \cdots \otimes \mathbf{v}_d \rangle \\ \vdots \\ \langle A, \mathbf{v}_1 \otimes \cdots \otimes \mathbf{v}_{i-1} \otimes \mathbf{e}_{n_i} \otimes \mathbf{v}_{i+1} \otimes \cdots \otimes \mathbf{v}_d \rangle \end{pmatrix} - \left(2 \prod_{j \neq i} \|\mathbf{v}_j\|^2 \right) \mathbf{v}_i,
\end{aligned} \tag{12.7}$$

where $\mathbf{e}_1, \dots, \mathbf{e}_{n_i}$ denotes the standard basis of \mathbb{R}^{n_i} . By multilinearity we can assume that the \mathbf{v}_i all have the same norm, so that $\sigma := 2 \prod_{j \neq i} \|\mathbf{v}_j\|^2$ is constant for all i . It is then convenient to write the critical equation (12.7) using the short-hand notation $A \bullet (\mathbf{v}_1 \otimes \cdots \otimes \widehat{\mathbf{v}}_i \otimes \cdots \otimes \mathbf{v}_d) = \sigma \cdot \mathbf{v}_i$. For $d = 3$ we can visualize this as follows

$$\mathbf{v}_1 \quad \text{cube} \quad \mathbf{v}_2 = \sigma \cdot \mathbf{v}_3 \tag{12.8}$$

The critical points of the critical equations over the complex numbers are called singular vectors.

Definition 12.13 Let $A \in \mathbb{R}^{n_1 \times \cdots \times n_d}$. We say that $(\mathbf{v}_1, \dots, \mathbf{v}_d) \in \mathbb{C}^{n_1} \times \cdots \times \mathbb{C}^{n_d}$, $\mathbf{v}_i \neq 0$, is a *singular vector tuple* for A , if there exists $\sigma \in \mathbb{C}$, called *singular value*, with

$$A \bullet (\mathbf{v}_1 \otimes \cdots \otimes \widehat{\mathbf{v}}_i \otimes \cdots \otimes \mathbf{v}_d) = \sigma \cdot \mathbf{v}_i.$$

for $i = 1, \dots, d$.

For $d = 2$ this coincides with the classic definition of singular vector pairs for matrices. The singular value decomposition implies that for a general matrix $A \in \mathbb{R}^{n_1 \times n_2}$ there are precisely $\min\{n_1, n_2\}$ singular vector pairs that are all real. For higher order tensors not all singular vectors need to be real. The number of singular vectors – and hence the Euclidean Distance Degree of \mathcal{S} – is given by the following theorem due to Friedland and Ottaviani [61].

Theorem 12.14 Let $A \in \mathbb{R}^{n_1 \times \cdots \times n_d}$ be a general tensor. The number of singular vector tuples of A , up to scaling $(\mathbf{v}_1, \dots, \mathbf{v}_d) \mapsto (t_1 \mathbf{v}_1, \dots, t_1 \mathbf{v}_d)$, is the coefficient of the monomial $x_1^{n_1-1} \cdots x_d^{n_d-1}$ in the polynomial

$$\prod_{i=1}^d \frac{f_i^{n_i} - x_i^{n_i}}{f_i - x_i}, \quad f_i = \sum_{j \neq i} x_j.$$

Example 12.15 We consider the formula in Theorem 12.14 for binary tensors $A \in \mathbb{R}^{2 \times \cdots \times 2}$. In this case,

$$\prod_{i=1}^d \frac{f_i^2 - x_i^2}{f_i - x_i} = \prod_{i=1}^d (f_i + x_i) = (x_1 + \cdots + x_d)^d.$$

The coefficient of $x_1 \cdots x_d$ in this polynomial is $d!$. Consequently, the Euclidean Distance Degree of the Segre variety in $\mathbb{R}^{2 \times 2 \times 2}$ is $3! = 6$. \diamond

If we follow the approach above for symmetric tensors and the Veronese variety, we arrive at the notion of *eigenpairs of tensors*. In this case, the critical equations are $(\langle A, \mathbf{e}_1 \otimes \mathbf{v}^{\otimes(d-1)} \rangle, \dots, \langle A, \mathbf{e}_n \otimes \mathbf{v}^{\otimes(d-1)} \rangle) = \lambda \mathbf{v}$. We abbreviate this as $A \bullet \mathbf{v}^{\otimes(d-1)} = \lambda \mathbf{v}$. Similar to (12.8) we can visualize this in the case $d = 3$:

Definition 12.16 Let $A \in S^d(\mathbb{R}^n)$. We say $\mathbf{v} \in \mathbb{C}^n \setminus \{0\}$ is an *eigenvector* of A , if there exists $\lambda \in \mathbb{C}$ with

$$A \bullet \mathbf{v}^{\otimes(d-1)} = \lambda \mathbf{v}.$$

The pair (\mathbf{v}, λ) is called an *eigenpair* of A .

Eigenpairs have another interesting interpretation, next to being critical points for the Euclidean distance function on the real Veronese variety. Recall that, if $A \in S^d(\mathbb{R}^n)$ is symmetric, $F_A(\mathbf{x}) = \langle A, \mathbf{x}^{\otimes d} \rangle$ is a homogeneous polynomial of degree d in n variables. Eigenpairs correspond to fixed points of the rational map $\mathbb{P}^{n-1} \dashrightarrow \mathbb{P}^{n-1}, \mathbf{x} \mapsto (\partial F_A / \partial \mathbf{x}_1, \dots, \partial F_A / \partial \mathbf{x}_n)$ given by the gradient of F_A .

Example 12.17 Consider the symmetric matrix $A = \begin{pmatrix} 1 & 2 \\ 2 & 0 \end{pmatrix} \in S^2(\mathbb{R}^2)$ from Example 12.3. The eigenvectors equations of A are

$$\begin{pmatrix} \partial F_A / \partial x_1 \\ \partial F_A / \partial x_2 \end{pmatrix} = \begin{pmatrix} 2x_1 + 4x_2 \\ 4x_1 \end{pmatrix} = 2A\mathbf{x} = \lambda \mathbf{x}.$$

Consider also the tensor $B = \begin{pmatrix} 1 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 2 \end{pmatrix} \in S^3(\mathbb{R}^2)$ from Example 12.3. The eigenvector equations for B are

$$\begin{pmatrix} \partial F_B / \partial x_1 \\ \partial F_B / \partial x_2 \end{pmatrix} = \begin{pmatrix} 3x_1^2 - 6x_1x_2 \\ -3x_1^2 + 6x_2 \end{pmatrix} = \lambda \mathbf{x}.$$

◊

In fact, we can remove the assumption that A is symmetric from Definition 12.16 and define eigenpairs for general tensors, as well. This way, we lose the interpretations above, but we have a more general definition. Let us count the number of eigenpairs of a general tensor. The following theorem was first proved by Cartwright and Sturmfels in [32] using intersection theory. Here, we give an alternative proof.

Theorem 12.18 Let $A \in (\mathbb{R}^n)^{\otimes d}$ be general. The number of eigenvectors of A , up to scaling $u \mapsto tu$, is

$$\sum_{i=0}^{n-1} (d-1)^i.$$

Proof We use the same proof strategy as for Corollary 3.13. Let $A \in S^d(\mathbb{R}^n)$ be the symmetric tensor with $F_A(\mathbf{x}) = x_1^d + \dots + x_n^d$ (for $d = 3, n = 3$ this gives the tensor from Example 12.19). The equations for eigenpairs are then

$$x_1^{d-1} - \xi^{d-2}x_1 = \dots = x_n^{d-1} - \xi^{d-2}x_n = 0.$$

We count that this system of homogeneous polynomial equations has precisely $(d-1)^n$ regular solutions in \mathbb{P}^n . By Bézout's theorem, a general system of n polynomials with degrees $(d-1, \dots, d-1)$ also has $(d-1)^n$ regular zeros. The Parameter Continuation (Theorem 3.16) then implies that the family of systems

$$\mathcal{F} := \{F_A(\mathbf{x}) - \xi^{d-2}\mathbf{v} \mid A \in \mathbb{R}^{n \times \dots \times n}\}$$

has $(d-1)^n$ regular zeros for a general A (Theorem 3.16 works for non-homogeneous systems; we can dehomogenize the systems in \mathcal{F}_A by considering a random affine patch in \mathbb{C}^{n+1}). Moreover, for general A and a zero $F_A(\mathbf{v}) - \xi^{d-2}\mathbf{v} = 0$ we must have $\xi \neq 0$, because $F_A(\mathbf{v}) \neq 0$, since it is a general system of n homogeneous equations in n variables). The number of eigenpairs for a general A therefore is

$$\frac{(d-1)^n - 1}{d-2} = \sum_{i=0}^{n-1} (d-1)^i,$$

because we have to remove $\mathbf{v} = 0$ from the count and divide the count by $(d-2)$ to account for scaling of ξ with $(d-2)$ -th roots of unity. □

Example 12.19 The polynomial $F_A(\mathbf{x}) = x_1^3 + x_2^3$ corresponds to a $2 \times 2 \times 2$ -tensor A . The eigenpairs of A are solutions to the system of equations

$$v_1^2 - \lambda v_1 = v_2^2 - \lambda v_2 = 0.$$

If $\lambda = 0$, then $\mathbf{v} = 0$, which by definition is not an eigenvector. So, we can set $\lambda = 1$. The other solutions are $\mathbf{v} \in \{(1, 1), (0, 1), (1, 0)\}$. So, we have 3 eigenvectors up to scaling, which is consistent with the formula in Theorem 12.18. \diamond

Observe that for $d = 2$ the formula of Theorem 12.18 gives n , which is the number of eigenpairs of a general matrix $A \in \mathbb{R}^{n \times n}$. For matrices every n -tuple of linearly independent vectors can be eigenvectors of a matrix. For tensors this is not so. Abo, Sturmfels and Seigal proved in [1] that a set of d points $\mathbf{v}_1, \dots, \mathbf{v}_d$ in \mathbb{C}^2 is the eigenconfiguration of a symmetric tensor in $S^d(\mathbb{C}^2)$ if and only if d is odd, or $d = 2k$ is even and for every of the points \mathbf{v} the differential operator $(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2})^k$ annihilates the binary form $f(x, y) = \prod_{i=1}^d (b_i x - a_i y)$, where $\mathbf{u}_i = (a_i, b_i)$.

12.3 Volumes of Rank-One Varieties

In the second part of the lecture we will now address the problem of computing the volumes of the complex Segre variety $\mathcal{S}_{\mathbb{C}} := \overline{\mathcal{S}}$ and of the complex Veronese variety $\mathcal{V}_{\mathbb{C}} := \overline{\mathcal{V}}$, where $\overline{}$ denotes complex Zariski closure. This is an important problem in metric algebraic geometry by itself. We measure volumes in $\mathbb{C}^{n_1 \times \dots \times n_d}$ relative to the Euclidean inner product $\text{Re}(\langle A, B \rangle_{\mathbb{C}})$, where the Hermitian inner product is

$$\langle A, B \rangle_{\mathbb{C}} := \sum_{i_1=1}^{n_1} \cdots \sum_{i_d=1}^{n_d} \overline{a_{i_1, \dots, i_d}} \cdot b_{i_1, \dots, i_d}$$

The complex Segre variety $\mathcal{S}_{\mathbb{C}}$ consists of rank-one vectors $\mathbf{v}_1 \otimes \dots \otimes \mathbf{v}_d$, where the $\mathbf{v}_i \in \mathbb{C}^{n_i}$ are complex vectors. Similarly, $\mathcal{V}_{\mathbb{C}}$ consists of vectors $\mathbf{v}^{\otimes d}$ for $\mathbf{v} \in \mathbb{C}^n$. We observe that both $\mathcal{S}_{\mathbb{C}}$ and $\mathcal{V}_{\mathbb{C}}$ are cones; i.e., closed under scaling. In particular, they are not compact and do not have finite volume. To make a meaningful computation we pass to complex projective space \mathbb{P}^N where $N = n_1 \cdots n_d - 1$ (or $N = n^d - 1$ if the n_i are all equal) and measure the volume of the projective Segre variety and projective Veronese variety. Let us denote them by

$$\mathcal{S}_{\mathbb{P}} := \{\mathbf{v}_1 \otimes \dots \otimes \mathbf{v}_d \in \mathbb{P}^N \mid \mathbf{v}_i \in \mathbb{P}^{n_i-1}, 1 \leq i \leq d\} \quad \text{and} \quad \mathcal{V}_{\mathbb{P}} := \{\mathbf{v}^{\otimes d} \in \mathbb{P}^N \mid \mathbf{v}_i \in \mathbb{P}^n\}.$$

Furthermore, let us denote the sphere in \mathbb{C}^n by

$$\mathbb{S}^{2n-1} := \{\mathbf{a} \in \mathbb{C}^n \mid \langle \mathbf{a}, \mathbf{a} \rangle_{\mathbb{C}} = 1\},$$

where, as above in the space of tensors, $\langle \mathbf{a}, \mathbf{b} \rangle_{\mathbb{C}} = \mathbf{a}^* \mathbf{b}$ is the standard Hermitian inner product. The sphere is a real manifold of real dimension $\dim_{\mathbb{R}} \mathbb{S}^{2n-1} = 2n - 1$. We have the projection $\pi : \mathbb{S}^{2n-1} \rightarrow \mathbb{P}^{n-1}$ that sends a point $\mathbf{a} \in \mathbb{S}^{2n-1}$ to its projective class. The tangent space of \mathbb{S}^{2n-1} at a point \mathbf{a} is

$$T_{\mathbf{a}} \mathbb{S}^{2n-1} = \{\mathbf{t} \in \mathbb{C}^n \mid \text{Re}(\langle \mathbf{a}, \mathbf{t} \rangle_{\mathbb{C}}) = 0\}.$$

We have $\text{Re}(\langle \mathbf{a}, \mathbf{b} \rangle_{\mathbb{C}}) = 0$ if and only if $\langle \mathbf{a}, \mathbf{b} \rangle_{\mathbb{C}} = 0$ or $\mathbf{a} = \sqrt{-1} \cdot \mathbf{b}$. Thus, the tangent space of projective space is

$$T_{\mathbf{x}} \mathbb{P}^{n-1} = \{\mathbf{t} \in \mathbb{C}^n \mid \langle \mathbf{a}, \mathbf{t} \rangle_{\mathbb{C}} = 0\}, \quad \mathbf{x} = \pi(\mathbf{a}) \text{ for } \mathbf{a} \in \mathbb{S}^{2n-1}.$$

Complex projective space \mathbb{P}^{n-1} is a Riemannian manifold relative to the Euclidean structure $\text{Re}(\langle \mathbf{a}, \mathbf{b} \rangle)_{\mathbb{C}}$. This induces a notion of volume for subsets of \mathbb{P}^{n-1} . We have defined the metric structures of \mathbb{S}^{2n-1} and \mathbb{P}^{n-1} so that the projection π is a Riemannian submersion. This implies that the m -dimensional real volume of a measurable subset $U \subset \mathbb{P}^{n-1}$ is

$$\text{vol}_m(U) = \frac{1}{2\pi} \text{vol}_{m+1}(\pi^{-1}(U)),$$

since the preimage $\pi^{-1}(\mathbf{x})$ for $\mathbf{x} \in \mathbb{P}^{n-1}$ is a circle. For instance, the volume of projective space is

$$\text{vol}_{2(n-1)}(\mathbb{P}^{n-1}) := \frac{1}{2\pi} \text{vol}_{2n-1}(\mathbb{S}^{2n-1}) = \frac{\pi^{n-1}}{(n-1)!}. \quad (12.9)$$

In the following, we will sometimes omit the subscript from vol when the dimension is clear from the context.

We have the following result.

Proposition 12.20 Denote $m := \dim_{\mathbb{R}} \mathcal{S}_{\mathbb{P}}$. The m -dimensional volume of $\mathcal{S}_{\mathbb{P}}$ is

$$\text{vol}(\mathcal{S}_{\mathbb{P}}) = \text{vol}(\mathbb{P}^{n_1-1}) \cdots \text{vol}(\mathbb{P}^{n_d-1}).$$

Proof We define the Segre map (12.5) for projective space: $\psi_{\mathbb{P}} : \mathbb{P}^{n_1-1} \times \cdots \times \mathbb{P}^{n_d-1} \rightarrow \mathcal{S}_{\mathbb{P}}$. Then, $\psi_{\mathbb{P}}$ is a smooth embedding. Let $(\mathbf{x}_1, \dots, \mathbf{x}_d) \in \mathbb{P}^{n_1-1} \times \cdots \times \mathbb{P}^{n_d-1}$ and $\mathbf{a}_i \in \mathbb{S}^{2n_i-1}$ with $\pi(\mathbf{a}_i) = \mathbf{x}_i$ be a fixed representative for \mathbf{x}_i . Let also $\mathbf{t}_i \in \mathbb{C}^{n_i}$ with $\langle \mathbf{a}_i, \mathbf{t}_i \rangle = 0$. Then, the derivative of $\psi_{\mathbb{P}}$ maps $(\mathbf{t}_1, \dots, \mathbf{t}_d) \in T_{(x_1, \dots, x_d)}(\mathbb{P}^{n_1-1} \times \cdots \times \mathbb{P}^{n_d-1})$ to

$$\theta := \mathbf{t}_1 \otimes \mathbf{a}_2 \otimes \cdots \otimes \mathbf{a}_d + \mathbf{a}_1 \otimes \mathbf{t}_2 \otimes \cdots \otimes \mathbf{a}_d + \cdots + \mathbf{a}_1 \otimes \mathbf{a}_2 \otimes \cdots \otimes \mathbf{t}_d.$$

It follows from (12.3) that the terms in this sum are pairwise orthogonal. Therefore

$$\|\theta\|^2 = \|\mathbf{t}_1\|^2 + \|\mathbf{t}_2\|^2 + \cdots + \|\mathbf{t}_d\|^2.$$

This shows that the derivative of $\psi_{\mathbb{P}}$ preserves norms. This implies that $\psi_{\mathbb{P}}$ is volume preserving. \square

For the Veronese variety we have the following result.

Proposition 12.21 The $2(n-1)$ -dimensional volume of the projective Veronese variety is

$$\text{vol}(\mathcal{V}_{\mathbb{P}}) = d^{n-1} \cdot \text{vol}(\mathbb{P}^{n-1}).$$

Proof The proof is similar to that of Theorem 12.20. We denote the Veronese map (12.6) for projective space: $\nu_{\mathbb{P}} : \mathbb{P}^{n-1} \rightarrow \mathcal{V}_{\mathbb{P}}$. Then, also $\nu_{\mathbb{P}}$ is a smooth embedding. Let $\mathbf{x} \in \mathbb{P}^{n-1}$ and $\mathbf{a} \in \mathbb{S}^{2n-1}$ be a representative for \mathbf{x} ; i.e., $\pi(\mathbf{a}) = \mathbf{x}$. Let $\mathbf{t} \in \mathbb{C}^n$ with $\langle \mathbf{a}, \mathbf{t} \rangle = 0$. The derivative of $\nu_{\mathbb{P}}$ maps $\mathbf{t} \in T_{\mathbf{x}} \mathbb{P}^{n-1}$ to

$$\theta := \mathbf{t} \otimes \mathbf{a} \otimes \cdots \otimes \mathbf{a} + \mathbf{a} \otimes \mathbf{t} \otimes \cdots \otimes \mathbf{a} + \cdots + \mathbf{a} \otimes \mathbf{a} \otimes \cdots \otimes \mathbf{t},$$

It follows from (12.3) that the terms in this sum are pairwise orthogonal, so $\|\theta\|^2 = d\|\mathbf{t}\|^2$. This shows that the derivative of $\nu_{\mathbb{P}}$ scales norms by \sqrt{d} . This implies that

$$\text{vol}(\mathcal{V}_{\mathbb{P}}) = (\sqrt{d})^{\dim_{\mathbb{R}} \mathbb{P}^{n-1}} \cdot \text{vol}(\mathbb{P}^{n-1}) = d^{n-1} \cdot \text{vol}(\mathbb{P}^{n-1}).$$

Propositions 12.20 and 12.21 can be applied to intersection theory using Howard's *Kinematic Formula* [80]. This is a general formula for the average volume of intersections of submanifolds in homogeneous spaces. For complex projective space we have the following; see [80, Theorem 3.8 & Corollary 3.9].

Let $M \subset \mathbb{P}^N$ be a smooth manifold of complex dimension m . Then, the Kinematic formula for complex projective space is

$$\mathbb{E}_U \#(M \cap U \cdot (\mathbb{P}^{N-m} \times \{0\}^m)) = \frac{\text{vol}_{2m}(M)}{\text{vol}_{2(N-m)}(\mathbb{P}^{N-m})},$$

where the expectation is taken relative to the probability measure on the unitary group $U(n+1)$ induced by the Haar measure. If $X \subset \mathbb{P}^N$ is a smooth algebraic variety of complex dimension m , then the number of intersection points $\#(X \cap U \cdot (\mathbb{P}^{N-m} \times \{0\}^m))$ equals the degree of X for almost all U . Thus, we are taking the expected value of a constant function. This shows

$$\deg(X) = \frac{\text{vol}_{2m}(X)}{\text{vol}_{2(N-m)}(\mathbb{P}^{N-m})}, \quad m = \dim_{\mathbb{C}}(X). \quad (12.10)$$

Combined with the theorems above we obtain the following result.

Corollary 12.22

1. $\deg(\mathcal{S}_{\mathbb{P}}) = \frac{(n_1 + \cdots + n_d - d)!}{(n_1 - 1)! \cdots (n_d - 1)!}.$
2. $\deg(\mathcal{V}_{\mathbb{P}}) = d^{n-1}.$

Proof The second formula follows directly from Proposition 12.21 and (12.10). For the second formula, we recall from (12.9) the volume of projective space: $\text{vol}_{2(n-1)}(\mathbb{P}^{n-1}) = \frac{\pi^{n-1}}{(n-1)!}$. Denote

$$m = n_1 + \cdots + n_d - d = \dim_{\mathbb{C}} \mathcal{S}_{\mathbb{P}}.$$

Using Proposition 12.20 and (12.10) we then have

$$\begin{aligned} \deg(\mathcal{S}_{\mathbb{P}}) &= \frac{\text{vol}(\mathbb{P}^{n_1-1}) \cdots \text{vol}(\mathbb{P}^{n_d-1})}{\text{vol}(\mathbb{P}^m)} = \frac{\pi^{\sum_{i=1}^d (n_i - 1)}}{\pi^m} \cdot \frac{m!}{(n_1 - 1)! \cdots (n_d - 1)!} \\ &= \frac{(n_1 + \cdots + n_d - d)!}{(n_1 - 1)! \cdots (n_d - 1)!}. \end{aligned}$$

Remark 12.23 By (12.1), a linear equation on $\deg(\mathcal{V}_{\mathbb{P}})$ corresponds to the evaluation of a homogeneous polynomial of degree d in n variables. Thus, $\deg(\mathcal{V}_{\mathbb{P}}) = d^{n-1}$ means that a general system of $n-1$ homogeneous polynomials of degree d has d^{n-1} zeros.

Remark 12.24 Howard's Kinematic Formula from [80] also provides the following result for real projective space. Let $\mathbb{P}_{\mathbb{R}}^N$ denote real projective space and let $M \subset \mathbb{P}_{\mathbb{R}}^N$ be a real submanifold of real dimension m . Then, $\mathbb{E}_U \#(M \cap U \cdot (\mathbb{P}_{\mathbb{R}}^{N-m} \times \{0\}^m)) = \frac{\text{vol}_m(M)}{\text{vol}_{N-m}(\mathbb{P}_{\mathbb{R}}^{N-m})}$, where here the expectation is taken relative to the probability measure on the orthogonal group $O(n+1)$. Thus, the volume of real projective varieties can be interpreted as an "average degree". We can use the same proof strategies as above to show that the projective volume of the real Segre variety \mathcal{S} is equal to $\text{vol}(\mathbb{P}_{\mathbb{R}}^{n_1-1}) \cdots \text{vol}(\mathbb{P}_{\mathbb{R}}^{n_d-1})$ and the projective volume of the real Veronese \mathcal{V} is $\sqrt{d^{n-1}} \cdot \text{vol}(\mathbb{P}_{\mathbb{R}}^{n-1})$. The latter result was first observed by Edelman and Kostlan in their seminal paper [58] to show that a homogeneous polynomial of degree d in n variables has on the average \sqrt{d} many real zeros.

Chapter 13

Computer Vision

This lecture will be based on the survey [89].

Chapter 14

Volumes

In this chapter we discuss the problem of computing the volume of a subset X of \mathbb{R}^n that is full-dimensional and semialgebraic. Being *semialgebraic* means that X is described by a finite Boolean combination of polynomial inequalities. We say that X is *basic semialgebraic* if that description is a conjunction of polynomial inequalities. This means that our set admits a representation of the form

$$X = \{\mathbf{x} \in \mathbb{R}^n : f_1(\mathbf{x}) \geq 0 \text{ and } f_2(\mathbf{x}) \geq 0 \text{ and } \dots \text{ and } f_k(\mathbf{x}) \geq 0\},$$

where f_1, f_2, \dots, f_k are polynomials in n unknowns with real coefficients. Our task is to compute the volume of X , as reliably and accurately as possible, when the input consists of the polynomials f_1, f_2, \dots, f_k .

14.1 Calculus and Beyond

The simplest scenario arises when $k = 1$, so our semialgebraic set X is the domain of nonnegativity of one polynomial $f(\mathbf{x}) = f(x_1, \dots, x_n)$ with real coefficients. We wish to evaluate the integral

$$\text{Vol}(X) = \int_X 1 \cdot d\mathbf{x}, \quad (14.1)$$

where $d\mathbf{x}$ denotes Lebesgue measure on \mathbb{R}^n . Of course, it makes perfect sense to also consider integrals $\int_X g(\mathbf{x})d\mathbf{x}$, where $g(\mathbf{x})$ is some polynomial function. The value of such an integral is a real number which is called a *period* [98]. Our integrals are special cases of *period integrals*.

We begin with an instance where the volume can be computed explicitly using calculus.

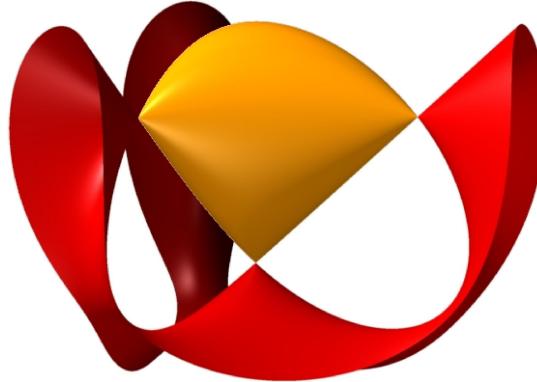


Fig. 14.1: The yellow convex body is the ellipote. It is bounded by Cayley's cubic surface.

Example 14.1 (Ellipote) Consider the set X of all points (x, y, z) in \mathbb{R}^3 such that the matrix

$$M = \begin{pmatrix} 1 & x & y \\ x & 1 & z \\ y & z & 1 \end{pmatrix}$$

is positive semidefinite. The set X is convex and semialgebraic: it consists of all points (x, y, z) in the cube $[-1, 1]^3$ such that $\det(M) = 2xyz - x^2 - y^2 - z^2 + 1$ is nonnegative. Figure 14.1 appears in [111, Figure 1.1] and it serves as the logo of the Nonlinear Algebra group at the Max-Planck Institute for Mathematics

in the Sciences in Leipzig. It illustrates several applications of algebraic geometry. In statistics, the convex set X is the set of all correlation matrices. In optimization, it is the feasible region of a semidefinite programming problem [111, Chapter 12], and it is known as the *elliptope*.

We now compute the volume of the elliptope. We begin by rewriting of its boundary surface. Solving the equation $\det(M) = 0$ for z with the quadratic formula, we obtain

$$z = xy \pm \sqrt{x^2y^2 - x^2 - y^2 + 1} = xy \pm \sqrt{(1-x^2)(1-y^2)} \quad \text{for } (x, y) \in [-1, 1]^2,$$

The plus sign gives the upper yellow surface and the minus sign gives the lower yellow surface. The volume of the elliptope X is obtained by integrating the difference between the upper function and the lower function over the square. Hence the desired volume equals

$$\text{vol}(X) = \int_{-1}^1 \int_{-1}^1 2 \sqrt{(1-x^2)(1-y^2)} dx dy = 2 \left[\int_{-1}^1 \sqrt{1-t^2} dt \right]^2.$$

The univariate integral on the right gives the area of a semicircle with radius 1. We know from trigonometry that this area equals $\pi/2$, where $\pi = 3.14159265\dots$. We conclude that

$$\text{vol}(X) = \pi^2/2 = 4.934802202\dots$$

Thus our elliptope covers about 61.7 % of the volume of the cube $[-1, 1]^3$ that surrounds it.

The number $\pi^2/2$ we found is an example of a period. It is generally much more difficult to accurately evaluate such integrals. In fact, this challenge has played an important role in the history of mathematics. Consider the problem of computing the arc length of an ellipse. This requires us to integrate the reciprocal square root of cubic polynomial $f(t)$. Such integrals are called *elliptic integrals*, and they represent periods of elliptic curves. Furthermore, in an 1841 paper, Abel introduced *abelian integrals*, where $g(t)$ is an algebraic function in one variable t . How to evaluate such an integral? This question leads us to Riemann surface and then to their Jacobians. And, violà, we arrived at the theory of *abelian varieties*.

This chapter presents two current paradigms for accurately computing integrals like (14.1). The first method rests on the theory of D -modules, that is, on the algebraic study of linear differential equations with polynomial coefficients. Our volume is found as a special value of a parametric volume function that is encoded by means of its *Picard-Fuchs differential equation*. This method, which tends to appeal to algebraic geometers, was introduced by Lairez, Mezzarobba and Safey El Din in [99].

The second approach is due to Lasserre and his collaborators [73, 146, 147]. On first glance it might appeal more to analysts and optimizers, but there is also plenty of deep algebraic structure under the hood. The idea is to consider all moments $m_{\mathbf{a}} = \int_X \mathbf{x}^{\mathbf{a}} d\mathbf{x}$ of our semialgebraic set X , where again $d\mathbf{x}$ is Lebesgue measure, and to use relations among these moments to infer an accurate approximation of $m_0 = \text{vol}(X)$. That numerical inference rests on semidefinite programming [111, Chapter 12].

14.2 D-Modules

In calculus, we learn about definite integrals in order to determine the area under a graph. Likewise, in multivariable calculus, we examine the volume enclosed by a surface. We are here interested in areas and volumes of semi-algebraic sets. When these sets depend on one or more parameters, their volumes are holonomic functions of the parameters. We explain what this means and how it can be used for accurate evaluation of volume functions. We present the method of [99], following the exposition given in [136].

Suppose that M is a D -module. The letter D denotes the *Weyl algebra* (cf. [132, 136]), written here as

$$D = \mathbb{C}\langle x_1, \dots, x_n, \partial_1, \dots, \partial_n \rangle.$$

In applications, M is usually a space of infinitely differentiable functions on a subset of \mathbb{R}^n or \mathbb{C}^n . Such D -modules are torsion-free. For a function $f \in M$, its *annihilator* is the D -ideal

$$\text{Ann}_D(f) := \{P \in D \mid P \bullet f = 0\}.$$

In general, it is a non-trivial task to compute this annihilating ideal. But, in some cases, computer algebra systems can help us to compute holonomic annihilating ideals. For rational functions $r \in \mathbb{Q}(x_1, \dots, x_n)$ this can be done in Macaulay2 with a built-in command as follows:

```
needsPackage "Dmodules"; D = QQ[x1,x2,d1,d2, WeylAlgebra => {x1=>d1,x2=>d2}];  
rnum = x1; rden = x2; I = RatAnn(rnum,rden)
```

This code fragment shows that $r = x_1/x_2$ has $\text{Ann}_D(r) = D\{\partial_1^2, x_1\partial_1 - 1, x_2\partial_1\partial_2 + \partial_1\}$.

Suppose now that $f(x_1, \dots, x_n)$ is an algebraic function. This means that f satisfies some polynomial equation $F(f, x_1, \dots, x_n) = 0$. Using the polynomial F as its input, the Mathematica package `HolonomicFunctions` can compute a holonomic representation of f . The output is a linear differential operator of lowest degree annihilating f . See Example 14.3.

Let M be a D -module and $f \in M$. We say that f is *holonomic* if, for each $i \in \{1, \dots, n\}$, there is an operator $P_i \in \mathbb{C}[x_1, \dots, x_n]\langle\partial_i\rangle \setminus \{0\}$ that annihilates f . If this holds then we say that $\text{Ann}_D(f)$ is a *holonomic D -ideal*. Suppose this is the case, and fix a general point $x_0 \in \mathbb{C}^n$. Let m_1, \dots, m_n denote the orders of the differential operators P_1, \dots, P_n in the definition of holonomic. Thus, P_k is an operator in ∂_k of order m_k whose coefficients are polynomials in x_1, \dots, x_n .

We fix initial conditions for f by specifying the following $m_1 m_2 \cdots m_n$ numerical values:

$$(\partial_1^{i_1} \cdots \partial_n^{i_n} \bullet f)|_{x=x_0} \quad \text{where } 0 \leq i_k < m_k \text{ for } k = 1, \dots, n. \quad (14.2)$$

Then the operators P_1, \dots, P_n together with the initial conditions (14.2) specify the function f .

Many interesting functions are holonomic. To begin with, every rational function r in $\mathbf{x} = (x_1, \dots, x_n)$ is holonomic, because r is annihilated by $r(\mathbf{x})\partial_i - \partial r / \partial x_i$ for $i = 1, 2, \dots, n$. By clearing denominators in this operator, we obtain a non-zero $P_i \in \mathbb{C}[\mathbf{x}]\langle\partial_i\rangle$ with $m_i = 1$ that annihilates r . See the Macaulay2 example above. These operators, together with fixing the value $r(\mathbf{x}_0)$ at a general point $\mathbf{x}_0 \in \mathbb{C}^n$, constitute a canonical holonomic representation of the rational function r .

Holonomic functions in one variable are solutions to ordinary linear differential equations with rational function coefficients. Examples include algebraic functions, some elementary trigonometric functions, hypergeometric functions, Bessel functions, period integrals, and many more. But, not every nice function is holonomic. A necessary condition for a meromorphic function $f(x)$ to be holonomic is that it has only finitely many poles in \mathbb{C} . For a concrete example, we start with the holonomic function $\sin(x)$. This is annihilated by the operator $\partial^2 + 1$. Its reciprocal $f(x) = \frac{1}{\sin(x)}$ has infinitely many poles, so is not holonomic. Hence the class of holonomic functions is not closed under division. It is also not closed under composition of functions, since both $\frac{1}{x}$ and $\sin(x)$ are holonomic. We record the following fact:

Proposition 14.2 *Let $f(\mathbf{x})$ be holonomic and $g(\mathbf{x})$ algebraic. Then $f(g(\mathbf{x}))$ is holonomic.*

For the proof see [136, Proposition 2.3]. The term ‘‘holonomic function’’ is due to Zeilberger [154]. Koutschan [97] developed practical algorithms for manipulating holonomic functions. These are implemented in his Mathematica package `HolonomicFunctions`, as seen below.

Example 14.3 Every algebraic function $f(\mathbf{x})$ in n variables is holonomic. Let $n = 2$ and consider the function $y = f(x)$ that is defined by $y^4 + x^4 + \frac{xy}{100} - 1 = 0$. Its annihilator in D can be computed as follows:

```
<< RISC`HolonomicFunctions`
q = y^4 + x^4 + x*y/100 - 1
ann = Annihilator[Root[q, y, 1], Der[x]]
```

This Mathematica code determines an operator P of lowest order in $\text{ann}_D(f)$. We find

$$\begin{aligned} P = & (2x^4 + 1)^2 (25600000000x^{12} - 76800000000x^8 + 76799999973x^4 - 25600000000) \partial^3 \\ & + 6x^3(2x^4 + 1)(51200000000x^{12} + 76800000000x^8 - 30719999946x^4 + 17919999973) \partial^2 \\ & + 3x^2(102400000000x^{16} + 204800000000x^{12} + 289279999572x^8 - 350719999444x^4 + 30719999953) \partial \\ & - 3x(102400000000x^{16} + 204800000000x^{12} + 145919999796x^8 - 104959999828x^4 + 5119999993). \end{aligned}$$

This operator is an encoding of the algebraic function $y = f(x)$ as a holonomic function.

In computer algebra, one represents a real algebraic number as a root of a polynomial with coefficients in \mathbb{Q} . However, this *minimal polynomial* does not specify the number uniquely. For that, one also needs an isolating interval or sign conditions on derivatives. The situation is analogous for encoding a holonomic function f in n variables. We specify f by a holonomic system of linear PDEs together with a list of initial conditions. The canonical holonomic representation is one possibility. Initial conditions such as (14.2) are designed to determine the function uniquely inside the linear space $\text{Sol}(I)$, where $I \subseteq \text{Ann}_D(f)$.

For instance, in Example 14.3, we would need three initial conditions to specify the function $f(\mathbf{x})$ uniquely inside the 3-dimensional solution space to our operator P . We could fix the values at three distinct points, or we could fix the value and the first two derivatives at one special point.

To be more precise, we generalize the canonical representation (14.2) as follows. A *holonomic representation* of a function f is a holonomic D -ideal $I \subseteq \text{ann}_D(f)$ together with a list of linear conditions that specify f uniquely inside the finite-dimensional solution space of holomorphic solutions. The existence of this representation makes f a *holonomic function*. The next example is meant to show the relevance of holonomic functions for metric algebraic geometry.

Example 14.4 (The area of a TV screen) Fix the quartic polynomial

$$q(x, y) = x^4 + y^4 + \frac{1}{100}xy - 1. \quad (14.3)$$

We are interested in the semi-algebraic set $S = \{(x, y) \in \mathbb{R}^2 \mid q(x, y) \leq 0\}$. This convex set is a slight modification of a set known in the optimization literature as “the TV screen”. Our aim is to compute the area of the semi-algebraic convex set S as accurately as is possible.

One can get a rough idea of the area of S by sampling. This is illustrated in Figure 14.2. From the polynomial $q(x, y)$ we read off that S is contained in the square defined by $-1.2 \leq x, y \leq 1.2$. We sampled 10000 points uniformly from that square, and for each sample we checked the sign of q . Points inside S are drawn in blue and points outside S are drawn in pink. By multiplying the area $(2.4)^2 = 5.76$ of the square with the fraction of the number of blue points among the samples, we learn that the area of the TV screen is approximately 3.7077.

We now compute the area more accurately using D -modules. Let $\text{pr}: S \rightarrow \mathbb{R}$ be the projection on the x -coordinate, and write $v(x) = \ell(\text{pr}^{-1}(x) \cap S)$ for the length of a fiber. This function is holonomic and it satisfies the third-order differential operator in Example 14.3.

The map pr has two branch points $x_0 < x_1$. They are the real roots of the resultant

$$\text{Res}_y(q, \partial q / \partial y) = 25600000000x^{12} - 76800000000x^8 + 76799999973x^4 - 25600000000. \quad (14.4)$$

These values can be written in radicals, but we take an accurate floating point representation:

$$x_1 = -x_0 = 1.000254465850258845478545766643566750080196276158976351763236\dots$$

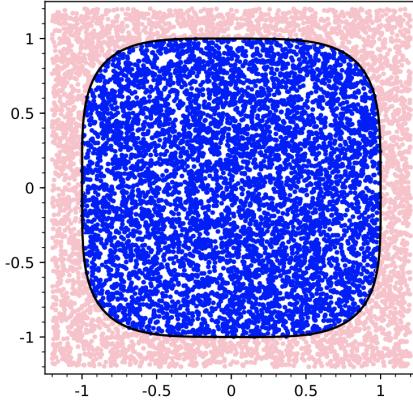


Fig. 14.2: The TV screen is the convex region consisting of the blue points.

The desired area equals $\text{vol}(S) = w(x_1)$, where w is the holonomic function

$$w(x) = \int_{x_0}^x v(t) dt.$$

One operator that annihilates w is $P\partial$, where $P \in \text{ann}_D(v)$ is the third-order operator above. To get a holonomic representation of w , we also need some initial conditions. Clearly, $w(x_0) = 0$. Further initial conditions on w' are derived by evaluating v at other points. By plugging values for x into (14.3) and solving for y , we find $w'(0) = 2$ and $w'(\pm 1) = 1/\sqrt[3]{100}$. Thus, we now have four linear constraints on our function w , albeit at different points.

Our goal is to determine a unique function $w \in \text{Sol}(P\partial)$ by incorporating these four initial conditions, and then to evaluate w at x_1 . To this end, we proceed as follows. Let $x_{\text{ord}} \in \mathbb{R}$ be any point at which $P\partial$ is not singular. Using the command `local_basis_expansion` that is built into the SAGE package `ore_algebra`, we compute a basis of local series solutions to $P\partial$ at the point x_{ord} . Since that point is non-singular, that basis has the following form:

$$\begin{aligned} s_{x_{\text{ord}},0}(x) &= 1 + O((x - x_{\text{ord}})^4), \\ s_{x_{\text{ord}},1}(x) &= (x - x_{\text{ord}}) + O((x - x_{\text{ord}})^4), \\ s_{x_{\text{ord}},2}(x) &= (x - x_{\text{ord}})^2 + O((x - x_{\text{ord}})^4), \\ s_{x_{\text{ord}},3}(x) &= (x - x_{\text{ord}})^3 + O((x - x_{\text{ord}})^4). \end{aligned} \quad (14.5)$$

Locally at x_{ord} , our solution is given by a unique choice of four coefficients $c_{x_{\text{ord}},i}$, namely

$$w(x) = c_{x_{\text{ord}},0} \cdot s_{x_{\text{ord}},0}(x) + c_{x_{\text{ord}},1} \cdot s_{x_{\text{ord}},1}(x) + c_{x_{\text{ord}},2} \cdot s_{x_{\text{ord}},2}(x) + c_{x_{\text{ord}},3} \cdot s_{x_{\text{ord}},3}(x).$$

At a regular singular point x_{rs} , complex powers of x and $\log(x)$ can appear in the local basis at x_{rs} . Any initial condition at that point determines a linear constraint on these coefficients. For instance, $w'(0) = 2$ implies $c_{0,1} = 2$, and similarly for our initial conditions at $-1, 1$ and x_0 . One challenge is that the initial conditions pertain to different points. To address this, we calculate transition matrices that relate the basis (14.5) of series solutions at one point to the basis at another point. These are invertible 4×4 matrices.

With the method described above, we find the basis of series solutions at x_1 , along with a system of four linear constraints on the four coefficients $c_{x_1,i}$. These constraints are derived from the initial conditions at $0, \pm 1$ and x_0 , using the 4×4 transition matrices. By solving these linear equations, we compute the

desired function value up to any desired precision:

$$w(x_1) = 3.708159944742162288348225561145865371243065819913934709438572\dots$$

In conclusion, this number is the area of the TV screen S defined by the polynomial $q(x, y)$.

Before computing an example in 3-space, let us first come back to properties of holonomic functions. Holonomic functions are very well-behaved with respect to many operations. They turn out to have remarkable closure properties. In the following, let f and g be functions in n variables $\mathbf{x} = (x_1, \dots, x_n)$.

Proposition 14.5 *If f, g are holonomic functions, then both $f + g$ and $f \cdot g$ are holonomic.*

Proof For each index $i \in \{1, 2, \dots, n\}$, there exist non-zero operators P_i and Q_i in $\mathbb{C}[\mathbf{x}]\langle\partial_i\rangle$ which satisfy $P_i \bullet f = Q_i \bullet g = 0$. Set $n_i = \text{order}(P_i)$ and $m_i = \text{order}(Q_i)$. The $\mathbb{C}(\mathbf{x})$ -linear span of the set $\{\partial_i^k \bullet f\}_{k=0, \dots, n_i}$ has dimension $\leq n_i$. Similarly, the span of the set $\{\partial_i^k \bullet g\}_{k=0, \dots, m_i}$ has dimension $\leq m_i$.

Now consider $\partial_i^k \bullet (f + g) = \partial_i^k \bullet f + \partial_i^k \bullet g$. The $\mathbb{C}(\mathbf{x})$ -linear span of $\{\partial_i^k \bullet (f + g)\}_{k=0, \dots, n_i+m_i}$ has dimension $\leq n_i + m_i$. Hence, there exists a non-zero operator $S_i \in \mathbb{C}[\mathbf{x}]\langle\partial_i\rangle$, such that $S_i \bullet (f + g) = 0$. Since this holds for all indices i , we conclude that the sum $f + g$ is holonomic.

A similar proof works for the product $f \cdot g$. For each $i \in \{1, 2, \dots, n\}$, we now consider the set $\{\partial_i^k \bullet (f \cdot g)\}_{k=0, 1, \dots, n_i m_i}$. By applying Leibniz' rule for taking derivatives of a product, we find that the $m_i n_i + 1$ generators are linear dependent over the rational function field $\mathbb{C}(\mathbf{x})$. Hence, there is a non-zero operator $T_i \in \mathbb{C}[\mathbf{x}]\langle\partial_i\rangle$ such that $T_i \bullet (f \cdot g) = 0$. We conclude that the product $f \cdot g$ is holonomic. \square

The proof above gives a linear algebra method for computing an annihilating D -ideal I of finite holonomic rank for $f + g$ (resp. of $f \cdot g$), starting from such D -ideals for f and g . The following example, similar to one in [154, Section 4.1], illustrates Proposition 14.5.

Example 14.6 ($n = 1$) Consider the functions $f(x) = \exp(x)$ and $g(x) = \exp(-x^2)$. Their canonical holonomic representations are $I_f = \langle\partial - 1\rangle$ with $f(0) = 1$ and $I_g = \langle\partial + 2x\rangle$ with $g(0) = 1$. We are interested in the function $h = f + g$. Its first partial derivatives are

$$\begin{pmatrix} h \\ \partial \bullet h \\ \partial^2 \bullet h \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & -2x \\ 1 & 4x^2 - 2 \end{pmatrix} \cdot \begin{pmatrix} f \\ g \end{pmatrix}.$$

By computing the left kernel of this 3×2 -matrix, we find that $h = f + g$ is annihilated by

$$I_h = \langle(2x + 1)\partial^2 + (4x^2 - 3)\partial - 4x^2 - 2x + 2\rangle, \quad \text{with } h(0) = 2, h'(0) = 1.$$

For the product $j = f \cdot g$ we have $j' = f'g + fg' = f \cdot g + f \cdot (-2xg) = (1 - 2x)j$, so the canonical holonomic representation of j is the D -ideal $I_j = \langle\partial + 2x - 1\rangle$ with $j(0) = 1$.

Proposition 14.7 *Let f be holonomic in n variables and $m < n$. Then the restriction of f to the coordinate subspace $\{x_{m+1} = \dots = x_n = 0\}$ is a holonomic function in the first m variables x_1, \dots, x_m .*

Proof For $i \in \{m + 1, \dots, n\}$, we consider the right ideal $x_i D$ in the Weyl algebra D . This ideal is a left module over $D_m = \mathbb{C}\langle x_1, \dots, x_m, \partial_1, \dots, \partial_m \rangle$. The sum of these ideals with $\text{Ann}_D(f)$ is hence a left D_m -module. Its intersection with D_m is called the *restriction ideal*:

$$(\text{Ann}_D(f) + x_{m+1}D + \dots + x_nD) \cap D_m. \tag{14.6}$$

By [132, Prop. 5.2.4], this D_m -ideal is holonomic and it annihilates $f(x_1, \dots, x_m, 0, \dots, 0)$. \square

Proposition 14.8 *The partial derivatives of a holonomic function are holonomic functions.*

Proof Let f be holonomic and $P_i \in \mathbb{C}[x]\langle\partial_i\rangle \setminus \{0\}$ with $P_i \bullet f = 0$ for all i . We can write P_i as $P_i = \tilde{P}_i \partial_i + a_i(x)$, where $a_i \in \mathbb{C}[x]$. If $a_i = 0$, then $\tilde{P}_i \bullet \frac{\partial f}{\partial x_i} = 0$ and we are done. Assume $a_i \neq 0$. Since both a_i and f are holonomic, by Proposition 14.5, there is a non-zero linear operator $Q_i \in \mathbb{C}[x]\langle\partial_i\rangle$ such that $Q_i \bullet (a_i \cdot f) = 0$. Then $Q_i \tilde{P}_i$ annihilates $\partial f / \partial x_i$. \square

A key insight from the theory of D -modules (see [132, Section 5.5]) is that integration is dual, in the sense of the Fourier transform, to restriction. Here is the dual to Proposition 14.7.

Proposition 14.9 *Let $f: \mathbb{R}^n \rightarrow \mathbb{C}$ be a holonomic function. Then the definite integral*

$$F(x_1, \dots, x_{n-1}) = \int_a^b f(x_1, \dots, x_{n-1}, x_n) dx_n$$

is a holonomic function in $n - 1$ variables, assuming the integral converges.

By dualizing (14.6), we obtain the following D_m -ideal, known as the *integration ideal*:

$$(\text{Ann}_D(f) + \partial_{m+1} D + \dots + \partial_n D) \cap D_m \quad \text{for } m < n.$$

The expression is dual to the restriction ideal (14.6) under the Fourier transform. This exchanges x_i and ∂_i . If $m = n - 1$ then the integration ideal annihilates the holonomic function F above.

Equipped with our tools for holonomic functions, we now return to computing volumes of compact semi-algebraic sets. We follow the work of P. Lairez, M. Mezzarobba and M. Safey El Din in [99]. They compute this volume by deriving a differential operator that encodes the period of a certain integral [98]. Here is the definition. Let $R(t, x_1, \dots, x_n)$ be a rational function and consider the formal period integral

$$\oint R(t, x_1, \dots, x_n) dx_1 \cdots dx_n. \quad (14.7)$$

Fix an open subset Ω of either \mathbb{R} or \mathbb{C} . An analytic function $\phi: \Omega \rightarrow \mathbb{C}$ is a *period* of the integral (14.7) if, for any $s \in \Omega$, there exists a neighborhood $\Omega' \subseteq \Omega$ of s and an n -cycle $\gamma \subset \mathbb{C}^n$ with the following property. For all $t \in \Omega'$, γ is disjoint from the poles of $R_t := R(t, \bullet)$ and

$$\phi(t) = \int_{\gamma} R(t, x_1, \dots, x_n) dx_1 \cdots dx_n. \quad (14.8)$$

If this holds, then there exists an operator $P \in D \setminus \{0\}$ of the Fuchsian class annihilating $\phi(t)$.

Let $S = \{f \leq 0\} \subset \mathbb{R}^n$ be a compact basic semi-algebraic set, defined by a polynomial $f \in \mathbb{Q}[x_1, \dots, x_n]$. Let $\text{pr}: \mathbb{R}^n \rightarrow \mathbb{R}$ denote the projection on the first coordinate. The set of *branch points* of pr is the following subset of the real line, which is assumed to be finite:

$$\Sigma_f = \{p \in \mathbb{R} \mid \exists x = (x_2, \dots, x_n) \in \mathbb{R}^{n-1} : f(p, x) = 0 \text{ and } \frac{\partial f}{\partial x_i}(p, x) = 0 \text{ for } i = 2, \dots, n\}.$$

The polynomial in the unknown p that defines Σ_f is obtained by eliminating x_2, \dots, x_n . It can be represented as a multivariate resultant, generalizing the Sylvester resultant in (14.4).

Fix an open interval I in \mathbb{R} with $I \cap \Sigma_f = \emptyset$. For any $x_1 \in I$, the set $S_{x_1} := \text{pr}^{-1}(x_1) \cap S$ is compact and semi-algebraic in $(n - 1)$ -space. We are interested in its volume. By [99, Theorem 9], the function $v: I \rightarrow \mathbb{R}$, $x_1 \mapsto \text{vol}_{n-1}(S_{x_1})$ is a period of the rational integral

$$\frac{1}{2\pi i} \oint \frac{x_2}{f(x_1, x_2, \dots, x_n)} \frac{\partial f(x_1, x_2, \dots, x_n)}{\partial x_2} dx_2 \cdots dx_n. \quad (14.9)$$

Let $e_1 < e_2 < \dots < e_K$ be the branch points in Σ_f and set $e_0 = -\infty$ and $e_{K+1} = \infty$. This specifies the pairwise disjoint open intervals $I_k = (e_k, e_{k+1})$. They satisfy $\mathbb{R} \setminus \Sigma_f = \bigcup_{k=0}^K I_k$. Fix the holonomic functions $w_k(t) = \int_{e_k}^t v(x_1) dx_1$. The volume of S then is obtained as

$$\text{vol}_n(S) = \int_{e_1}^{e_K} v(x_1) dx_1 = \sum_{k=1}^{K-1} w_k(e_{k+1}).$$

How does one compute such an expression? As a period of the rational integral (14.9), the volume v is a holonomic function on each interval I_k . A key step is to find an operator $P \in D_1$ that annihilates $v|_{I_k}$ for all k . Then the product $P\partial$ annihilates the functions $w_k(x_1)$ for all k . By imposing sufficiently many initial conditions, we can reconstruct the functions w_k from the operator $P\partial$. One initial condition that comes for free for each k is $w_k(e_k) = 0$.

The differential operator P is known as the *Picard–Fuchs equation* of the period in question. The following software packages can be used to compute such Picard–Fuchs equations:

- `HolonomicFunctions` by C. Koutschan in **Mathematica**,
- `ore_algebra` by M. Kauers in **SAGE**,
- `periods` by P. Lairez in **MAGMA**,
- `Ore_Algebra` by F. Chyzak in **Maple**.

We now apply this to compute volumes. Starting from the polynomial f , we compute the Picard–Fuchs operator $P \in D_1$ along with sufficiently many compatible initial conditions. For each interval I_k , where $k = 1, \dots, K-1$, we perform the following steps, here described for the `ore_algebra` package in **SAGE**:

1. Using the command `local_basis_expansion`, compute a local basis of series solutions for the linear differential operator $P\partial$ at various points in $[e_k, e_{k+1}]$.
2. Using the command `op.numerical_transition_matrix`, numerically compute a transition matrix for the series solution basis from one point to another one.
3. From the initial conditions construct linear relations between the coefficients in the local basis extensions. Using step (ii), transfer them to the branch point e_{k+1} .
4. Plug in to the local basis extension at e_{k+1} and thus evaluate the volume of $S \cap \text{pr}^{-1}(I_k)$.

We illustrate this recipe by computing the volume of a convex body in 3-space, shown in Figure 14.3.

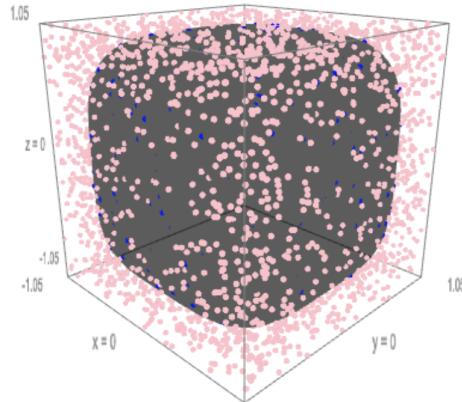


Fig. 14.3: The quartic bounds the convex region consisting of the gray points.

Example 14.10 (Quartic surface) Fix the quartic polynomial

$$f(x, y, z) = x^4 + y^4 + z^4 + \frac{x^3y}{20} - \frac{xyz}{20} - \frac{yz}{100} + \frac{z^2}{50} - 1, \quad (14.10)$$

and consider the set $S = \{(x, y, z) \in \mathbb{R}^3 \mid f(x, y, z) \leq 0\}$. Our aim is to compute $\text{vol}_3(S)$.

As in Example 14.4 with the TV screen, we can get a rough idea of the volume of S by sampling. This is illustrated in Figure 14.3. Our set S is compact, convex, and contained in the cube defined by $-1.05 \leq x, y, z \leq 1.05$. We sampled 10000 points uniformly from that cube. For each sample we checked the sign of $f(x, y, z)$. By multiplying the volume $(2.1)^3 = 9.261$ of the cube by the fraction of the number of gray points and the number of sampled points, SAGE found within few seconds that $\text{vol}(S) \approx 6.4771$. In order to obtain a higher precision, we now compute the volume of our set S with help of D -modules.

Let $\text{pr}: \mathbb{R}^3 \rightarrow \mathbb{R}$ be the projection onto the x -coordinate. Let $v(x) = \text{vol}_2(\text{pr}^{-1}(x) \cap S)$ denote the area of the fiber over any point x in \mathbb{R} . We write $e_1 < e_2$ for the two branch points of the map pr restricted to the quartic surface $\{f = 0\}$. They can be computed with resultants. The projection has 36 complex branch points. The first two of them are real and therefore are the branch points of pr . We obtain $e_1 \approx -1.0023512$ and $e_2 \approx 1.0024985$. By [99, Theorem 9], the area function $v(x)$ is a period of the rational integral

$$\frac{1}{2\pi i} \oint \frac{y}{f(x, y, z)} \frac{\partial f(x, y, z)}{\partial y} dy dz.$$

We set $w(t) = \int_{e_1}^t v(x) dx$. The desired 3-dimensional volume equals $\text{vol}_3(S) = w(e_2)$.

Using Laierez' implementation periods in MAGMA, we compute a differential operator P of order eight that annihilates $v(x)$. Again, $P\partial$ then annihilates $w(x)$. One initial condition is $w(e_1) = 0$. We obtain eight further initial conditions $w'(x) = \text{vol}_2(S_x)$ for points $x \in (e_1, e_2)$ by running the same algorithm for the 2-dimensional semi-algebraic slices $S_x = \text{pr}^{-1}(x) \cap S$. In other words, we make eight subroutine calls to an area measurement as in Example 14.4. From these nine initial conditions we derive linear relations of the coefficients in the local basis expansion at e_2 . These computations are run in SAGE as described in steps (i), (ii), (iii) and (iv) above. We find the approximate volume of our convex body S to be

$$\begin{aligned} &\approx 6.438832480572893544740733895969956188958420889235116976266328923128826 \\ &9155273887642162091495583989038294311376088934526903525560097601024171 \\ &190804769405534826558114212766135380613959757935305271022089419155701 \\ &52158647017087400219438452914068685622775954171509711339913473405961 \\ &7632892206072085516332397969163383760070738760107318247752061504714 \\ &367250460900923409066377732273390396822296235214963623286613117557 \\ &930687544148360721225681053481178760058264738867105810326818911 \\ &578448323758536767168707442532146029753762594261578920477859. \end{aligned}$$

This numerical value is guaranteed to be accurate up to 550 digits.

14.3 Lasserre's Method

In this section present the second method for computing volumes, based on semidefinite programming. This was developed by Lasserre and his collaborators. See [73, 146, 147] and references therein. We consider an inclusion of semialgebraic sets $K \subset B \subset \mathbb{R}^n$, where K and B are compact. Here B is a set that serves as a bounding box, like $B = [-1, 1]^n$. We assume that the moments of Lebesgue measure on B are known or easy-to-compute. In other words, we assume that we have access to the values of the integrals

$$\beta_{\mathbf{u}} = \int_B \mathbf{x}^{\mathbf{u}} d\mathbf{x} = \int_B x_1^{u_1} x_2^{u_2} \cdots x_n^{u_n} dx_1 dx_2 \cdots dx_n \quad \text{for } \mathbf{u} \in \mathbb{N}^n.$$

The moments $m_{\mathbf{u}}$ of Lebesgue measure on X are unknown. These will be our decision variables:

$$m_{\mathbf{u}} = \int_K \mathbf{x}^{\mathbf{u}} dx = \int_X x_1^{u_1} x_2^{u_2} \cdots x_n^{u_n} dx_1 dx_2 \cdots dx_n \quad \text{for } \mathbf{u} \in \mathbb{N}^n. \quad (14.11)$$

Our aim is to compute $m_0 = \text{vol}(K)$. The idea is to use the following infinite-dimensional linear program: *Maximize the integral $\int d\mu$, where μ and $\hat{\mu}$ range over measures on \mathbb{R}^n , where μ is supported on K , $\hat{\mu}$ is supported on B , and the sum $\mu + \hat{\mu}$ is Lebesgue measure on B .*

The unique optimal solution $(\mu, \hat{\mu})$ to this linear program can be characterized as follows: μ^* is Lebesgue measure on K , $\hat{\mu}^*$ is Lebesgue measure on $B \setminus K$, and the optimal value is $\text{vol}(K) = \int d\mu^*$. This is described in [147, equation (1)]. The linear programming (LP) dual is given in [147, equation (2)].

We can express our linear program in terms of the moment sequences $\mathbf{m} = (m_{\mathbf{u}})$ and $\hat{\mathbf{m}} = (\hat{m}_{\mathbf{u}})$ of the two unknown measures μ and $\hat{\mu}$. Namely, we paraphrase: *Maximize m_0 subject to $m_{\mathbf{u}} + \hat{m}_{\mathbf{u}} = \beta_u$ for all $\mathbf{u} \in \mathbb{N}^d$, where \mathbf{m} and $\hat{\mathbf{m}}$ are valid moment sequences of measures on \mathbb{R}^n , with m supported on X .* This brings us to the moment problem, which is the question how to characterize valid moment sequences. This is a problem with a long history in mathematics, and an exact characterization is very difficult. However, in recent years, it has been realized that there are effective necessary conditions. These involve semidefinite programming formulations in finite dimensions, which are built via the *localizing matrices* we now define.

Let $K = \{\mathbf{x} \in \mathbb{R}^n : f(\mathbf{x}) \geq 0\}$ be defined by a single polynomial $f = \sum_{\mathbf{w}} c_{\mathbf{w}} \mathbf{x}^{\mathbf{w}}$ in n variables. Fix an integer d that exceeds the degree of f . We shall construct three symmetric matrices of format $\binom{n+d}{d} \times \binom{n+d}{d}$ whose entries are linear in the decision variables. The rows and columns of our matrices are indexed by elements $\mathbf{u} \in \mathbb{N}^n$ with $|\mathbf{u}| = u_1 + \cdots + u_n$ at most d . These correspond to monomials $\mathbf{x}^{\mathbf{u}}$ of degree $\leq d$.

Our first matrix $M_d(\mathbf{m})$ has the entry $m_{\mathbf{u}+\mathbf{v}}$ in row \mathbf{u} and column \mathbf{v} . Our second matrix $M_d(\hat{\mathbf{m}})$ as the entry $\hat{m}_{\mathbf{u}+\mathbf{v}}$ in row \mathbf{u} and column \mathbf{v} . And, finally, our third matrix $M_d(f\mathbf{m})$ has the entry $\sum_{\mathbf{w}} c_{\mathbf{w}} m_{\mathbf{u}+\mathbf{v}+\mathbf{w}}$ in row \mathbf{u} and column \mathbf{v} . We consider the following semidefinite program:

$$\begin{aligned} & \text{Maximize } m_0 \text{ subject to } m_{\mathbf{u}} + \hat{m}_{\mathbf{u}} = \beta_u \text{ for all } \mathbf{u} \in \mathbb{N}^d \text{ with } |\mathbf{u}| \leq d, \text{ where} \\ & \text{the symmetric matrices } M_d(m), M_d(\hat{m}) \text{ and } M_d(f\mathbf{m}) \text{ are positive semidefinite.} \end{aligned} \quad (14.12)$$

Here, the third matrix is usually replaced by $M_{d'}(f\mathbf{m})$ where $d' = d - \lceil \deg(f)/2 \rceil$. The objective function value depends on d , and it decreases as d increases. The limit for $d \rightarrow \infty$ is equal to the volume of X . Indeed, this sequence of SDP problems is an approximation to the infinite-dimensional linear programming problem above. The convergence property was proved in [73].

The remainder of this section will demonstrate how one can solve (14.12) in practice. It is based on [73, 146, 147], and we discuss an implementation in **Mathematica**. This material was developed by Chiara Meroni, and we are very grateful to her for allowing us to include it in these lecture notes.

Our point of departure is the following question: given a sequence of real numbers $\mathbf{m} = (m_{\alpha})_{\alpha}$, does there exist a set S and a measure μ_S supported on S such that (14.11) holds? Given $d \in \mathbb{N}$, denote by \mathbb{N}_d^n the set of multiindices $\alpha \in \mathbb{N}^n$ such that $|\alpha| = \alpha_1 + \dots + \alpha_n \leq d$. Fix a semialgebraic set K as above, let $r = \lceil \frac{\deg f}{2} \rceil$, and consider an arbitrary sequence of real numbers $\mathbf{m} = (m_{\alpha})_{\alpha}$ that is indexed by \mathbb{N}_d^n .

The *moment matrix* and the *localizing matrix* associated with this sequence are respectively

$$M_d(\mathbf{m}) = \left(m_{\alpha+\beta} \right)_{\alpha, \beta \in \mathbb{N}_d^n}, \quad M_{d-r}(f\mathbf{m}) = \left(\sum_{\mathbf{w} \in W} c_{\mathbf{w}} m_{\mathbf{w}+\alpha+\beta} \right)_{\alpha, \beta \in \mathbb{N}_d^n}. \quad (14.13)$$

The moment matrix has size $\binom{n+d}{d} \times \binom{n+d}{d}$ whereas the localizing matrix has size $\binom{n+d-r}{d-r} \times \binom{n+d-r}{d-r}$. A necessary condition for a sequence $\mathbf{m} = (m_{\alpha})_{\alpha}$ to have a representing measure supported on K is that for

every $d \in \mathbb{N}$ the matrix inequalities $M_d(\mathbf{m}) \succeq 0$ and $M_{d-r}(f\mathbf{m}) \succeq 0$ hold. This result is a formulation of Putinar's Positivstellensatz [73, Theorem 2.2]. In particular, the positive definiteness of the moment matrix is a necessary condition for \mathbf{m} to have a representing measure; the inequality with the localizing matrix forces the support of the representing measure to be contained in the superlevel set $\{f(\mathbf{x}) \geq 0\}$, namely K .

Example 14.11 As a sanity check, consider the disc $K = \{(x, y) \in \mathbb{R}^2 \mid f = 1 - x^2 - y^2 \geq 0\}$. Its moments are

$$m_{(\alpha_1, \alpha_2)} = ((-1)^{\alpha_1} + 1)((-1)^{\alpha_2} + 1) \frac{\Gamma\left(\frac{\alpha_1+1}{2}\right)\Gamma\left(\frac{\alpha_2+1}{2}\right)}{4\Gamma\left(\frac{1}{2}(\alpha_1 + \alpha_2 + 4)\right)},$$

where Γ denotes the usual Gamma function. For $d = 3$, the moment and localizing matrices in (14.13) are

$$M_3(\mathbf{m}) = \begin{pmatrix} \pi & 0 & \frac{\pi}{4} & 0 & 0 & 0 & 0 & \frac{\pi}{4} & 0 & 0 \\ 0 & \frac{\pi}{4} & 0 & \frac{\pi}{8} & 0 & 0 & 0 & 0 & \frac{\pi}{24} & 0 \\ \frac{\pi}{4} & 0 & \frac{\pi}{8} & 0 & 0 & 0 & 0 & \frac{\pi}{24} & 0 & 0 \\ 0 & \frac{\pi}{8} & 0 & \frac{5\pi}{64} & 0 & 0 & 0 & 0 & \frac{\pi}{64} & 0 \\ 0 & 0 & 0 & \frac{\pi}{4} & 0 & \frac{\pi}{24} & 0 & 0 & 0 & \frac{\pi}{8} \\ 0 & 0 & 0 & 0 & \frac{\pi}{24} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\pi}{24} & 0 & \frac{\pi}{64} & 0 & 0 & \frac{\pi}{64} \\ 0 & 0 & 0 & 0 & \frac{\pi}{24} & 0 & 0 & \frac{\pi}{64} & 0 & 0 \\ \frac{\pi}{4} & 0 & \frac{\pi}{24} & 0 & 0 & 0 & \frac{\pi}{8} & 0 & 0 & 0 \\ 0 & \frac{\pi}{24} & 0 & \frac{\pi}{64} & 0 & 0 & 0 & \frac{\pi}{64} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\pi}{8} & 0 & \frac{\pi}{64} & 0 & 0 & \frac{5\pi}{64} \end{pmatrix}, \quad M_2(f\mathbf{m}) = \begin{pmatrix} \frac{\pi}{2} & 0 & \frac{\pi}{12} & 0 & 0 & \frac{\pi}{12} \\ 0 & \frac{\pi}{12} & 0 & 0 & 0 & 0 \\ \frac{\pi}{12} & 0 & \frac{\pi}{32} & 0 & 0 & \frac{\pi}{96} \\ 0 & 0 & 0 & \frac{\pi}{12} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\pi}{96} & 0 \\ \frac{\pi}{12} & 0 & \frac{\pi}{96} & 0 & 0 & \frac{\pi}{32} \end{pmatrix},$$

These two matrices are symmetric and positive definite.

We consider the infinite-dimensional *linear program* on measures whose optimal value is the volume of $K \subset B$. The program was stated above. We use the formulation in [73, Equation 3.1] and [147, Equation 1]:

$$\begin{aligned} P : \quad & \max_{\mu_K, \mu_{B \setminus K}} \int d\mu_K \\ & \text{s.t. } \mu_K + \mu_{B \setminus K} = \mu_B^*. \end{aligned} \tag{14.14}$$

Here μ_S is a positive finite Borel measure supported on S , and μ_B^* is the Lebesgue measure on B . The adjective "infinite-dimensional" refers to the fact that we are optimizing over a set of measures, which is uncountable. Based on the theory of dual Banach spaces, one can talk about dual convex bodies, and construct a duality theory for LP. In our case, the dual to the space of positive finite Borel measures is the set of positive continuous functions. This observation leads to the definition of an LP dual to P :

$$\begin{aligned} P^* : \quad & \inf_{\gamma} \int \gamma d\mu_B^* \\ & \text{s.t. } \gamma \geq \mathbf{1}_K, \end{aligned} \tag{14.15}$$

where γ is a positive continuous function on B and $\mathbf{1}_K$ is the indicator function of K . There is no duality gap between P and P^* , i.e. the optimal values of (14.14) and (14.15) coincide. Notice that the optimal value of P^* is an infimum and not a minimum, since we are approximating the *discontinuous* indicator function $\mathbf{1}_K$ using continuous functions. This detail explains the slow rate of approximation of the basic method.

The infinite-dimensional LP can be approximated by a hierarchy of finite-dimensional *semidefinite programs* [100]. The optimal values of the hierarchy converge monotonically to the optimal value of the LP [73, Theorem 3.2]. There is again a primal and dual version of the SDP. In our setting, the primal is

$$\begin{aligned} P_d : \quad & \max_{\mathbf{m}, \widehat{\mathbf{m}}} m_0 \\ \text{s.t. } & \mathbf{m} + \widehat{\mathbf{m}} = \mathbf{b}, \quad M_d(\mathbf{m}) \geq 0, \quad M_d(\widehat{\mathbf{m}}) \geq 0, \quad M_{d-r}(f\mathbf{m}) \geq 0. \end{aligned} \quad (14.16)$$

Here $\mathbf{m} = (m_\alpha)_{\alpha \in \mathbb{N}_{2d}^n}$, $\widehat{\mathbf{m}} = (\widehat{m}_\alpha)_{\alpha \in \mathbb{N}_{2d}^n}$, and \mathbf{b} contains the moments of B indexed by \mathbb{N}_{2d}^n . This formulation is [147, Equation 3]. The optimal value of P_d is an upper bound for $\text{vol}(K)$, since we are optimizing over a larger set. The dual SDP is [73, Equation 3.6], which is formulated using sums of squares of polynomials. The authors of [73, 146, 147] implemented the SDPs using **GloptiPoly** MATLAB. Our computations in the next examples are performed in **Mathematica**. We are going to include the linear condition $\mathbf{m} + \widehat{\mathbf{m}} = \mathbf{b}$ inside the condition on the moment matrix of $\widehat{\mathbf{m}}$, by imposing directly that $M_d(\mathbf{b} - \mathbf{m}) \geq 0$.

Example 14.12 (TV screen) Fix $K_1 = \{(x, y) \in [-1.2, 1.2]^2 \mid f_1(x, y) \geq 0\} \subset \mathbb{R}^2$ where $f_1 = -q$ is the quartic in (14.3). This convex set shown in Figures 14.2 and 14.4. Recall that $\text{vol}(K_1) = 3.7081599447\dots$

Let us now try the SDP formulation above, with $d = 10$. The moment matrices $M_{10}(\mathbf{m})$ and $M_{10}(\mathbf{b} - \mathbf{m})$ have format 66×66 . For instance, the second matrix looks like

$$M_{10}(\mathbf{b} - \mathbf{m}) = \begin{pmatrix} 4-m_{(0,0)} & -m_{(0,1)} & \frac{4}{3}-m_{(0,2)} & -m_{(0,3)} & \cdots \\ -m_{(0,1)} & \frac{4}{3}-m_{(0,2)} & -m_{(0,3)} & \frac{4}{5}-m_{(0,4)} & \cdots \\ \frac{4}{3}-m_{(0,2)} & -m_{(0,3)} & \frac{4}{5}-m_{(0,4)} & -m_{(0,5)} & \cdots \\ -m_{(0,3)} & \frac{4}{5}-m_{(0,4)} & -m_{(0,5)} & \frac{4}{7}-m_{(0,6)} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

The localizing matrix $M_8(f_1\mathbf{m})$ has format 45×45 . Its (α, β) entry equals

$$m_{\alpha+\beta} - m_{(4,0)+\alpha+\beta} - m_{(0,4)+\alpha+\beta} - \frac{1}{100}m_{(1,1)+\alpha+\beta}.$$

The optimal value of the semidefinite program P_{10} is $4.4644647361\dots$, the optimal value of P_{14} is $4.3679560947\dots$, and for P_{18} we get $4.3241824171\dots$. These numbers are upper bounds for the actual volume, as predicted. However, these bounds are still far from the truth.

Example 14.13 (Elliptope) Set $f_2(x, y) = 1 - x^2 - y^2 - z^2 + 2xyz$. This defines the elliptope $K_2 = \{x, y \in [-1, 1]^3 \mid f_2(x, y) \geq 0\} \subset \mathbb{R}^3$, which is shown in Figures 14.1 and 14.4. We already know $\text{vol } K_2 = \frac{\pi^2}{2} = 4.934802202\dots$. The upper bounds computing from the semidefinite program for $d = 4, 8, 12$ are respectively $7.3254012963\dots$, $6.6182632506\dots$, and $6.303035372\dots$. This is still pretty bad.

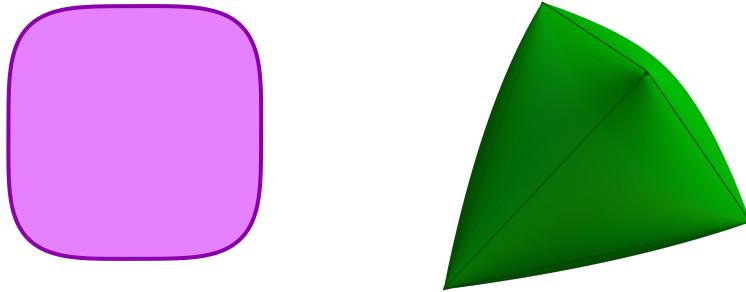


Fig. 14.4: Left: the TV screen from Example 14.12. Right: the elliptope from Example 14.13.

Examples 14.12 and 14.13 suggest that the convergence of the SDP approximation is quite slow. To improve the convergence, one uses the method of *Stokes constraints*. This was introduced and analyzed

in [146, 147] and we shall now explain it. In the infinite-dimensional linear program P^* (and in the SDP hierarchy) we aim to approximate a piecewise-differentiable function, $\mathbf{1}_K$ with continuous functions (respectively, polynomials). This produces the well-known *Gibbs effect*, creating many oscillations near the boundary of K in the polynomial solutions of the SDP. To remedy this, we add linear constraint that do not modify the infinite-dimensional LP problem but add more information to the finite-dimensional SDP. One concrete way to do this uses Stokes' theorem and the fact that f vanishes on the boundary ∂K of K .

Let U be an open region in \mathbb{R}^n such that the Euclidean closure of U is our semialgebraic set K . Since ∂K is smooth almost everywhere, the classical Stokes Theorem applies. This theorem states that

$$\int_{\partial K} \omega = \int_K d\omega$$

for any $(n - 1)$ -differential form ω on \mathbb{R}^n . One consequence of Stokes' Theorem is *Gauss' formula*

$$\int_{\partial K} V(\mathbf{x}) \cdot \hat{n}(\mathbf{x}) d\mathcal{H}^{n-1}(\mathbf{x}) = \int_K \operatorname{div} V(\mathbf{x}) d\mathbf{x}.$$

Here $V(\mathbf{x})$ is a vector field, div denotes divergence, $\hat{n}(\mathbf{x})$ is the exterior normal vector at $\mathbf{x} \in \partial K$, and \mathcal{H}^{n-1} is $(n - 1)$ -dimensional Hausdorff measure. If the vector field is a scalar field times a constant vector $\mathbf{c} \in \mathbb{R}^n$, say $V(\mathbf{x}) = v(\mathbf{x})\mathbf{c}$, then we obtain the following equations:

$$\mathbf{c} \cdot \left(\int_{\partial K} v(\mathbf{x}) \hat{n}(\mathbf{x}) d\mathcal{H}^{n-1}(\mathbf{x}) \right) = \int_K \operatorname{div}(v(\mathbf{x})\mathbf{c}) d\mathbf{x} = \mathbf{c} \cdot \left(\int_K \nabla v(\mathbf{x}) d\mathbf{x} \right).$$

This holds because $\operatorname{div}(v(\mathbf{x})\mathbf{c}) = \nabla v(\mathbf{x}) \cdot \mathbf{c} + v(\mathbf{x}) \operatorname{div} \mathbf{c}$ and the divergence of a constant vector is zero. Since this identity holds for every $\mathbf{c} \in \mathbb{R}^n$, we have

$$\int_{\partial K} v(\mathbf{x}) \hat{n}(\mathbf{x}) d\mathcal{H}^{n-1}(\mathbf{x}) = \int_K \nabla v(\mathbf{x}) d\mathbf{x}. \quad (14.17)$$

If $v = 0$ on ∂K , then the left hand side of (14.17) is zero. This condition can be expressed in terms of measures and distributions, and added to (14.14) and (14.15) as in [147, Equation 17 and Remark 3].

In the setting of our SDP hierarchy, the Stokes constraints are written as follows. Let $v(\mathbf{x}) = f(\mathbf{x})\mathbf{x}^\alpha$ for any multiindex $\alpha \in \mathbb{N}^n$ with $|\alpha| \leq d + 1 - \deg f$. Then we require

$$\nabla(f(\mathbf{x})\mathbf{x}^\alpha)|_{\mathbf{x}^\beta \rightarrow m_\beta} = 0.$$

We now replace each monomial by its moment. This yields n new linear conditions for each α as above.

Example 14.14 For the SDP in Examples 14.12 and 14.13, the Stokes constraints for a given α are:

K_1 :

$$\begin{aligned} \alpha_1 m_{\alpha+(-1,0)} - (\alpha_1 + 4)m_{\alpha+(3,0)} - \alpha_1 m_{\alpha+(-1,4)} - \frac{\alpha_1 + 1}{100}m_{\alpha+(0,1)} &= 0, \\ \alpha_2 m_{\alpha+(0,-1)} - \alpha_2 m_{\alpha+(4,-1)} - (\alpha_2 + 4)m_{\alpha+(0,3)} - \frac{\alpha_2 + 1}{100}m_{\alpha+(1,0)} &= 0, \end{aligned}$$

K_2 :

$$\begin{aligned} \alpha_1 m_{\alpha+(-1,0,0)} - (\alpha_1 + 2)m_{\alpha+(1,0,0)} - \alpha_1 m_{\alpha+(-1,2,0)} - \alpha_1 m_{\alpha+(-1,0,2)} + 2(\alpha_1 + 1)m_{\alpha+(0,1,1)} &= 0, \\ \alpha_2 m_{\alpha+(0,-1,0)} - \alpha_2 m_{\alpha+(2,-1,0)} - (\alpha_2 + 2)m_{\alpha+(0,1,0)} - \alpha_2 m_{\alpha+(0,-1,2)} + 2(\alpha_2 + 1)m_{\alpha+(1,0,1)} &= 0, \\ \alpha_3 m_{\alpha+(0,0,-1)} - \alpha_3 m_{\alpha+(2,0,-1)} - \alpha_3 m_{\alpha+(0,2,-1)} - (\alpha_3 + 2)m_{\alpha+(0,0,1)} + 2(\alpha_3 + 1)m_{\alpha+(1,1,0)} &= 0. \end{aligned}$$

Table 14.1 compares the optimal values of the SDP (14.13) with and without Stokes constraints.

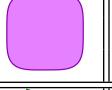
K	Volume	d	without Stokes		with Stokes	
			$\max P_d$	time	$\max P_d$	time
	3.708159...	10	4.464464...	0.621093	3.709994...	0.482376
		15	4.367956...	3.545369	3.708191...	3.738137
		20	4.324182...	14.906281	3.708163...	20.592531
	4.934802...	4	7.325401...	0.124392	5.612716...	0.077315
		8	6.618263...	7.222441	4.976796...	7.178571
		12	6.303035...	696.886298	4.937648...	1105.619231

Table 14.1: The optimal values of (14.13) with and without Stokes constraints for Examples 14.12 and 14.13. The column “ $\max P_d$ ” displays the optimal value, whereas the column “time” gives the time, in seconds, for running the command `SemidefiniteOptimization` in `Mathematica`.

As Table 14.1 shows, the convergence with Stokes constraints is much faster than without them. The intuition is that now, with the (dual) Stokes constraints added to P^* , the function we approximate is not just the indicator function of K . A detailed explanation, for a variant of the Stokes constraints, is given in [146]. The authors prove that, when adding this new type of constraints, the optimal solution of the new P^* becomes a minimum. This eliminates any kind of Gibbs effect, and guarantees faster convergence. In [146], the authors mention that, from numerical experiments, it is reasonable to expect that the original Stokes constraints and the new Stokes constraints are equivalent, but there is no formal proof of this statement yet. We close with the remark that general semialgebraic sets fit into this framework; see [73, 146, 147].

Chapter 15

Sampling

This chapter is about methods for sampling from a real algebraic variety $X \subset \mathbb{R}^n$. This means we want to compute a finite subset $S \subset X$, which we call a *sample*. An example of a sample on a curve is shown in Figure 15.1. The sample S yields a discrete approximation of X that can be used to explore properties of the variety. For instance, if $g : X \rightarrow \mathbb{R}$ is a function we can find a lower bound for the optimization problem $\max_{x \in X} g(x)$ by computing $\max_{s \in S} g(s)$, or we can estimate the integral $\int_{x \in X} g(x) dx / \text{vol}(X)$ (provided X has finite volume) by $\frac{1}{|S|} \sum_{s \in S} g(s)$. Asmussen and Glynn [7] underline the importance of sampling methods as follows:

“Sampling-based computational methods are a fundamental part of the numerical toolset across an enormous number of different applied domains”.

In Section 15.1 we discuss in detail how samples can be used to compute topological information of X .

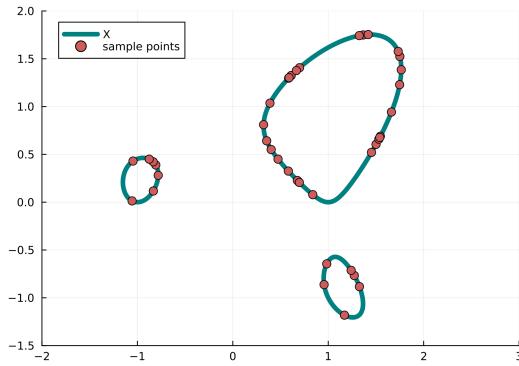


Fig. 15.1: A sample of points on the curve $X = \{x^4 + y^4 - 2x^2 - 2xy^2 - y + 1 = 0\}$.

We will discuss two approaches to sampling. The first approach concerns sampling methods with density guarantees. These methods have in common that they generate a (possibly random) sample $S \subset X$ that is ε -dense in X . This property of the sample S is defined next.

Definition 15.1 A finite subset $S \subset X$ is called ε -dense in X or a ε -sample for X , if for all $x \in X$ there exists $s \in S$ with $\|x - s\| < \varepsilon$.

The second approach to sampling is to generate points from a prescribed probability distribution on X . For instance, if X is compact, we could be interested in sampling from the uniform distribution.

In fact, since we are computing random samples, it is enough to replace the variety X by its smooth locus $\text{Reg}(X)$ and sample from $\text{Reg}(X)$. To keep the notation simple, though, in the following we will simply assume that X is a smooth manifold embedded in \mathbb{R}^n .

15.1 Computing the Homology from Finite Samples

We first recall a theorem due to Niyogi, Smale and Weinberger [119]. Their result gives conditions for when the homology of a smooth manifold X embedded in \mathbb{R}^n can be computed from a finite sample S . The idea is to compute the homology of the union of ε -balls $U = \bigcup_{s \in S} B_\varepsilon(s)$ of an ε -sample S . The homology groups of a union of balls U can be computed from the associated Čech-complex. The theorem explains how small ε must be for this to work.

Theorem 15.2 Let $\varepsilon > 0$, $S \subset X$ be a ε -sample for X , and $U = \bigcup_{s \in S} B_\varepsilon(s)$ be the union of ε -balls around points in S . Let τ be the reach of X . If $\varepsilon < \sqrt{\frac{3}{20}}\tau$, then X is a deformation retract of U . In particular, the homology of X equals the homology of U .

Proof See [119, Proposition 3.1]. \square

It was shown in [130] that we can replace the reach τ in Theorem 15.2 by what is called the *local reach* $\tau(\mathbf{x})$. For $\mathbf{x} \in X$ the local reach is defined as

$$\tau(\mathbf{x}) := \sup \{r \geq 0 \mid \text{for all } \mathbf{u} \in B_r(\mathbf{x}) \text{ there is a unique minimizer of } X \rightarrow \mathbb{R}, \mathbf{x} \mapsto \|\mathbf{x} - \mathbf{u}\|\}$$

If $\varepsilon < \frac{4}{5}\tau(s)$ for all points s in a ε -dense sample $S \subset X$, then X is a deformation retract of $U = \bigcup_{s \in S} B_\varepsilon(s)$ (see [130] for a proof). Notice that $\tau = \inf_{\mathbf{x} \in X} \tau(\mathbf{x})$, so using the local reach instead of the reach for upper bounding ε can give make significant difference.

Interestingly, if we only want to compute homology for small dimensions we can relax the conditions on ε even more. For this we recall the definition of *weak feature size* from [38]. The weak feature size is always greater or equal than the reach. For the definition we first need to introduce the notion of k -bottlenecks.

Definition 15.3 Let $k \geq 2$. For $B = \{\mathbf{x}_1, \dots, \mathbf{x}_k\} \subset X$, $\#B = k$, let $\Gamma(B)$ be the union of the centers of all $(n-1)$ -spheres passing through $\mathbf{x}_1, \dots, \mathbf{x}_k$. If $N_{\mathbf{x}_1}X \cap \dots \cap N_{\mathbf{x}_k}X \cap \Gamma(B) \cap \text{conv}(B) \neq \emptyset$, we call B a k -bottleneck of X . Its size is $\ell(B) := \inf_{\mathbf{u} \in \Gamma(B)} \|\mathbf{x}_1 - \mathbf{u}\|$.

If k is larger than the Euclidean Distance Degree $\text{EDD}(X)$, then there are not k -bottlenecks, because there exists no center of a sphere $\mathbf{u} \in \mathbb{R}^n$ with more than $\text{EDD}(X)$ many critical points on X . The weak feature size is then the smallest size of all k -bottlenecks:

$$\text{wfs}(X) := \min_{2 \leq k \leq \text{EDD}(X)} \inf \{\ell(B) \mid B \text{ is a } k\text{-bottleneck of } X\}.$$

The following was proved in [130].

Theorem 15.4 Let $\varepsilon < \text{wfs}(X)$ and $S \subset X$ be an ε -dense sample. Construct the 2-dimensional Vietoris-Rips complex C with vertices S as follows: Add the edge spanned by $\mathbf{x}, \mathbf{y} \in S$ to C , if and only if:

1. $\|\mathbf{x} - \mathbf{y}\| \leq 2\varepsilon$, or
2. $\|\mathbf{x} - \mathbf{y}\| \leq \sqrt{32}\varepsilon$ and there is $\mathbf{z} \in S$ with $\|\mathbf{x} - \mathbf{z}\|, \|\mathbf{y} - \mathbf{z}\| < 2\varepsilon$.

Moreover, add the 2-simplex spanned by $\mathbf{x}, \mathbf{y}, \mathbf{z} \in S$ to C , if and only if there is an edge between \mathbf{x} and \mathbf{y} , between \mathbf{x} and \mathbf{z} , and between \mathbf{y} and \mathbf{z} . Then, $H_0(X) \cong H_0(C)$ and $H_1(X) \cong H_1(C)$.

Remark 15.5 Theorem 15.4 is based on [38, Theorem 1], where it is shown that for $\varepsilon < \text{wfs}(X)$ the tubular neighborhood $\bigcup_{\mathbf{x} \in X} B_\varepsilon(\mathbf{x})$ is homotopy equivalent to X .

15.2 Sampling with Density Guarantees

This section presents two sampling algorithms that guarantee to compute an ε -sample. Both algorithms compute a sample of $X \cap R$, where

$$R = [a_1, b_1] \times \dots \times [a_n, b_n] \subset \mathbb{R}^n$$

is a box. If X is compact, we can compute a box R such that $X \subset R$ as follows. We first sample a point $\mathbf{u} \in \mathbb{R}^n$ at random. Then, we compute the ED critical points on X with respect to \mathbf{u} ; i.e., the critical points

of the Euclidean distance function $X \rightarrow \mathbb{R}, \mathbf{x} \mapsto \|\mathbf{x} - \mathbf{u}\|$. From this we infer $r := \max_{\mathbf{x} \in X} \|\mathbf{x} - \mathbf{u}\|$ and set R to be the box with center q and side length $2r$.

The first sampling algorithm we present is from [56]. Let $R = [a_1, b_1] \times \cdots \times [a_n, b_n]$ be a box. The basic idea for sampling from $X \cap R$ is to sample points $\mathbf{u} \in \mathbb{R}^n$ and then to collect the ED critical points with respect to \mathbf{u} . The complexity of this approach therefore depends on the Euclidean Distance Degree of X .

The algorithm in [56] works recursively by dividing the sides of the box R in half, thus splitting R into 2^n subboxes. In addition, one implements a database \mathcal{D} that contains information about all the regions in R that already have been covered by at least one sample point. Algorithm 4 provides a complete description. The correctness of this algorithm is proved in [56].

Theorem 15.6 (Theorem 4.4 in [56]) *Algorithm 4 terminates and outputs an ε -dense sample of $X \cap R$.*

Algorithm 4: The algorithm from [56].

```

1 Input: A real algebraic variety  $X \subset \mathbb{R}^n$ , a real number  $\varepsilon > 0$  and a box  $R = [a_1, b_1] \times \cdots \times [a_n, b_n]$ 
2 Output: An  $\varepsilon$ -dense sample  $S \subset X \cap R$ .
3 Initialize  $S = \emptyset$  and  $\mathcal{D} = \emptyset$ . The set  $S$  will contain the sample points. The set  $\mathcal{D}$  serves as a database containing
   balls in  $\mathbb{R}^n$  that have already been covered in the process of the algorithm.
4 for each subbox  $R'$  of  $R$  that is not yet covered do
5   Compute the midpoint  $\mathbf{u}$  of  $R'$ .
6   Compute the real ED critical points  $E \subset X$  with respect to  $\mathbf{u}$  and compute  $r := \min_{\mathbf{x} \in X} \|\mathbf{x} - \mathbf{u}\|$ .
7   Add the points in  $E$  to  $S$ .
8   Add  $B_r(\mathbf{u})$  to  $\mathcal{D}$  (this ball does not contain any point in  $X$ , so we do not need to consider this region any
      further and can label it as being covered).
9   Add  $B_\varepsilon(\mathbf{y})$  for  $\mathbf{y} \in E$  to  $\mathcal{D}$ .
10  if the union of balls in  $\mathcal{D}$  cover  $R'$  then
11    | Label  $R'$  and all of its subboxes as covered.
12  else
13    | Split  $R'$  into  $2^n$  smaller subboxes.
14  end
15 end
16 if all subboxes of  $R$  are labeled as covered then
17  | return  $S$ .

```

The second algorithm we present is from [130]. This algorithm is also based on computing Euclidean critical points on X , but in addition adds linear slices to the sampling. We need a few definitions. We denote $d := \dim X$. For every $1 \leq k \leq d$ denote by \mathcal{T}_k be the set of subsets of $\{1, \dots, n\}$ with k elements. Given a set $T = \{t_1, \dots, t_k\} \in \mathcal{T}_k$ we let $V_T \subseteq \mathbb{R}^n$ be the k -dimensional coordinate plane spanned by $\mathbf{e}_{t_1}, \dots, \mathbf{e}_{t_k}$. For $\delta > 0$ consider the grid

$$G_T(\delta) := \{\delta \cdot (a_1 \cdot \mathbf{e}_{t_1} + \cdots + a_d \cdot \mathbf{e}_{t_k}) \mid a_1, \dots, a_k \in \mathbb{Z}\} \cong \delta \cdot \mathbb{Z}^k.$$

Let $\pi_T : \mathbb{R}^n \rightarrow V_T$ be the projection. Then, the linear spaces $\pi_T^{-1}(g)$ for $g \in G_T(\delta)$ are given by the faces of a cubical tessellation with side length δ .

Let b be the width of the smallest bottleneck of X (we have defined and discussed bottlenecks in detail in Section 7.1). The algorithm from [130] takes as input a number $0 < \delta < \frac{1}{\sqrt{n}} \min\{\varepsilon, 2b\}$. Then, the sample is given by

$$S_\delta := \bigcup_{T \in \mathcal{T}_d} \bigcup_{g \in G_T(\delta)} X \cap \pi_T^{-1}(g); \quad (15.1)$$

i.e., S_δ consists of the points of that are obtained by intersecting X with the collection of linear spaces $\pi_T^{-1}(g)$ ranging over $T \in \mathcal{T}_d$ and $g \in G_T(\delta)$. The dimension of $\pi_T^{-1}(g)$ equals the codimension of X . To ensure transversal intersections we can always modify $G_T(\delta)$ by a random translation.

If $d = \dim X > 1$, the algorithm computes an additional sample. First, we sample a random point $\mathbf{u} \in \mathbb{R}^n$. Denote by $E(T, g, \mathbf{u})$ the ED critical points on $X \cap \pi_T^{-1}(g)$ with respect to \mathbf{u} . The additional sample is

$$S'_\delta = \bigcup_{k=1}^d \bigcup_{T \in \mathcal{T}_d} \bigcup_{g \in G_T(\delta)} E(T, g, \mathbf{u}), \quad (15.2)$$

The motivation for this extra sample is that $E(T, g, \mathbf{u})$ contains a point on every connected component of $X \cap \pi_T^{-1}(g)$. The algorithm is summarized in Algorithm 5.

Theorem 15.7 (Theorem 4.6 in [130]) Algorithm 5 outputs an ε -dense sample of $X \cap R$.

Algorithm 5: The algorithm from [130].

```

1 Input: A real algebraic variety  $X \subset \mathbb{R}^n$ , a real number  $\delta > 0$  with  $\delta < \frac{1}{\sqrt{n}} \min\{\varepsilon, 2b\}$ , where  $b$  is the width of the
smallest bottleneck of  $X$ , and a box  $R = [a_1, b_1] \times \cdots \times [a_n, b_n]$ 
2 Output: An  $\varepsilon$ -dense sample  $S \subset X \cap R$ .
3 Initialize  $S_\delta = \emptyset$  and  $S'_\delta$ .
4 for  $T \in \mathcal{T}_d$  and  $g \in G_T(\delta)$  do
5   | Compute  $X \cap \pi_T^{-1}(g)$ .
6   | Add the points in  $X \cap \pi_T^{-1}(g)$  to  $S_\delta$ .
7 end
8 if  $\dim X > 1$  then
9   | Set  $d := \dim X$ .
10  | for  $1 \leq k \leq d$  do
11    |   | for  $T \in \mathcal{T}_k$  and  $g \in G_T(\delta)$  do
12    |   |   | Sample a random point  $\mathbf{u} \in \mathbb{R}^n$ .
13    |   |   | Compute  $E(T, g, \mathbf{u})$ , which are the ED critical points on  $X \cap \pi_T^{-1}(g)$  with respect to  $\mathbf{u}$ .
14    |   |   | Add the points in  $E(T, g, \mathbf{u})$  to  $S'_\delta$ .
15  | end
16 end
17 Set  $S := S_\delta \cup S'_\delta$ .
18 return  $S$ .

```

15.3 Sampling from Probability Distributions

Let π be a probability measure on X . In this section we discuss algorithms for sampling from π . In this context, π is also called the *target distribution*. We will review one popular class of methods for sampling from probability distributions on X , namely *Markov-Chain Monte Carlo* (MCMC) methods. In the following, \mathcal{A} denotes the σ -algebra of X .

Example 15.8 Let X be compact and dx be the Lebesgue measure on X . For a measurable set $A \in \mathcal{A}$ let $\text{vol}(A) = \int_A \text{dx} < \infty$ be the volume of A . The probability distribution with probability measure given by $\pi(A) := \text{vol}(A) / \text{vol}(X)$ is called the *uniform distribution* on X . For instance, the sample in Figure 15.1 consists of i.i.d. (independent and uniformly distributed) points from the uniform distribution on a plane curve $X = \{x^4 + y^4 - 2x^2 - 2xy^2 - y + 1 = 0\}$.

Before we discuss sampling algorithms let us briefly recall the following result by Niyogi, Smale and Weinberger [119], which implies that sampling from the uniform distribution on X can be used to generate ε -samples with high probability.

Proposition 15.9 *Let $\varepsilon > 0$ and $0 < \delta < 1$. Suppose X is compact and has reach $\tau > 0$. Set*

$$\theta := \arcsin\left(\frac{\varepsilon}{\tau}\right), \quad \omega := \frac{\text{vol}(X)}{\cos^k \theta}, \quad \beta_1 := \frac{\omega}{\text{vol}(B_\varepsilon(\mathbf{0}))}, \quad \beta_2 := \frac{\omega}{\text{vol}(B_{\varepsilon/8}(\mathbf{0}))}$$

(here, $B_\varepsilon(\mathbf{0})$ is the unit ball of radius ε). Let $n > \beta_1(\log \beta_2 - \log \delta)$. For a sample of i.i.d. points $S = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ from the uniform distribution on X we have $\text{Prob}(S \text{ is a } \varepsilon\text{-sample for } X) > 1 - \delta$.

Let us now put the focus on sampling by using MCMC methods. These methods set up a *Markov process* on X . Let us recall some basic definitions from the theory of Markov chains; see, e.g., [109, Chapter 3]. In this context, X is also called a *state space*. A *Markov kernel* is a map $p : X \times \mathcal{A} \rightarrow [0, 1]$, such that

1. $p(\mathbf{x}, \cdot)$ is a probability measure for all $\mathbf{x} \in X$.
2. $p(\cdot, A)$ is measurable function for all $A \in \mathcal{A}$.

A stochastic process $\mathbf{x}_0, \mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \dots$ on X is a sequence of random points on X . Markov processes encompass a special type of stochastic processes. Let $x \in X$ be a fixed point. A (time-homogeneous) Markov process with starting point \mathbf{x} is the stochastic process defined by $\mathbf{x}_0 = \mathbf{x}$ and for $k \geq 1$:

$$\text{Prob}(\mathbf{x}_1 \in A_0, \dots, \mathbf{x}_k \in A_k \mid \mathbf{x}_0 = \mathbf{x}) := \int_{\mathbf{y}_1 \in A_1} \cdots \int_{\mathbf{y}_{k-1} \in A_{k-1}} p(\mathbf{x}, d\mathbf{y}_1) \cdot p(\mathbf{y}_1, d\mathbf{y}_2) \cdots p(\mathbf{y}_{k-1}, A_k).$$

For fixed $\mathbf{z} \in X$ we have

$$\text{Prob}(\mathbf{x}_k \in A \mid \mathbf{x}_{k-1} = \mathbf{z}, \mathbf{x}_{k-2}, \dots, \mathbf{x}_0) = \text{Prob}(\mathbf{x}_k \in A \mid \mathbf{x}_{k-1} = \mathbf{z}) = \int_{\mathbf{y} \in A} p(\mathbf{z}, d\mathbf{y}); \quad (15.3)$$

see, e.g., [109, Proposition 3.4.3]. Equation (15.3) is called the *Markov property*. It means that the probability law of the next point in the process only depends on the current state, but not on earlier states. Due to its role in (15.3) the kernel p is also called *transition probability*.

Example 15.10 (Markov Chains in \mathbb{R}^2) Let us consider two examples of Markov Chains in \mathbb{R}^2 starting at the origin. For the first we take the kernel $p_1(\mathbf{x}, d\mathbf{y}) = (2\pi)^{-1} \cdot \exp(-\frac{1}{2}\|\mathbf{y}\|^2) d\mathbf{y}$. The stochastic process arising from this passes from the state $\mathbf{x} \in \mathbb{R}^2$ to the next state by sampling a normal vector in \mathbb{R}^2 with covariance matrix the identity and mean value $\mathbf{0}$. In particular, the transition probability is independent of the current state.

The second example has the kernel $p_2(\mathbf{x}, d\mathbf{y}) = (2\pi)^{-1} \exp(-\frac{1}{2}\|\mathbf{x} - \mathbf{y}\|^2) d\mathbf{y}$. In this case, passing from a state $\mathbf{x} \in \mathbb{R}^2$ to the next state works by sampling a normal vector in \mathbb{R}^2 with covariance matrix the identity and mean value \mathbf{x} . We can simulate the first $n = 10$ steps in this chain in Julia as follows.

```

x0 = [0; 0]
states = []
push!(states, x0)

n = 10
for k in 1:n
    x = states[k]
    y = x + randn(2)
    push!(states, y)
end

```

Figure 15.2 shows one realization of this chain.

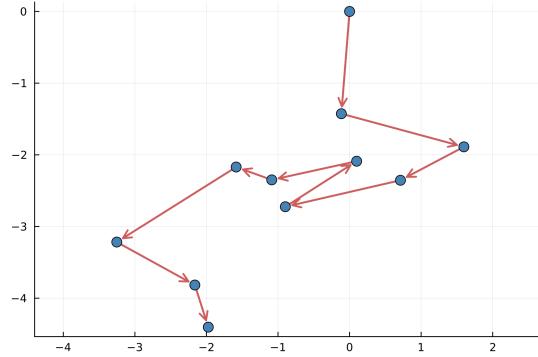


Fig. 15.2: The picture shows one sample of the first 10 steps of the Markov Chain with transition probability at state \mathbf{x} given by sampling a normal vector in \mathbb{R}^2 with covariance matrix the identity and mean value \mathbf{x} . See Example 15.10.

Example 15.11 (A Markov Chain on a Real Variety) Let $X \subset \mathbb{R}^n$ be a real variety of dimension d . We can create a Markov chain on X as follows. Suppose that chain is in state $\mathbf{x} \in X$. We sample a random linear space L of complimentary dimension. If L intersects X , we sample a point uniformly at random from $X \cap L$. This is the next state. Otherwise, we reject and sample L again. As an example, we take the surface defined by $z - xy = 0$. Given a point \mathbf{x} on this surface, we sample the line $L = \{\mathbf{Ax} = \mathbf{b}\}$ by sampling A with Gaussian entries and setting $\mathbf{b} = A\mathbf{x}$. In addition, we only accept states in the box $R = [-8, 8] \times [-8, 8] \times [-64, 64]$. The first few steps in this chain starting at $\mathbf{x}_0 = (0, 0, 0)$ are implemented in Julia as follows.

```
using HomotopyContinuation
@var x y z
f = System([z - x * y], variables = [x; y; z])
is_in_R(p) = abs(p[1])<8 && abs(p[2])<8 && abs(p[3])<64

n = 10
states = []
x0 = [0.0; 0.0; 0.0]
push!(states, x0)
for k in 1:n
    p = last(states)
    A = randn(2,3); b = A*p
    L = LinearSubspace(A, b)

    S = solve(f, target_subspace = L)
    points = real_solutions(S)
    filter!(is_in_R, points)
    if !isempty(points)
        push!(states, rand(points))
    end
end
```

One realization of this example is shown in Figure 15.3.

Let us now work towards sampling. We will recall results from the survey [129] by Roberts and Rosenthal. A probability measure π on X is called a *stationary distribution*, if

$$\int_X \pi(dx) \cdot p(x, dy) = \pi(dy) \quad \text{for all } y \in X. \quad (15.4)$$

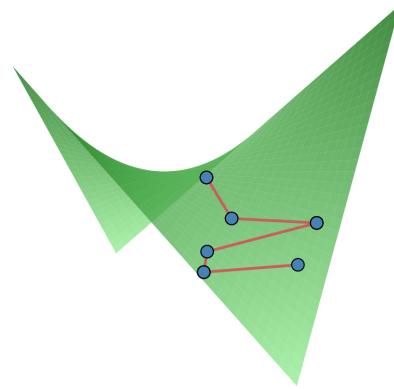


Fig. 15.3: The picture shows first few steps of the Markov Chain from Example 15.11 on the surface $z - xy = 0$.

The idea of MCMC methods for sampling from a probability distribution π is to set up a Markov process on X starting at \mathbf{x} that has stationary measure π and such that the probability measure

$$\mu^k(\mathbf{x}, \cdot) : A \mapsto \text{Prob}(\mathbf{x}_k \in A \mid \mathbf{x}_0 = \mathbf{x})$$

converges to π as $k \rightarrow \infty$. Convergence is measured by the *total variation distance*. The total variation distance between two measures μ and ν is $d_{\text{TV}}(\mu, \nu) := \sup_{A \in \mathcal{A}} |\mu(A) - \nu(A)|$. Thus, we want to define a Markov process starting at a point $\mathbf{x} \in X$ such that $\lim_{k \rightarrow \infty} d_{\text{TV}}(\pi, \mu^k(\mathbf{x}, \cdot)) = 0$. The key properties for achieving this are *irreducibility* and *aperiodicity*.

Definition 15.12 A Markov chain with kernel p is called irreducible, if for all states $\mathbf{x} \in X$ and all measurable sets $A \in \mathcal{A}$ with $\text{vol}(A) > 0$ there exists $k \in \mathbb{N}$ such that $\mu^k(\mathbf{x}, A) > 0$.

The interpretation of irreducibility is that all sets with positive volume can be reached eventually by the Markov chain starting at any point $x \in X$.

Remark 15.13 One can replace the Lebesgue measure in the definition by any other measure ϕ . In this case, one speaks of ϕ -irreducible Markov chains.

Definition 15.14 Consider a Markov chain with kernel p and suppose that it has a stationary distribution π . Let $d \geq 2$. We call the chain *periodic* with period d , if there exist disjoint subsets $A_1, \dots, A_d \in \mathcal{A}$ such that for all i we have

1. $\pi(A_i) = 0$, and
2. $p(\mathbf{x}, A_{i+1 \text{ mod } d}) = 1$ for all $\mathbf{x} \in A_i$.

Otherwise, the chain is called *aperiodic*.

The geometric interpretation of aperiodicity is that the Markov process does not move periodically between disjoint subset A_1, \dots, A_d .

Given an irreducible and aperiodic Markov chain with stationary distribution π we have the following convergence result.

Theorem 15.15 Let $\mathbf{x}_0, \mathbf{x}_1, \mathbf{x}_2, \dots$, be a Markov chain with kernel p and stationary distribution π . Suppose that the chain is irreducible and aperiodic. Then,

$$\lim_{k \rightarrow \infty} d_{\text{TV}}(\pi, \mu^k(\mathbf{x}, \cdot)) = 0$$

for almost all $\mathbf{x} \in X$.

Proof See [129, Theorem 4]. □

Remark 15.16 For this theorem it is enough that X is a state space with countably generated σ -algebra. Smooth submanifolds of \mathbb{R}^n always satisfy this hypothesis.

The next result gives, under some assumptions, the speed of convergence in Theorem 15.15. Roberts and Rosenthal [129] attribute the this theorem to Doeblin, Doob and also to Markov.

Theorem 15.17 Consider a Markov Chain with stationary distribution π . Suppose that there exist $n \in \mathbb{N}$, $\varepsilon > 0$ and a probability measure ν on X such that

$$\mu^n(\mathbf{x}, A) \geq \varepsilon \cdot \nu(A) \quad \text{for all } \mathbf{x} \in X \text{ and } A \in \mathcal{A}.$$

Then, we have

$$d_{\text{TV}}(\pi, \mu^k(\mathbf{x}, \cdot)) < (1 - \varepsilon)^{\lfloor \frac{k}{n} \rfloor}.$$

Proof See [129, Theorem 8]. □

The condition in Theorem 15.17 intuitively means, that all n step transitions have a component of probability at least ε in common.

Theorems 15.15 and 15.17 have the following algorithmic consequence. For sampling from a distribution π we set up an irreducible and aperiodic Markov chain with stationary distribution π . Then, if we let the Markov chain run long enough, the points in the process will have a probability distribution close to π . This is the idea underlying MCMC methods. The key task is thus to find and implement such a chain. The first subtask is to find a chain whose stationary is π . It is often easier to show that a Markov chain is *reversible* with respect to π .

Definition 15.18 A Markov chain with kernel p is reversible with respect to the probability distribution π , if $\pi(dx) \cdot p(x, dy) = \pi(dy) \cdot p(y, dx)$ for all $x, y \in X$.

Lemma 15.19 If a Markov chain with kernel p is reversible with respect to the probability distribution π , then π is a stationary distribution.

Proof We have to check the equation in (15.4). Fix $y \in X$. Then

$$\int_X \pi(dx) \cdot p(x, dy) = \int_X \pi(dy) \cdot p(y, dx) = \pi(dy) \cdot \int_X p(y, dx) = \pi(dy),$$

since $p(y, \cdot)$ is a probability measure. □

Using Lemma 15.19 it is straightforward to show that the *Metropolis Hastings algorithm* (Algorithm 6) creates a Markov chain with stationary distribution π ; see, e.g., [129, Proposition 2].

The Metropolis Hastings algorithm works for a target distribution π that has a density ϕ . The basic idea is to take another Markov chain whose kernel $p(x, A)$ has a density $q(x, y)$; i.e., $p(x, dy) = q(x, y) dy$. The density q is called a *proposal density*. Sampling from the proposal density creates a random proposal point y , which is either accepted or rejected depending on how likely it is that the proposal point y was sampled from π . Notice that in the algorithm we only need to evaluate $\phi(y)$ and $q(x, y)$ up to scaling.

Algorithm 6: The Metropolis Hastings algorithm.

```

1 Input: A probability measure  $\pi$  on  $X$  with a density  $\varphi(\mathbf{y})$ . A Markov kernel  $p(\mathbf{x}, A)$  on  $X$  with density  $q(\mathbf{x}, \mathbf{y})$ . A
   fixed starting point  $\mathbf{x} \in X$ .
2 Output: A Markov chain on  $X$  with stationary distribution  $\pi$ .
3 Set  $\mathbf{x}_0 = \mathbf{x}$ .
4 for  $k = 0, 1, 2, \dots$  do
5   Sample  $\mathbf{y} \sim p(\mathbf{x}_k, \cdot)$ .
6   if  $\phi(\mathbf{x}_k) = 0$  or  $q(\mathbf{x}_k, \mathbf{y}) = 0$  then
7     | Set  $w(\mathbf{x}_k, \mathbf{y}) = 0$ 
8   else
9     | Compute  $w(\mathbf{x}_k, \mathbf{y}) = \min \left\{ 1, \frac{\phi(\mathbf{y}) \cdot q(\mathbf{y}, \mathbf{x}_k)}{\phi(\mathbf{x}_k) \cdot q(\mathbf{x}_k, \mathbf{y})} \right\}$ .
10  end
11  Sample a Bernoulli random variable  $\beta \in \{0, 1\}$  with  $\text{Prob}\{\beta = 1\} = w(\mathbf{x}_k, \mathbf{y})$ .
12  if  $\beta = 1$  then
13    | Set  $\mathbf{x}_{k+1} := \mathbf{y}$ .
14  else
15    | Return to line 5.
16  end
17 end

```

Example 15.20 (The Symmetric Metropolis Algorithm) For a symmetric density $q(\mathbf{x}, \mathbf{y}) = q(\mathbf{y}, \mathbf{x})$, the Metropolis Hastings algorithm (Algorithm 6) is called *Symmetric Metropolis Algorithm*. For instance, the Markov kernel with density $q(\mathbf{x}, \mathbf{y}) \propto \exp(-\frac{1}{2}\|\mathbf{x} - \mathbf{y}\|^2)$ from Example 15.10 is symmetric.

Example 15.21 (Random Walks) We speak of a *Random Walk Metropolis-Hastings Algorithm*, if the proposal density $q(\mathbf{x}, \mathbf{y})$ has the form $q(\mathbf{x}-\mathbf{y})$. An example for this is the density $q(\mathbf{x}, \mathbf{y}) \propto \exp(-\frac{1}{2}\|\mathbf{x}-\mathbf{y}\|^2)$ from Example 15.10.

Example 15.22 (Independence Sampler) We call Algorithm 6 an *independence sampler*, if $q(\mathbf{x}, \mathbf{y})$ does not depend on \mathbf{x} . In this case, the samples obtained from Algorithm 6 are independent.

Example 15.23 (The Langevin Algorithm) The Langevin Algorithm works for sampling in $X = \mathbb{R}^n$. Suppose that the density $\phi(\mathbf{y})$ of the target distribution π in Algorithm 6 is differentiable. Denote by $\nabla\phi(\mathbf{y})$ the gradient. The Langevin Algorithm generates a proposal \mathbf{y} by sampling $\mathbf{y} \sim N(\mathbf{x}_k + \delta \cdot \nabla\phi(\mathbf{x}_k), 2\delta)$, where \mathbf{x}_k is the current state. This choice is motivated by a discrete approximation to a Langevin diffusion processes.

One issue with Algorithm 6 when sampling from a nonlinear manifold X is to find a suitable proposal distribution with a density. Take, for instance, the Markov chain from Example 15.11, where the next step $\mathbf{x}_{k+1} \in X$ was computed from the current step \mathbf{x}_k by taking a random linear space L through \mathbf{x}_k and sampling uniformly from the intersections points in $X \cap L$. It is straightforward to describe the generation of this random variable. But it is not clear how to compute its density (or if such a density even exists). In such a scenario we must prove that the chain is reversible with respect to π . A further complication arises when X is not connected. In this case, the proposals must be chosen in a way that no connected component of X is missed.

These points illustrates the importance of defining an appropriate proposal distribution. In the remainder of this section we present two approaches from the literature. The first is the algorithm in [21] using an independence sampler. Next, we consider the algorithm in [104] based on a random walk.

The algorithm in [21] is based on the idea of linear slicing. However, instead of considering a Markov chain in X the paper considers a Markov chain in the Grassmannian $G(c, \mathbb{R}^n)$, where $c = \text{codim } X$ is

the codimension of X . The algorithm is an independence sampler. The following theorem describes the density with which we have to sample $L \in G(c, \mathbb{R}^n)$. As before, we assume that the target distribution π has a density $\phi(\mathbf{y})$. For $(A, \mathbf{b}) \in \mathbb{R}^{d \times n} \times \mathbb{R}^d$ we introduce the new function

$$\bar{\phi}(A, \mathbf{b}) := \sum_{\mathbf{x} \in X : A\mathbf{x} = \mathbf{b}} \frac{\phi(\mathbf{x})}{\alpha(\mathbf{x})}, \quad \text{where } \alpha(\mathbf{x}) := \frac{\sqrt{1 + \langle \mathbf{x}, P_{\mathbf{x}} \mathbf{x} \rangle}}{(1 + \|\mathbf{x}\|^2)^{(d+1)/2}} \frac{\Gamma\left(\frac{d+1}{2}\right)}{\sqrt{\pi}^{d+1}},$$

and $P_{\mathbf{x}}$ is the orthogonal projection onto the normal space $N_{\mathbf{x}}X$. As before, $d = \dim X$ is the dimension of X . The additional factor α is related to the change of variables when embedding \mathbb{R}^n into the n -dimensional real projective space.

Theorem 15.24 *Let $d := \dim X$ and $c = n - d = \text{codim } X$. Let $\varphi(A, b)$ be the probability density for which the entries of $(A, \mathbf{b}) \in \mathbb{R}^{d \times n} \times \mathbb{R}^d$ are i.i.d. standard Gaussian. Denote*

$$\psi(A, \mathbf{b}) := \frac{\varphi(A, \mathbf{b}) \cdot \bar{\phi}(A, \mathbf{b})}{\mathbb{E}_{(A, \mathbf{b}) \sim \varphi} \bar{\phi}(A, \mathbf{b})}.$$

Then, ψ is a probability density and the random linear space $L = \{\mathbf{x} \in \mathbb{R}^n \mid A\mathbf{x} = \mathbf{b}\} \in G(c, \mathbb{R}^n)$ for $(A, \mathbf{b}) \sim \psi$ has the properties:

1. $X \cap L$ is finite with probability one.
2. If we choose one of the finitely many points in $\mathbf{x} \in X \cap L$ with probability

$$\text{Prob}\{\mathbf{x}\} := \frac{\phi(\mathbf{x})}{\alpha(\mathbf{x}) \cdot \bar{\phi}(A, \mathbf{b})},$$

the random point \mathbf{x} is distributed according to the density ϕ .

Proof See [21, Theorem 1.1]. □

We review another algorithm from the literature. The algorithm in [104] is similar to the Metropolis-Hastings algorithm. The basic idea is as follows. Suppose we want to sample from a target density $\phi(\mathbf{y})$. Write this as $\phi(\mathbf{y}) = \exp(-V(\mathbf{y}))$ and assume that $V(\mathbf{y})$ is smooth. The function V is called a *potential function*. Given a point $\mathbf{x} \in X$ we create a proposal by sampling first in a random tangent direction $\mathbf{v} \in T_{\mathbf{x}}X$ and then computing the intersection of X with the random linear space

$$L = \mathbf{x} + \mathbf{v} + N_{\mathbf{x}}X \in G(c, \mathbb{R}^n).$$

This creates a Markov chain on X , but as we have discussed before, it is not clear how to compute the density for this random proposal. Instead, the authors in [104] prove directly reversibility of their Markov chain, so that they can apply Lemma 15.19. Algorithm 7 shows a (simplified version) of their algorithm.

Remark 15.25 The sampling of the random tangent vector \mathbf{v} in line 5 of Algorithm 7 can be achieved as follows. Let $U \in \mathbb{R}^{n \times d}$ be a matrix whose columns form an orthonormal basis of $T_{\mathbf{x}}X$. Such a matrix can be computed by using the Gram-Schmidt algorithm. Sample $\mathbf{z} \in \mathbb{R}^d$ with i.i.d. $N(0, \sigma^2)$ -entries. Then $\mathbf{v} = U\mathbf{z}$.

The following theorem asserts that Algorithm 7 works correctly.

Theorem 15.26 *Algorithm 7 produces a Markov chain that is reversible with respect to π . In particular, by Lemma 15.19 the Markov chain has π as stationary distribution.*

Proof See [104, Theorem 1]. □

Algorithm 7: The algorithm from [104].

1 **Input:** A probability measure π on X with a density $\exp(-V(\mathbf{y}))$, where V is smooth. A variance parameter $\sigma^2 > 0$. A fixed starting point $\mathbf{x} \in X$.
 2 **Output:** A Markov chain on X with stationary distribution π .
 3 Set $\mathbf{x}_0 = \mathbf{x}$.
 4 **for** $k = 0, 1, 2, \dots$ **do**
 5 Randomly draw $\mathbf{v} \in T_{\mathbf{x}_k}X$ by sampling \mathbf{v} from the multivariate normal distribution on $T_{\mathbf{x}_k}X$ with mean $\mathbf{0}$ and covariance matrix $\sigma^2 \cdot \mathbf{I}$.
 6 Set $L = \mathbf{x}_k + \mathbf{v} + N_{\mathbf{x}_k}X$.
 7 Sample a point $\mathbf{y} \in X \cap L$ uniformly.
 8 Compute $\mathbf{w} \in T_{\mathbf{y}}X$ such that $\mathbf{x}_k \in K := \mathbf{y} + \mathbf{w} + N_{\mathbf{y}}X$.
 9 Compute $w(\mathbf{x}_k, \mathbf{y}) = \min \left\{ 1, \frac{|X \cap L|}{|X \cap K|} \cdot \exp \left(- (V(\mathbf{y}) - V(\mathbf{x})) \right) \cdot \exp \left(- \frac{1}{2\sigma^2} (\|\mathbf{w}\|^2 - \|\mathbf{v}\|^2) \right) \right\}$.
 10 Sample a Bernoulli random variable $\beta \in \{0, 1\}$ with $\text{Prob}\{\beta = 1\} = w(\mathbf{x}_k, \mathbf{y})$.
 11 **if** $\beta = 1$ **then**
 12 Set $\mathbf{x}_{k+1} := \mathbf{y}$.
 13 **else**
 14 Return to line 5.
 15 **end**
 16 **end**

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