Department of Mathematics and Systems Analysis

Geometry of Real Tensors and Phylogenetics

Emanuele Ventura

Aalto University

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Geometry of Real Tensors and Phylogenetics

Emanuele Ventura

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Abstract

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Abstract

This thesis is devoted to the study of special algebraic varieties arising from the theory of tensors and phylogenetics. The main motivations for analyzing these objects come from both pure and applied mathematics.

In the context of tensors, the Waring problem is a classical question going back to the work of Hilbert, Scorza, Sylvester, and many other geometers and algebraists of the nineteenth century. We contribute to the solution of the real and complex Waring problem for some classes of homogeneous polynomials. More specifically, we classify the Waring ranks of real and complex reducible cubics, extending a result by Segre. Furthermore, we give upper bounds for the real Waring rank of any monomial; as a by-product we characterize monomials whose least exponent is one as the only ones whose real and complex Waring ranks coincide.
Finally, for plane curves of low degree we introduce the space of real sums of powers, parametrizing real Waring decompositions and we analyze the real rank boundary of such curves.

We also study an intriguing invariant of abelian groups from algebraic geometry applied to computational phylogenetics. This invariant constitutes an upper bound for the degree of equations of toric varieties; the latter describe the group-based models on n taxa. We show that this invariant is finite for any abelian group, thus proving that such an upper bound on degree exists. We achieve this result by the means of the combinatorial structure of special matrices, corresponding to binomials in the ideals of these toric varieties. This solves a conjecture by Sturmfels and Sullivant.

Keywords Phylogenetics, Secant varieties, Tensors, Waring problems

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In memory of my grandmother

Preface

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Infine, vorrei dedicare questo lavoro a mia nonna, Antonia Ielo, con indescrivibile amore ed ammirazione.

Helsinki, November 17, 2016,

Emanuele Ventura

Contents

List of Publications

This thesis consists of an overview and of the following publications which are referred to in the text by their Roman numerals.

I Enrico Carlini, Cheng Guo, and Emanuele Ventura. Real and complex Waring rank of reducible cubic forms. *J. Pure Appl. Algebra*, **220**(11):3692–3701, November 2016.

II Enrico Carlini, Mario Kummer, Alessandro Oneto, and Emanuele Ventura. On the real rank of monomials. *Math. Z.*, to appear, arXiv:1602.01151, 8 pp., March 2016.

III Mateusz Michałek, Hyunsuk Moon, Bernd Sturmfels, and Emanuele Ventura. Real rank geometry of ternary forms. *Ann. Mat. Pura Appl.*, appeared online, 1–30, August 2016.

IV Mateusz Michałek and Emanuele Ventura. Finite phylogenetic complexity and combinatorics of tables. *Algebra Number Theory*, to appear, arXiv:1606.07263, 17 pp., June 2016.

Author's Contribution

Publication I: "Real and complex Waring rank of reducible cubic forms"

The authors have equally contributed to the paper.

Publication II: "On the real rank of monomials"

The authors have equally contributed to the paper.

Publication III: "Real rank geometry of ternary forms"

The authors have equally contributed to the paper. The author of the thesis contributed less to the introduction and more to the technical part of the paper.

Publication IV: "Finite phylogenetic complexity and combinatorics of tables"

The authors have equally contributed to the paper.

1. Introduction

This thesis is devoted to the study of special varieties arising from the theory of tensors and phylogenetics. While the main motivations for the study of these objects come from both pure and applied mathematics, the main source of inspiration underlying the present research is the glorious Italian school of algebraic geometry [26]. Their results, ideas, and geometrical intuition have contributed to most of the topics underlying these fields of research. Indeed, one of the main contributions of this school was the introduction of many interesting algebraic varieties whose properties are unexpected. While these geometrical objects have a mathematical interest on their own, they seem to be crucial also for many applications of algebraic geometry. An instance of this phenomenon is represented by secant varieties, which are ubiquitous in this overview.

Algebraic geometry primarily deals with systems of polynomial equations, which are fundamental in many applied sciences such as biology, computer science, economics, statistics, and many others [141]. Originally studied by the German and Italian algebraic geometers during the last century, the subject developed enormously following the abstract approach of the French school. During the last decades, a wealth of new ideas coming from other disciplines of pure and applied mathematics has led to an increased interest in concrete geometrical constructions, many times introduced and already studied by the classical geometers. Recently, the research directed towards establishing explicit properties of projective varieties has been enormous, see for example [46].

Our research project follows the line of this renewed interest in complex and real varieties with exceptional behaviour and in their applications. More specifically, in the context of tensors, the main questions we study are related to the Waring problem and semialgebraic sets, which naturally appear when the Waring problem is considered over the real numbers. In the context of phylogenetics, we study the degree bound for equations of a family of toric varieties encoding probabilistic models on phylogenetic trees.

The subsequent overview is structured into two parts. The first reviews real tensors, forms, and their Waring problems. Here we present the results in Papers I, II, and III. The second part introduces phylogenetics, phylogenetic models, and explains their connection to algebraic varieties. In this part, we explain the results in Paper IV.

2. Real Tensors

In this part we overview the background, methods, and main results related to Papers I, II, and III. The main references for tensors and Waring problems are the books by Geramita [75], Iarrobino and Kanev [79], and Landsberg [89]. For basic notions of real algebraic geometry and semialgebraic sets we refer to the book by Bochnak, Coste, and Roy [22].

2.1 Tensors and ranks

We start introducing the main character of this part. Let $\mathbb{K}$ be a field. Let $V_1, \dots, V_k, U$ be $\mathbb{K}$-vector spaces. A function

$$T : V_1 \times \cdots \times V_k \to U$$

is multilinear if it is linear in each of the factors V_j. The vector space of multilinear functions T is the tensor product $V_1^* \otimes \cdots \otimes V_k^* \otimes U$, whose elements are called *tensors*.

Let V be a $\mathbb{K}$-vector space and let $V^{\otimes d}$ denote the d-fold tensor product $V \otimes \cdots \otimes V$. The symmetric group $\mathcal{S}_d$ acts on $V^{\otimes d}$ by permuting the factors. We define the map $\pi : V^{\otimes d} \to V^{\otimes d}$ as

$$\pi(v_1 \otimes \cdots \otimes v_d) = \frac{1}{d!} \sum_{\sigma \in \mathcal{S}_d} v_{\sigma(1)} \otimes \cdots \otimes v_{\sigma(d)}.$$

The image of π is the dth symmetric power of V, denoted by $S^d V$. The elements of $S^d V$ are called *symmetric d-tensors*. The space $S^d V^*$ can be identified with the vector space of homogeneous polynomials, or *forms*, of degree d on V. Details of the role and the basics of tensors in algebraic geometry may be found in [89].

A tensor $T \in V_1 \otimes \cdots \otimes V_k$ of the form $v_1 \otimes \cdots \otimes v_k$ is said to be of rank one. The *rank* of a tensor T, denoted by $\mathbf{rk}_{\mathbb{K}}(T)$, is the minimum integer s such that

$$T = \sum_{i=1}^{s} T_i,$$

where the T_i are tensors of rank one. For instance, matrices are tensors in $V_1 \otimes V_2$. The usual matrix rank coincides with the tensor rank defined above for $k = 2$. Tensor rank is a field-dependent notion.

Similarly, one can define the analogous notion for symmetric tensors $F \in S^d V$, or forms $F \in R = \mathbb{K}[x_1, \ldots, x_n]$ of degree d. The vector space consisting of homogeneous polynomials of degree d is denoted by R_d.

The *symmetric* or *Waring rank* of $F \in R_d$ is the smallest integer s, denoted by $\mathrm{rk}_{\mathbb{K}}(F)$, such that F can be written as a sum of powers of linear forms,

$$F = \sum_{i=1}^{s} \lambda_i L_i^d,$$

where $L_i \in R_1$ are linear forms, and $\lambda_i \in \mathbb{K}$. This expression is called a *Waring decomposition* of F. The λ_i-coefficients are needed when the field $\mathbb{K}$ is not algebraically closed. The Waring rank is a field-dependent notion, see [52]. The *Waring problem* over a field $\mathbb{K}$ for a form F is the determination of $\mathrm{rk}_{\mathbb{K}}(F)$. The computation of some Waring ranks is a familiar task in linear algebra. The Waring problem for a quadratic form Q is equivalent to the computation of the rank of the associated matrix to Q.

Remarkably, the relationship between the tensor and the Waring rank is still an open question. The conjectural relationship over the complex numbers between these two notions of rank was proposed by Comon [50]: For any symmetric tensor $T \in S^d V$, the equality $\mathrm{rk}_{\mathbb{C}}(T) = \mathbf{rk}_{\mathbb{C}}(T)$ holds. It is known to be true for $d = 2$, $n = 1$, and other sporadic cases.

The origin of the Waring problem can be traced back to the 1770 treatise *Meditationes algebraicæ* by Waring [149]. In this notable work, various statements, without proof, regarding the decomposition of every natural number as a sum of at most 9 positive cubes, as a sum of 19 biquadratics, and so forth, made their first appearance. Waring believed that for every natural number $d \geq 2$, there exists a number $N(d)$ such that every positive integer n can be written as a *sum of powers* $n = m_1^d + \cdots + m_{N(d)}^d$, for some $m_i \geq 0$. It was only in 1909 that Hilbert [78] proved the existence of such $N(d)$ for every d.

Since its origins, the Waring problem has been a delightful chapter of classical geometry and algebra, and its first developments were achieved in the pioneering work of Sylvester [145]. In the latter, Sylvester completely solved the case of forms in two variables over the complex numbers. Even this case over any field is an active area of research. Reznick [125] studied the Waring rank of a fixed form in two variables, over $\mathbb{K} \subset \mathbb{C}$, as $\mathbb{K}$ varies.

Waring problems for several classes of forms have been the subject of intensive research in the last decade [27, 31, 32, 42, 48, 51, 69, 93, 99, 100, 110, 120]. Algorithms to produce Waring decompositions appear in [14, 24, 50, 79, 109]. For geometric aspects of the Waring problem connected to linear systems, we refer to the overview by Ciliberto [45].

One of the main objectives of the thesis is to study of the Waring problem for special families of forms. Apart from an algebraic and geometrical interest, Waring and tensor ranks along with their geometrical counterparts are motivated by applications in algebraic statistics [73], dynamical systems [3], geometric complexity [30], matrix multiplication complexity [88], phylogenetics [65], quantum information [43], and signal processing [49, 76]. In addition to Landsberg's book [89], see the overview by Carlini, Grieve, and Oeding [33] for more references.

The majority of the current results in the literature concern ranks over the complex numbers, but most of the applications are in the real case. The Waring problem for real forms in two variables is investigated in [17, 39, 52]. Real monomials in two variables are treated in [14].

The results in Papers I and II contribute to the theory of Waring ranks over the real numbers.

2.2 Varieties and ranks

Now we introduce some remarkable classical varieties and other rank notions, which are fundamentally linked with the Waring problem. We refer to textbooks in classical algebraic geometry for details and properties of these costructions, for example the books by Beltrametti, Carletti, Gallarati, and Monti Bragadin [12], and Dolgachev [57].

In these definitions we assume $\mathbb{K} = \mathbb{C}$. Let $V_1, \ldots, V_k$ be vector spaces and let $V = V_1 \otimes \cdots \otimes V_k$. The k-factor *Segre variety* is the image of the embedding

$$\mathrm{Seg}\ : \mathbb{P}V_1 \times \cdots \times \mathbb{P}V_k \to \mathbb{P}V,$$

mapping $([v_1], \ldots, [v_n]) \mapsto [v_1 \otimes \cdots \otimes v_k]$. For instance, for $k = 2$, the Segre variety can be thought of as the projectivization of the set of matrices, whose usual rank is one. More generally, the Segre variety can be regarded as the projectivization of the set of rank one tensors.

Let V be a vector space. The dth Veronese embedding is the image of the embedding

$$v_d : \mathbb{P}V \to \mathbb{P}(S^d V),$$

mapping $[v] \mapsto [v^d]$. This is the symmetrized version of the Segre variety.

The join $J(X, Y)$ of two projective varieties $X, Y \subset \mathbb{P}^n$ is the Zariski closure of the union of linear spans of pairs of points in X and Y:

$$J(X,Y) = \overline{\bigcup_{x \in X, y \in Y, x \neq y} \langle x, y \rangle}.$$

For instance, if $X \subset \mathbb{P}^3$ is a curve and Y is a point q outside the curve, the join $J(X, q)$ is a cone over the curve. The join of k varieties $X_1, \ldots, X_k$ is defined similarly. The kth secant variety σ_k of a projective variety X is defined as the k-fold join $\sigma_k(X) = J(X, \ldots, X)$. The secant $\sigma_2(X)$ is called the secant line variety of X. Dimensions and equations of secants are in general mysterious and have been studied intensively in the last decades, starting with the work of Palatini [116], Scorza [134, 135], and Terracini [148]. Geometrical properties of these special projective varieties along with many applications of those within algebraic geometry are for example in the books by Russo [128] and Zak [150].

The first issue in this context is to determine, given a projective variety X, the dimension of the secants $\sigma_k(X)$. The dimensions of all secant varieties of Veronese varieties have been obtained in the work of Alexander and Hirschowitz [4]. Their result can be rephrased in terms of a Waring problem for general forms. A general form $F \in R_d$ is a sum of $s = \lceil \frac{1}{n+1}\binom{n+d}{n} \rceil$ powers of linear forms, unless

(i) $d = 2$, where $s = n + 1$ instead of $\lceil \frac{n+2}{2} \rceil$;

(ii) $d = 3$ and $n = 4$, where $s = 8$ instead of 7;

(iii) $d = 4$ and $n = 2, 3, 4$, where $s = 6, 10, 15$ instead of $5, 9, 14$, respectively.

For a simplified proof of this result with historical remarks, see [25].

The Grassmannian is the projective variety whose points are linear subspaces of fixed dimension in a given projective space. Dimensions of secant varieties of Segre varieties and Grassmannians are largely unknown. A conjectural list of secants of those not with the expected dimensions are presented in [2, 11]. There is a vast literature of partial results on dimensions of these varieties [1, 2, 37, 38]. Nice results on lower bounds for the degree of secants appear in [47].

A trend in current reseach is the focus on the description of ideals of secant varieties of Segre varieties and Grassmannians. Motivated by the computational complexity of matrix multiplication, Strassen showed some instances in [139]. Further studies were performed in [90, 91, 92]. Raicu [119] recently provided an explicit description of the ideal of the secant line variety of Segre varieties. Further references may be found in [33].

Another exciting recent line of research focuses on showing that for a family of varieties $X(d, n)$ and fixed k the degrees of the minimal generators of the ideal of the kth secant variety of $X(d, n)$ are bounded by a constant not depending on d or n. Sam [129] showed that the ideal of kth secants of dth Veronese embeddings of a projective variety is generated in bounded degree that is independent of d. This was done with an unexpected use of Hopf rings. In [130], the same statement is shown to hold for syzygies of secants. The latter statements are ideal-theoretic. Analogous set-theoretic results are known for Segre embeddings and Plücker embeddings of Grassmannians by the work of Draisma and Kuttler [63], and by Draisma and Eggermont [60]. Interestingly, the corresponding ideal-theoretic generation in bounded degree for secants of Segre varieties and Grassmannians is still not settled.

We shift gears and consider more general notions of rank from the literature, including the tensor and the Waring rank as particular cases. This generalization will put the theory of ranks under a more geometric light. For this purpose, we assume $\mathbb{K}$ to be an infinite field, and we denote by $\mathbb{P}^n_{\mathbb{K}} = \mathbb{P}^n$ the projective space over $\mathbb{K}$. Let $X \subset \mathbb{P}^n$ be a projective variety and consider a point $p \in \mathbb{P}^n$. The X-***rank*** of p, denoted by $\mathrm{rk}_X(p)$, is the minimum integer s such that p belongs to the linear span of

s points of X [29]. Blekherman and Sinn [19] showed that if X is a real variety, then for any $p \in \mathbb{P}^n_{\mathbb{R}}$, the real rank $\mathrm{rk}_X(p)$ satisfies the inequality $\mathrm{rk}_X(p) \leq \mathrm{codim}(X) + 2$.

The X-*border rank* is the smallest s such that $p \in \sigma_s(X)$. The geometric counterpart of the border rank is incarnated by secant varieties. The X-rank coincides with the tensor rank when X is a Segre variety. Analogously, the X-rank coincides with the Waring rank over $\mathbb{K}$ when X is a Veronese variety.

An integer s is an X-*generic rank* if the set of points in $\mathbb{P}^n$ of X-rank equal to s contains a Zariski open dense subset. It is known that for any non-degenerate variety X over an algebraically closed field, the X-generic rank is unique [20]. Moreover, the X-generic rank is the smallest s such that $\sigma_s(X) = \mathbb{P}^n$. Assuming $\mathbb{K} = \mathbb{C}$ and X to be a Veronese variety, the X-generic rank is known by the Alexander-Hirschowitz theorem mentioned before: The computation of the X-generic rank, when X is a Veronese variety, is equivalent to determining the Waring rank of a general form of fixed degree in a fixed number of variables.

2.3 Typical ranks and real rank boundaries

Let $\mathbb{K}$ be the field of real numbers. An integer s is said to be a *typical rank* if the set of forms in $R = \mathbb{R}[x_0, \ldots, x_n]$ of degree d of real Waring rank s contains an open Euclidean ball. Unlike the complex generic rank, that is unique, there may exist more than one typical rank. The smallest typical rank is the generic rank over $\mathbb{C}$, see [20].

The case $n = 1$ of forms in two variables has been analyzed in [17, 52]: For all d and $\lfloor \frac{d+2}{2} \rfloor \leq s \leq d$, there exists a form F in two variables of degree d whose real Waring rank is s and all forms in an open neighborhood of F satisfy this property as well. That is equivalent to such s being a typical rank. Bernardi, Blekherman, and Ottaviani [13] showed the following property of typical ranks: Let $X \subset \mathbb{P}^n_{\mathbb{R}}$ be a real projective variety. Then each X-rank between the lowest typical rank and the highest typical rank is also typical. In addition, various interesting results on ternary forms are proven. They proved that four is the unique typical rank of real ternary cubics, which was implicit in [8]. For quaternary cubics, they demonstrated that five and six are the only typical ranks. For ternary quartics, six and seven were shown to be typical ranks, and eight was proven to be the maximal possible typical rank. It is still unknown if eight is an actual typical rank for quartics. Even an example of a quartic ternary form of Waring rank eight is unknown. Finally, for ternary quintics, they showed that the typical ranks are between seven and thirteen.

Paper III deals with typical ranks in the case $n = 2$, the case of ternary forms, along the lines of Bernardi, Blekherman, and Ottaviani above. Let $\mathcal{R}_d$ be the set of forms of degree d whose Waring rank is the complex generic rank. This is a semialgebraic set, whose topological boundary $\partial\mathcal{R}_d$ is either empty or of codimension one. One of the goals of Paper III is to study the variety defined as the complex Zariski closure of $\partial\mathcal{R}_d$, called the *real rank boundary* and denoted by $\partial_{\text{alg}}\mathcal{R}_d$. The question of describing this algebraic boundary was addressed and completely solved for forms in two variables by Lee and Sturmfels [94], where the components of the real rank boundary were identified.

As mentioned above, the real rank of a general ternary cubic is four, as in this case there exists a unique typical rank. Consequently, the boundary $\partial\mathcal{R}_3$ is empty.

In Paper III we start the description of the real rank boundary for ternary quartics. The algebraic boundary $\partial_{\text{alg}}\mathcal{R}_4$ is a reducible hypersurface in the $\mathbb{P}^{14}_{\mathbb{R}}$ of real quartics. One of its irreducible components has degree 51. The latter component divides the quartics F that can be written as

$$F = \sum_{i=1}^{5} \lambda_i L_i^4 - \lambda_6 L_6^4,$$

where the λ_i are positive real numbers. Another irreducible component divides the region of hyperbolic quartics. The complete list of all irreducible components of this algebraic boundary is still unknown.

A complete answer for ternary quintics is provided. The algebraic boundary $\partial_{\text{alg}}\mathcal{R}_5$ of the set $\mathcal{R}_5 = \{F : \text{rk}_{\mathbb{R}}(F) = 7\}$ is an irreducible hypersurface of degree 168 in the $\mathbb{P}^{20}_{\mathbb{R}}$ of real quintics. It is a unirational variety having a parametric representation

$$G \ = \ L_1^5 + L_2^5 + L_3^5 + L_4^5 + L_5^5 \ + \ L_6^4 L_7, \ \ \text{where} \ \ L_1, \ldots, L_7 \in R_1.$$

Quartics are more difficult than quintics, since their decompositions are parameterized by a threefold, while quintics have a unique Waring decomposition up to scaling.

We now consider ternary sextics. The generic complex rank for sextics is ten. We show that eleven is a typical real rank. Indeed, the algebraic boundary is non-empty and we show that $\partial_{\mathrm{alg}}\mathcal{R}_6$ is a hypersurface in the $\mathbb{P}^{27}_{\mathbb{R}}$ of real ternary sextics. One of its irreducible components is the dual to the Severi variety of rational sextics. This Severi variety has dimension 17 and degree 26312976 in the $\mathbb{P}^{27}_{\mathbb{R}}$ of all sextic curves [18]. The same proof technique to show the non-emptiness of the algebraic boundary in the case of ternary sextics applies also to octics. Indeed, fifteen is the smallest typical rank for octics and it coincides with the size of the fourth catalecticant of an octic form F, and we are able to conclude that there is an open set of octics of rank bigger than fifteen. However, for even integers $d \geq 10$, such arguments do not work, since the generic complex rank exceeds the size of the $\lfloor \frac{d}{2} \rfloor$th catalecticant. New techniques are needed to establish the existence of the hypersurface $\partial_{\mathrm{alg}}\mathcal{R}_d$ for $d \geq 9$.

Finally, for ternary septics, we show that the real rank boundary $\partial_{\mathrm{alg}}\mathcal{R}_7$ is a non-empty hypersurface in $\mathbb{P}^{35}_{\mathbb{R}}$. One of the components is equal to the join of the tenth secant variety and the tangential variety to the seventh Veronese variety of $\mathbb{P}^2$. We conjecture that the join of a secant and a tangential variety is a component of the real rank boundary, whenever a form has finitely many Waring decompositions. Moreover, we conjecture that it is the unique component of the real rank boundary when a form has a unique Waring decomposition.

2.4 Waring ranks, apolarity, and lower bounds

Let $R = \mathbb{K}[x_0, \dots, x_n]$ and $T = \mathbb{K}[\partial/\partial x_0, \dots, \partial/\partial x_n]$ be its dual ring of differential polynomial operators, acting by the usual (right) differentiation on R. This action is classically known as *apolar action*. The apolar action is a central notion in invariant theory [111].

For a given $F \in R_d$ form of degree d, the apolar ideal $F^{\perp}$ of F is the homogeneous ideal of all forms $G \in T$ such that $G \circ F = 0$, where $\circ$ denotes the differentiation. The ideals $F^{\perp}$ were called *principal systems* by

Macaulay [95]. He showed that the ideals $F^{\perp}$ are Gorenstein, that is, they are Artinian, graded and whose socle is one-dimensional. Moreover, Gorenstein ideals of socle degree d are in bijection with forms $F \in R_d$.

At the heart of apolarity stands the *apolarity lemma* [79, Lemma 1.15]. As before, let $F \in R_d$ be a form of degree d. The following are equivalent:

(i) $F = \sum_{i=1}^{s} \lambda_i L_i^d$, where the L_i are linear forms;

(ii) $I_{\mathbb{X}} \subset F^{\perp}$, where $I_{\mathbb{X}}$ is the ideal defining a zero-dimensional reduced scheme $\mathbb{X}$ of degree s. Equivalently, $\mathbb{X}$ consists of s reduced points.

In the classical literature the collection of these linear forms L_i is called *polar s-gon* or *polar polyhedron*. We call this collection of linear forms an *apolar scheme* to F. The apolarity lemma is one of the main devices to solve the Waring problem for forms.

In order to determine the Waring rank of a given form, it is useful to have powerful lower-bounds. A remarkable lower bound for the Waring rank is given by catalecticants. The rth *catalecticant* of $F \in R_d$ is a linear map $\phi_r : T_r \to R_{d-r}$ given by $\phi_r(G) = G \circ F$. Catalecticants were introduced by Sylvester [146]. Catalecticant matrices and their vanishing loci were studied by Iarrobino and Kanev in [79].

Another lower bound appears in [93, Theorem 1.3]. This lower bound takes into account not only the rank of the catalecticant, but also the dimension of the singular locus of the projective hypersurface whose equation is given by the form F.

The goal of Paper I is to develop other lower bounds for the Waring rank. The lower bound introduced in Paper I is as follows. We assume $\mathbb{K}$ to be of characteristic zero. Let $0 \le p \le n$ be an integer, $F \in \mathbb{K}[x_0, \ldots, x_n]$ be a form, and set $F_k = \partial F / \partial x_k$ for $0 \le k \le n$. If

$$\mathbf{rk}_{\mathbb{K}}(F_0 + \sum_{k=1}^{p} \lambda_k F_k) \ge m,$$

for all $\lambda_k \in \mathbb{K}$, and the forms $F_1, \ldots, F_p$ are linearly independent, then

$$\mathbf{rk}_{\mathbb{K}}(F) \ge m + p.$$

This lower bound is particularly effective in the case of real and complex reducible cubics. The main reason is that when F is a cubic form, the condition on the Waring rank of $F_0 + \sum_{k=1}^{p} \lambda_k F_k$ is a matrix rank condition. We also derive the classification of reducible cubics over the real numbers. This classification involves the signature of a quadric and the action of the orthogonal groups $\mathrm{O}(p, \mathbb{R}) \times \mathrm{O}(n+1-p, \mathbb{R})$. Segre proved that the reducible cubic surface $V(C) \subset \mathbb{P}^3$, whose components are a smooth quadric and a tangent plane, has rank seven and that this is the maximal rank among cubic surfaces [136]. Our classification result may be viewed as an extension of this classical result, without the maximality property of the rank.

2.5 Monomials and apolar schemes

Monomials are interesting since they are the sparsest symmetric tensors. In other words, they are the simplest forms to study. Over the complex numbers, we have the recent precise answer by Carlini, Catalisano, and Geramita [31]: If $M = x_0^{a_0} x_1^{a_1} \dots x_n^{a_n}$ with $0 < a_0 \leq a_1 \leq \dots \leq a_n$, then

$$\mathbf{rk}_{\mathbb{C}}(M) = \frac{1}{a_0+1} \prod_{i=0}^{n} (a_i + 1).$$

Over the real numbers, the situation is much more involved. In this context the only result is for monomials in two variables by Boij, Carlini, and Geramita [23]: If $M = x_0^{a_0} x_1^{a_1}$, then

$$\mathbf{rk}_{\mathbb{R}}(M) = a_0 + a_1.$$

The goal of Paper II is to obtain results toward a solution of the real Waring problem for monomials. Equipped with a Descartes' rule of signs type of result, we obtain the following upper bound. If $M = x_0^{a_0} \dots x_n^{a_n}$ with $0 < a_0 \leq \dots \leq a_n$, then

$$\mathbf{rk}_{\mathbb{R}}(M) \leq \frac{1}{2a_0} \prod_{i=0}^{n} (a_i + a_0).$$

This upper bound immediately implies that for a monomial M, whose least exponent is equal to one, the real and complex Waring ranks coincide. In order to show the lower bound, we introduce a symmetric bilinear form B on the finite $\mathbb{R}$-algebra A, whose spectrum consists of the reduced points apolar to M. If A consists only of $\mathbb{R}$-points, then B is positive definite [117]. The assumption that a reduced apolar scheme to $M = x_0^{a_0} x_1^{a_1} \dots x_n^{a_n}$, with $2 \leq a_0 \leq \dots \leq a_n$, consists of $\prod_{i=1}^{n}(a_i + 1)$ real points is shown to contradict the positive definiteness of B. We use that reduced apolar schemes to a monomial M of degree $\mathrm{rk}_{\mathbb{C}}(M)$ are complete intersections [20].

Moreover, Paper II gives an upper bound, which is better than the previous one, for the infinite family of monomials of type $M = x_0^2 \cdots x_n^2$. The real Waring rank of M satisfies $\mathrm{rk}_{\mathbb{R}}(M) \leq (3^{n+1} - 1)/2$. A reduced apolar scheme of degree $(3^{n+1} - 1)/2$ to M is constructed from specific apolar schemes of points to its partial derivatives $\partial M/\partial x_i$.

2.6 Varieties and spaces of sums of powers

For any form $F \in R = \mathbb{C}[x_0, \ldots, x_n]$ of degree d, the space parameterizing all the Waring decompositions of length s is called the *variety of sums of powers* and it is denoted by VSP(F, s). Suppose that $V(F)$, the vanishing locus of F, is a hypersurface in $\mathbb{P}^n$. If $F = \sum_{i=1}^{s} \lambda_i L_i^d$, by projective duality, each linear form L_i gives a point l_i in the dual projective space $\mathbb{P}^{n\vee}$. The variety of sums of powers VSP(F, s) parameterizes unordered collections of s points that can occur in a Waring decomposition of F, see [120] for a precise definition. In other words, each point of the variety of sums of powers corresponds to a collection of linear forms L_i appearing in a Waring decomposition of F.

These varieties received a lot of attention by algebraists and geometers in the nineteenth century: Dixon and Stuart [55], Hilbert [77], Reye [122, 123, 124], Rosanes [127], Scorza [132, 133], and Sylvester [145], see [79] for an account of the subject. After they had been forgotten for decades in the literature, Mukai [105] gave very nice appearances of varieties of sums of powers: For instance, for a general ternary quadric F, the variety of sums of powers of F is a del Pezzo threefold V_5. These results renewed the interest in these classical varieties. Old and new results concerning the varieties of sums of powers were later collected and explained with modern terminology by Ranestad and Schreyer in [120] by the means of apolarity and syzygies. More recently, they showed in [121] that for a quadric $Q \subset \mathbb{P}^n$, the variety of sums of powers is a smooth Fano variety of index two and Picard number one when $n < 5$, and singular otherwise.

Despite the fact that there are fascinating results for specific instances, very little is known in general about these schemes, for example about

Ternary forms	Generic rank	Variety of sums of powers	Reference
Quadrics	3	del Pezzo threefold V_5	Mukai [105]
Cubics	4	$\mathbb{P}^2$	Dolgachev and Kanev [56]
Quartics	6	Fano threefold V_{22} of genus 12	Mukai [105]
Quintics	7	1 point	Hilbert [77], Palatini [115], and Richmond [126]
Sextics	10	$K3$ surface V_{38} of genus 20	Mukai [106]
Septics	12	5 points	Dixon and Stuart [55]
Octics	15	16 points	Ranestad and Schreyer [120]

Table 2.1. Varieties of sums of powers for ternary forms of degree $d = 2, \ldots, 8$.

their degrees. As these intriguing results witness, the varieties of sums of powers constitute a peculiar family of very special varieties with marvellous properties. In Table 2.1, we state the current knowledge of varieties of sums of powers for ternary forms in small degrees.

For a general form, one of the natural questions related to the Waring problem is the identifiability or the uniqueness of a Waring decompositions of it. The finiteness of the number of decompositions corresponds to a zero-dimensional variety of sums of powers. Identifiability questions are also treated in the more general context of decompositions of tensors [21]. The cases when the decomposition for a general form is unique are particularly interesting, as they correspond to the variety of sums of powers being one point and guarantee the existence of a canonical form of it. In these regards, a general form $F \in R_d$ has a unique presentation as a sum of s powers of linear forms only in the following cases [72]:

(i) $n = 1$, $d = 2k - 1$ and $s = k$, by [145];

(ii) $n = 2$, $d = 5$ and $s = 7$, by [77, 126, 115];

(iii) $n = 3$, $d = 3$ and $s = 5$, the Sylvester Pentahedral Theorem [145].

In [98], Massarenti and Mella study the birational behaviour of the varieties of sums of powers: For a general quadric in R_2, the irreducible components of the variety of sums of powers are unirational for any s and rational for $s = n + 1$. Moreover, they show the rational connectedness of infinitely many varieties of sums of powers.

Generalizations of varieties of sums of powers are present and studied in the literature. One of those is due to Massarenti [97], it is analogous to the concept of X-rank of any projective variety X, and it was studied along with its birational behaviour. Another direction was presented by Gallet, Ranestad, and Villamizar in [71], where varieties of apolar schemes were introduced.

Paper III introduces the space parameterizing all real Waring decompositions of a form F. This is called the *space of real sums of powers* and it is denoted by $\mathrm{SSP}_{\mathbb{R}}(F)$. This space is a semialgebraic set sitting inside the variety of sums of powers, when $s = \mathrm{rk}_{\mathbb{C}}(F)$. This does not need to coincide with the real part of the variety of sums of powers. Indeed, the latter is defined as the variety of points in the variety of sums of powers which are invariant under complex conjugation. One goal of Paper III is to get an explicit description of the space of real sums of powers for general ternary forms of small degrees.

One of the main traits of these semialgebraic sets, studied in Paper III, is that they are described by hyperdeterminants. This is again a very classical notion, and it was introduced by Cayley [41]. Let $X \subset \mathbb{P}^n$ be a projective variety. The *dual variety* $X^\vee \subset \mathbb{P}^{n\vee}$ is the closure of all hyperplanes tangent to X in some smooth point [74, Chapter 1]. The *dual defect* δ_X of X is the natural number $n - 1 - \dim X^\vee$. A variety X is said to be *dual defective* if the dual defect is positive, it is said to be *non-defective* otherwise.

Let $X = \mathrm{Seg}(\mathbb{P}V_1 \times \cdots \times \mathbb{P}V_k)$ be the Segre variety, where $\dim V_i = r_i + 1$. If $r_j = \max\{r_i, 1 \leq i \leq k\}$, then X is non-defective if and only if $r_j \leq \sum_{i \neq j} r_i$, [74, Chapter 14]. When X is non-defective, the polynomial equation of the hypersurface $X^\vee$ is called the *hyperdeterminant* of format $(r_1 + 1) \times \ldots \times (r_k + 1)$, [74, 112]. In order to explicitly describe the space of real sums of powers, the hyperdeterminants of format $m \times (n+1) \times (m+n-1)$ are interpreted as Hurwitz forms [142]. More specifically, the case of interest is for $n = 2$: The hyperdeterminant of format $3 \times m \times (m+1)$ is an irreducible homogeneous polynomial of degree $12\binom{m+1}{3}$, and it is the discriminant of ideals of $\binom{m+1}{2}$ points in $\mathbb{P}^2$.

The case of ternary cubic forms was considered by Banchi [8]. In Paper III, we show that the space of real sums of powers is either a disk in the real projective plane or a disjoint union of a disk and a Möbius strip. The two cases are characterized in Table 2.2. The algebraic boundary of the space of real sums of powers is an irreducible sextic curve that has nine cusps.

The general ternary form F belongs to the *Hesse pencil* [7],

$$F = x_0^3 + x_1^3 + x_2^3 + \lambda x_0 x_1 x_3.$$

λ	$\lambda < -3$	$-3 < \lambda < 0$	$0 < \lambda < 6$	$6 < \lambda$
F	hyperbolic	not hyperbolic	not hyberbolic	not hyperbolic
$H(F)$	not hyperbolic	hyperbolic	hyperbolic	hyperbolic
$C(F)$	hyperbolic	hyperbolic	not hyperbolic	hyperbolic
Space of sums of powers	disk	disk ⊔ Möbius strip	disk	disk
Oriented matroid	$(+,+,+,+)$	$(+,+,+,+) \sqcup (+,+,-,-)$	$(+,+,+,-)$	$(+,+,+,+)$

Table 2.2. Four possible types of a real cubic F in the Hesse pencil.

There are two ternary forms classically associated to the cubic F, the *Hessian* $H(F)$ and the *Cayleyan* $C(F)$ [57, Chapter 3].

As shown in Table 2.2, the remarkable feature here is that the hyperbolicity behaviour of $F, H(F)$, and $C(F)$ determines the structure of the space of real sums of powers.

Here is a connection to combinatorics. Consider a ternary cubic $F = L_1^3 + L_2^3 + L_3^3 + L_4^3$, whose apolar ideal $F^{\perp}$ is generated by three quadrics. Then any three of the linear forms L_1, L_2, L_3, L_4 are linearly independent. As a consequence, there is unique vector $v = (v_1, v_2, v_3, v_4) \in (\mathbb{R}\backslash\{0\})^4$ satisfying $v_1 = 1$ and $\sum_{i=1}^4 v_i L_i = 0$. The oriented matroid [16] of (L_1, L_2, L_3, L_4) is given by the sign vectors $\big(+, \mathrm{sign}(v_2), \mathrm{sign}(v_3), \mathrm{sign}(v_4)\big) \in \{-,+\}^4$.
For a general cubic, every point in the space of real sums of powers is mapped to one of the three sign vectors above. By continuity, this map is constant on each connected component of the space of real sums of powers. The last row in Table 2.2 shows the resulting map from the five connected components to the three oriented matroids. For instance, the fiber over $(+,+,-,-)$ is the Möbius strip in the space of real sums of powers. This is the first of the following two cases. For a general ternary cubic F,

(i) the space of real sums of powers is disconnected if and only if F is isomorphic over $\mathbb{R}$ to a cubic of the form $x_0^3+x_1^3+x_2^3+(ax_0+bx_1-cx_2)^3$ where a, b, c are positive real numbers;

(ii) the Hessian $H(F)$ is hyperbolic and the Cayleyan $C(F)$ is not hyperbolic if and only if F is isomorphic to $x_0^3 + x_1^3 + x_2^3 + (ax_0 + bx_1 + cx_2)^3$ where a, b, c are positive real numbers.

Results on spaces of sums of powers from Paper III cover also the case of sextics. Here, we derive the space of real sums of powers and its boundary inside the real part of the variety of sums of powers, which is a real K3 surface, by the $3 \times 4 \times 5$-hyperdeterminant. It is a polynomial of degree at most 240 in local coordinates and it completely describes the boundary of the space of real sums of powers.

2.7 Quartics

Ternary quartics are beautiful creatures of classical algebraic geometry. A source is Ciani's monograph [44]. A modern approach can be found in Dolgachev's book [57, Chapter 6]. Ternary quartics are non-hyperelliptic curves of genus three with 28 complex bitangents. They are one of the exceptions to the Alexander-Hirschowitz theorem and their generic rank is six. In his wonderful thesis at the University of Pisa in 1898, Scorza [132] studied the properties of polar polyhedra of ternary quartics. Mukai [105] proved that for a general ternary quartic $F \subset \mathbb{P}^2$, the variety of sums of powers is a smooth Fano threefold V_{22}, and every V_{22} arises this way. This threefold is the intersection of the Grassmannian of four-dimensional subspaces in a five-dimensional space with a suitable thirteen-dimensional linear subspace [120]. A study of real Fano threefolds has been pursued by Kollár and Schreyer [85], and Schreyer [131].

Real ternary quartics in $\mathbb{P}^2_{\mathbb{R}}$ have six topological types, which were classified by Zeuthen [151]. This classification is reviewed in [118]. The types are: four ovals, three ovals, two non-nested ovals, hyperbolic, one oval, and the empty set. The topological types correspond to reality conditions on the 28 complex bitangents. Klein [84] proved that these types are connected subsets in $\mathbb{P}^{14}_{\mathbb{R}}$.

As for any smooth ternary form, on a general ternary quartic we may define a *theta characteristic*. This is a collection of points in the curve with special properties. Using the language of divisors, a theta characteristic is a divisor class θ such that 2θ is linearly equivalent to the canonical divisor K_F of the ternary form F. A theta characteristic θ on F is *even* or *odd*, depending on the parity of $h^0(F, \theta)$. If a ternary form has genus three, there are 28 odd theta characteristics and 36 even theta characteristics [57, Chapter 6].

Another intriguing divisor lying on a quartic curve is the intersection divisor given by contact cubics. A *contact cubic* for a ternary quartic F is a ternary cubic whose intersection with F is given by six non-reduced points, each of whom has multiplicity two. There are 56 contact cubics given by three bitangents for every even theta characteristic whose six points do not lie on a conic. In total there are $56 \times 36 = 2016$ contact cubics of this type [118]. Additionally, there are $45 \times 28 = 1260$ contact cubics whose six points lie on a conic. These are all the triples of the 28 bitangents of a general ternary quartic, and $1260 + 2016 = \binom{28}{3}$. Contact cubics of the first type can be used to construct a determinantal representation of a ternary quartic. A modern account of this result is presented by Plaumann, Sturmfels, and Vinzant [118]. They also discuss how to derive the 36 representation of it as a determinant of $Ax_0 + Bx_1 + Cx_2$, where A, B, C are symmetric matrices.

The Aronhold invariant of a ternary cubic is a homogeneous polynomial in the ten coefficients of the cubic. It vanishes on a ternary cubic C if and only if C is projectively equivalent to the Fermat cubic $x_0^3 + x_1^3 + x_2^3$.

The *Scorza map* associates to a general ternary quartic F a pair $(S(F), \theta)$ where $S(F)$ is another quartic, the Aronhold covariant, and θ is an even theta characteristic on $S(F)$. The quartic $S(F)$ is the Aronhold invariant of the ternary cubic obtained as the polar of F with respect to a general point in $\mathbb{P}^2$. Scorza [133] showed that $F \mapsto S(F)$ is a degree 36 covering map and that this map is a birational map between the moduli space of curves of genus three and the moduli space of curves of genus three equipped with an even theta characteristic. A modern and neat proof of this fact was given by Dolgachev and Kanev in [56].

Mukai [107] introduced the strictly biscribed triangles to a general quartic. These are contact cubics for the quartic. There are 288 biscribed triangles on a general ternary quartic. Each even theta characteristic on its Aronhold covariant $S(F)$ produces eight of them and, moreover, every strictly biscribed triangle corresponds to a Waring decomposition of F.

In Paper IV, we study the Scorza map over the reals. Among the 36 pairs of topological types of smooth ternary quartics in the real projective plane $\mathbb{P}^2_{\mathbb{R}}$, at least 30 pairs are realized by a quartic F and its Aronhold covariant quartic $S(F)$. Every pair not involving the hyperbolic type is realizable as $\big(F, S(F)\big)$. The result is obtained with computational methods.

We also analyze the space of real sums of powers for a real quartic. Let F be a general ternary quartic of real rank six. If it can be written as

$$F = \sum_{i=1}^{6} \lambda_i L_i^4,$$

where the λ_i are positive real numbers, then the space of real sums of powers equals the real part of its variety of sums of powers. If the space of real sums of powers is a proper subset of the real part of the variety of sums of powers, then its algebraic boundary has degree 84. It is the hyperdeterminant of format $4 \times 3 \times 3$.

3. Phylogenetics

In this part we overview the background, methods, and main results related to Paper IV. Our motivation here comes from applications of algebraic geometry in biology. The main reference is the book by Pachter and Sturmfels [114].

3.1 Markov processes and phylogenetics

A *Markov chain* is a sequence of random variables $\{X_i\}$ satisfying the *Markov property*

$$P(X_{k+1} = x_{k+1} | X_1 = x_1, \dots X_k = x_k) = P(X_{k+1} = x_{k+1} | X_k = x_k),$$

where $P(A|B)$ denotes the conditional probability of A given B. In other words, the Markov property is satisfied whenever the probability of X_{k+1} being in a specific state x_{k+1} depends only on the state of the previous random variable X_k in the sequence.

This construction can be generalized to rooted trees. In the definition of a Markov chain, the underlying rooted tree is a path. Let $\mathcal{T}$ be a directed rooted tree on the set of vertices (or nodes) V, that is, a directed connected graph without cycles on V, with a distinguished vertex $r \in V$. We denote by E the set of edges of $\mathcal{T}$. The degree of a vertex is the number of edges incident to the vertex. The leaves of $\mathcal{T}$ are the vertices of $\mathcal{T}$ whose degree is one. The set of leaves is denoted by L. The vertices that are not leaves are referred to as internal nodes.

To each vertex $v \in V$ we associate a random variable X_v, whose set of states is a finite set S_v. For each vertex v different from the root, there is a unique vertex u connected to v through an edge, directed from u to

v. Such a vertex u is the ancestor of v. Each edge $e \in E$, directed from u to v, comes equipped with a $|S_v| \times |S_u|$ matrix M_e, whose entries are the conditional probabilities for the states of X_v, given those of X_u. These matrices are called *transition matrices*. Analogously to the sequence of random variables $\{X_i\}$, on the tree $\mathcal{T}$, the states of X_v depend uniquely on the states of the random variable X_u, corresponding to the ancestor u of v.

This model is very useful in applied mathematics, since it is powerful to describe different phenomena such as Brownian motion, population growth, stock market fluctuations, and many others [80]. These tree models are used in computational biology to study the evolution process of species and the history of life. In this context, each vertex v of $\mathcal{T}$ represents a species (the random variable) and the states are usually the four nucleobases forming the DNA: *adenine*, *cytosine*, *guanine*, and *thymine* denoted by A, C, G, and T, respectively. The matrices of conditional probabilities M_e specify the model of evolution of the species in the tree.

The part of computational biology that models evolution and describes mutations in this process is called phylogenetics [137]. This is a fertile subject witnessing many connections to various parts of mathematics such as algebraic geometry [65, 96, 138, 144], combinatorics [15], and representation theory [86].

A remarkable structure modeling evolution is a phylogenetic tree. This is a binary tree, that is, all internal nodes have degree three, except for the root having degree two. The leaves of a phylogenetic tree are labelled by integers and called *taxa*. The leaves are observed variables, while the internal nodes are hidden variables. The tree models appearing in phylogenetics are very intriguing since they naturally give algebraic varieties. To be more specific, let us fix a tree $\mathcal{T}$ with n taxa. Assuming that each leaf has k possible states, there are k^n possible observations at the leaves. The probability ϕ_i of an observation i is a polynomial in the entries of the matrices M_e and the probability distribution of the root, see the example in Figure 3.1. Then we obtain a polynomial map $\phi = (\phi_1, \ldots, \phi_{k^n}) : \mathbb{R}^N \to \mathbb{R}^{k^n}$, where N is the number of entries of the matrices M_e and the probability distribution of the root. The first approach in phylogenetic algebraic geometry [65] is to study the Zariski closure of the image of ϕ over the complex numbers. From the probabilistic per-

Species	DNA
Human	CCCCGGTGTACTCTAACCACTGAAG CGGCCGTGTCGGGGACTCACGCGCTTCCCATTCAGCTCTGGATCTGGAAC
Mouse	CCCCGTCGCCT TGATCATTTAAACGGGCCCTGTAGCAGGCTAGCT ATCCTATACATTTCTGGGCCTGGAGC
Rat	CCCCGTCACCCCATGATCGTTTAAGCGGGCCCTGTAGCAGTCTAGGT GTCCTATTCATTTCTGGACATGGAGC

Table 3.1. Example of DNA alignment from [64].

spective, the relevant points are the real positive points lying in the standard simplex sitting in $\mathbb{R}^{k^n}$. In phylogenetic algebraic geometry, these relevant points sit inside the phylogenetic varieties together with extra points, coming from complex numbers and Zariski closure. The crucial advantage is that working with complex algebraic varieties makes all the machinery of algebraic geometry available.

The generators of ideals of these phylogenetic varieties are called *phylogenetic invariants*. They were introduced by Cavender and Felsenstein [40], and Lake [87] as algebraic tools to reconstruct evolutionary trees. In general, it is a very difficult task to explicitly compute phylogenetic invariants. Progress on their computation is subject of current intensive research [5, 28, 36, 58, 101, 103, 104].

Besides determining phylogenetic invariants, the other main issue is to infer phylogenetic trees. Suppose that we have a DNA alignment of n species, as in Table 3.1. Our aim is to reconstruct the phylogenetic tree underlying the evolution of these species.

The problem of reconstructing ancestral genomes, along with the related statistical and mathematical questions of comparative genomics, are treated by Pachter in [113]. To discuss some of the methods addressing the phylogenetic reconstruction, we mostly follow the overview by Casanellas [34]. We choose a model of evolution $\mathcal{M}$ and a set of invariants $f_{\mathcal{T}}$, for each binary tree $\mathcal{T}$ with n leaves. The data of the alignment give an empirical probability distribution $\hat{p} \in \mathbb{R}^{4^n}$, that comes from counting columns of every possible type in the alignment. Now, we evaluate each set of invariants at the point $\hat{p}$ and we pick the binary tree $\mathcal{T}$ such that $f_{\mathcal{T}}(\hat{p})$ is the smallest according to some measure. The problem is that the choice of the invariants $f_{\mathcal{T}}$ does not necessarily differentiate the topology of different phylogenetic trees [35, 64]. Only those invariants that are topologically informative, that is, they vanish on some tree topologies but not in others, can be seen as meaningful for a statistical test. Casanellas and Fernández-Sánchez [35] proved that some of these useful invariants for phylogenetics come from edges of the tree, called edge invariants.

One of the most common phylogenetic reconstruction methods is the MLE-algorithm. Given a DNA alignment $\mathcal{D}$ and an evolutionary model $\mathcal{M}$, the objective is to find a binary tree $\hat{\mathcal{T}}$ and parameters $\hat{\theta}$ maximizing the probability $P(\mathcal{D}|\mathcal{M},\mathcal{T},\theta)$ among all the possible tree topologies and parameters. The MLE-algorithm is performed separately on each tree topology using optimization methods. The weak point of this approach is due to the magnitude of the number of cases, there are $(2n-5)!!$ unrooted phylogenetic trees on n leaves [114, Lemma 2.32].

Another useful reconstruction method is the neighbor-joining method. A *dissimilarity function* d on a set of n species is a symmetric map on pairs of species that outputs a non-negative real number. This dissimilarity function can be interpreted as a distance between pairs of species. In other words, it is meant to give an estimate of the amount of mutations that separate apart two species. To approximate the amount of observed and unobserved mutations that occurred between two species, the *Jukes-Cantor distance* is typically chosen as distance function. It is defined as $-\frac{3}{4}\ln(1-\frac{4}{3}f)$, where f is the fraction of different nucleotides in both sequences.

Given a dissimilarity function d, the neighbor-joining algorithm chooses two species x and y minimizing the function

$$D(x,y) = d(x,y) - \frac{1}{n-2}\sum_z (d(x,z)+d(y,z)),$$

where z runs over all the species. Then the two species x and y are joined by two edges through an internal node. The algorithm introduces a species t at the internal node substituting x and y. At each step, the number of species decreases and the function D is redefined. The algorithm gives the correct phylogenetic tree if the species are actually organized in a tree and the distances used are the lengths of the paths between the species in the tree.

3.2 Models and varieties

Here we explore in more detail some phylogenetic models and we draw more formally the connection to algebraic geometry. Let $\mathcal{T}$ be a directed rooted tree, let X_v be the random variables corresponding to the vertices of $\mathcal{T}$, and S be their finite set of states. We define W to be the complex vector space spanned by the elements of S, that is $W = \oplus_{s \in S} \mathbb{C}_s$. To each vertex v we attach a vector space W_v isomorphic to W, whose basis is $\{\alpha_v\}$.

Defining a *model* $\mathcal{M}$ is equivalent to selecting a subspace $\hat{W} \subseteq \mathrm{End}(W)$ of matrices. To each edge $e \in E$ of $\mathcal{T}$, we associate an isomorphic copy of $\hat{W}$, denoted by $\hat{W}_e$. Each entry of any matrix in $\hat{W}_e$ is labelled by pairs of elements in S.

The models mostly used in the literature, listed in chronological order, are:

(i) The *Jukes-Cantor model*. It was introduced by Jukes and Cantor in [81]. In this model, S has four elements and the transition matrices are of the form:

$$\begin{bmatrix} a & b & b & b \\ b & a & b & b \\ b & b & a & b \\ b & b & b & a \end{bmatrix}.$$

(ii) The *Cavender-Farris-Neyman model*. It was introduced by Neyman in [108]. In this model, S has two elements and the transition matrices are of the form:

$$\begin{bmatrix} a & b \\ b & a \end{bmatrix}.$$

(iii) The *2-Kimura model*. It was introduced by Kimura in [82]. In this model, S has four elements and the transition matrices are of the form:

$$\begin{bmatrix} a & b & c & b \\ b & a & b & c \\ c & b & a & b \\ b & c & b & a \end{bmatrix}.$$

(iv) The *3-Kimura model*. It was introduced by Kimura in [83]. In this model, S has four elements and the transition matrices are of the form:

$$\begin{bmatrix} a & b & c & d \\ b & a & d & c \\ c & d & a & b \\ d & c & b & a \end{bmatrix}.$$

(v) The *general Markov model*. In this model, the space of matrices $\hat{W}$ coincides with $\mathrm{End}(W)$ and the number of states is arbitrary.

As an example, let us consider the following directed rooted tree $\mathcal{T}$ with a root r, two leaves l_1 and l_2, and two edges a and b.

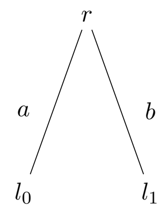

Figure 3.1. The rooted tree $\mathcal{T}$

We consider the Cavender-Farris-Neyman model on $\mathcal{T}$. Suppose that the probabilities of r to be 0 and 1 are, respectively, σ_0 and σ_1. Let us denote the transition matrices associated to the edges a and b in Figure 3.1, respectively, by:

$$A = \begin{bmatrix} a_0 & a_1 \\ a_1 & a_0 \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} b_0 & b_1 \\ b_1 & b_0 \end{bmatrix}.$$

Here a_0 is the conditional probability $P(l_0 = 0|r = 0) = P(l_0 = 1|r = 1)$, and a_1 is $P(l_0 = 0|r = 1) = P(l_0 = 1|r = 0)$, where l_0 is a leaf in Figure 3.1. Likewise b_0 and b_1 are conditional probabilities for the states of the leaf l_1 in Figure 3.1. The parameters of the model are $\sigma_0, \sigma_1, a_0, a_1, b_0, b_1$. The probability distribution at the leaves l_0, l_1 is encoded in the following matrix with four entries corresponding to the possible states $00, 01, 10, 11$:

$$\begin{bmatrix} \sigma_0 a_0 b_0 + \sigma_1 a_1 b_1 & \sigma_0 a_0 b_1 + \sigma_1 a_1 b_0 \\ \sigma_0 a_1 b_0 + \sigma_1 a_0 b_1 & \sigma_0 a_1 b_1 + \sigma_1 a_0 b_0 \end{bmatrix}.$$

This matrix can be understood as a projective morphism $\mathbb{P}^1 \times \mathbb{P}^1 \times \mathbb{P}^1 \to \mathbb{P}^3$. The closure of its image is the secant line variety of the Segre variety $\mathbb{P}^1 \times \mathbb{P}^1$.

We give a more algebraic framework for the models and the map given in the example, following [28, 101]. Let us define the following vector spaces,

$$W_V = \bigotimes_{v\in V} W_v,\ W_L = \bigotimes_{\ell\in L} W_\ell, \hat{W}_E = \bigotimes_{e\in E} \hat{W}_e.$$

Let $\hat{\psi} : \hat{W}_E \to W_V$ be the map whose dual is defined as

$$\hat{\psi}^*\Big(\bigotimes_{v\in V} \alpha_v\Big) = \bigotimes_{e\in E} \Big(\alpha_{u(e)} \otimes \alpha_{v(e)}\Big)^*_{|\hat{W}_e},$$

where the edge e connects $u(e)$ to $v(e)$. The map $\hat{\psi}$ is the map giving the probability distribution to the leaves. Now, we define the map $\pi_L : W_V \to W_L$ to be

$$\pi_L = \Big(\bigotimes_{v\in L} \mathrm{id}_{W_v}\Big) \otimes \Big(\bigotimes_{v\in N} \delta_{W_v}\Big),$$

where N denotes the set of internal nodes and δ_{W_v} is the sum of the duals of the basis $\{\alpha_v\}$, that is, δ_{W_v} is the sum of the coordinates. The map π is a contraction map and it sums up the probabilities of all states of vertices as long as they differ on the nodes. We obtain a map $\hat{\phi} = \pi_L \circ \hat{\psi} : \hat{W}_E \to W_L$ between vector spaces. The map $\hat{\phi}$ induces a rational (that is, it is not necessarily defined everywhere) map between the corresponding projective spaces. This map coincides with the one given in the example of the rooted tree $\mathcal{T}$ in Figure 3.1. The closure of the image of $\hat{\phi}$, denoted by $X(W, \hat{W}, \mathcal{T})$, is the algebraic variety of the model.

Examples of classical varieties that show up as varieties parameterizing probabilistic models are Veronese varieties, determinantal varieties, secant varieties, and joins. Particularly interesting instances of the latter family are secant varieties of Segre varieties, as in the example related to Figure 3.1. The special variety $\sigma_4(\mathbb{P}^3 \times \mathbb{P}^3 \times \mathbb{P}^3)$, that is the fourth secant variety of the Segre variety $\mathbb{P}^3 \times \mathbb{P}^3 \times \mathbb{P}^3$, is the variety of the mixture model with four states, corresponding to the nucleotides A, C, G, T. It describes the evolutionary tree of three species with a common ancestor. Conjecturally, such a projective variety is generated by polynomials of degrees five, six, and nine. This conjecture is known as *salmon conjecture*, since the prize for the hypothetical solver would be a smoked Copper river salmon. There has been some progress towards this conjecture by Friedland [67], who gave the first set-theoretic solution to the salmon conjecture. Friedland's solution used Strassen's equations of degrees five and nine, along with new equations of degree sixteen. Bates and Oeding [10] gave a different set-theoretic solution using equations of degrees five, nine, and six. This solution was in part based on computational methods carried with the software for numerical algebraic geometry Bertini [9]. Friedland and Gross [68] modified Friedland's original proof using degree six equations to play the role of the original Friedland's degree sixteen equations, providing a numeric-free proof of the set-theoretic statement. More recently, Daleo and Hauenstein [54] gave a numerical proof of the full salmon conjecture.

Another family of interesting explicit varieties is the one of toric varieties, see [53, 70, 140] for an introduction to those. They arise as varieties for group-based models, which we discuss next. Let G be an abelian group acting transitively and freely on the set of states S. A *general group-based model* is a maximal subspace $\hat{W}_G$ of invariant matrices under the group action. A subspace of this maximal subspace is called a *group-based model*. Examples of group-based models include the Cavender-Farris-Neyman model and the 3-Kimura model for the groups $G = \mathbb{Z}_2$ and $G = \mathbb{Z}_2 \times \mathbb{Z}_2$, respectively.

For group-based models, the variety of the model is the closure of the map

$$\hat{\phi} = \pi_L \circ \hat{\psi} : \prod_{e \in E} \mathbb{P}(\hat{W}_e) \to \mathbb{P}(W_L^G),$$

where W_L^G is the invariant subspace of W_L with respect to the action of G. In [101], it is shown that the target projective space has coordinates parameterized by group-based zero-sum sequences. Let G be a finite abelian group and n a natural number. A *group-based zero-sum sequence* is a sequence of n elements of G summing up to the 0 of G. The set of group-based zero-sum sequences is a group, via the coordinate-wise action, isomorphic to G^{n-1}.

The origin of group-based models can be traced back to the seminal work of Evans and Speed [66]. They realized that the Klein group $G = \mathbb{Z}_2 \times \mathbb{Z}_2$ acts on $\{A, C, G, T\}$ transitively and freely. A further generalization of their method was presented in [147], where the variety of the model was recognized to be toric, after a change of coordinates. More recently, Sturmfels and Sullivant [143] studied phylogenetic invariants for several group-based models: For Jukes-Cantor and Kimura models on a binary tree, they showed that their phylogenetic invariants form toric ideals, whose minimal generators and Gröbner bases were determined. For a binary tree, the ideal of phylogenetic invariants for the models below is generated by an explicit set of polynomials of given degrees:

(i) Cavender-Farris-Neyman model, degree 2;

(ii) Jukes-Cantor model, degrees $1, 2, 3$;

(iii) 2-Kimura model, degrees $1, 2, 3, 4$;

(iv) 3-Kimura model, degrees $2, 3, 4$.

Moreover, they proved that it is enough to consider stars $K_{1,n}$ in order to analyze arbitrary trees $\mathcal{T}$.

As already mentioned above, the group-based models encountered so far give rise to toric varieties, but this is not in general the case. In [101], Michałek gave a precise condition under which the phylogenetic variety of the model is toric. Let H be a normal, abelian subgroup of a group $G \subset \mathrm{Sym}(S)$, the symmetric group of a set S. Suppose that H acts transitively and freely on S. Then the phylogenetic variety $X(W, \hat{W}, \mathcal{T})$ is a toric variety for any tree $\mathcal{T}$, where $\hat{W}$ is the space of matrices invariant under the action of G. Moreover, he gave conditions for the normality of a toric variety from a model.

In the setting of more general models, some results are known. For a general Markov model on binary trees, Allman and Rhodes [6] determined the full ideal of invariants for the 2-state model. They showed that the ideal of the variety parameterizing the 2-state general Markov model is generated by 3×3-minors of certain matrices coming from tensor flattenings. The flattenings correspond to contracting internal edges and grouping the leaves. Raicu [119] proved the same type of result in the case of stars, which is equivalent to finding the vanishing ideal of the secant line variety of any Segre variety. Results of Draisma and Kuttler [62] showed that it is sufficient to know the case of stars in order to obtain the result for any tree. The last statement holds for all equivariant models, which include general Markov and group-based models.

3.3 Moves and phylogenetic complexity

The objects of interest in Paper IV are the toric varieties of group-based models whose trees are the stars $K_{1,n}$, and whose group G acts freely and transitively on the set of states. We denote them by $X(G, K_{1,n})$, for simplicity of notation.

The polytopes corresponding to these toric varieties are constructed as follows. Let $M \cong \mathbb{Z}^{|G|}$ be a lattice with a basis corresponding to elements of G. Consider M^n with the basis $e_{(i,g)}$ indexed by pairs in $[n] \times G$. We have an injective map of sets

$$\mathfrak{G} \to M^n, (g_1, \ldots, g_n) \longmapsto \sum_{i=1}^{n} e_{(i,g_i)},$$

where $\mathfrak{G}$ is the group of group-based zero-sum sequences. The image of this map defines the vertices of the polytope $P_{G,n}$, which correspond to group-based zero-sum sequences.

The phylogenetic complexity is an intriguing invariant of abelian groups, first analyzed in [143]. Let $\phi(G, n) = \phi(G, K_{1,n})$ be the maximal degree of a generator in a minimal generating set of $I(X(G, K_{1,n}))$. We define the phylogenetic complexity $\phi(G)$ of an abelian group G to be

$$\phi(G) = \sup_{n \in \mathbb{N}} \phi(G, n).$$

The main goal of Paper IV is to show that for any finite abelian group G, the phylogenetic complexity $\phi(G)$ is finite.

To achieve this, we use a more suitable way to look at the binomials in the ideal $I(X(G, K_{1,n}))$. Such binomials may be identified with a pair of matrices T_0 and T_1, or *tables*, of the same size filled with elements of G, regarded up to row permutation. Each row of such tables has to be a group-based flow. The identification is as follows. Every binomial is a pair of monomials. As mentioned above, the variables in such monomials correspond to group-based zero-sum sequences, given by a collection of n elements in G. Every monomial is viewed as a table, whose rows are the variables appearing in the monomial. The number of rows of the corresponding table is the degree of the monomial. A binomial is identified with the pair of tables encoding the two monomials. A binomial belongs to $I(X(G, K_{1,n}))$ if and only if the two tables are *compatible*, that is, for each i, the ith column of T_0 and the ith column of T_1 are equal as multisets. In order to generate a binomial, represented by a pair of tables T_0,

T_1, by binomials of degree at most d, we select a subset of rows in T_0 of cardinality at most d, and we replace it with a compatible set of rows. We repeat these replacements until both tables are equal. The procedure just described is a *move* of degree d.

For an instance of such moves, let us assume for the sake of simplicity $G = (\mathbb{Z}_2, +)$ and $n = 6$. Consider the compatible tables

$$T_0 = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \end{bmatrix} \text{ and } T_1 = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 \end{bmatrix}.$$

The red subtable of T_0 is compatible with the table

$$T' = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 1 \end{bmatrix}.$$

We may exchange them obtaining

$$\tilde{T_0} = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

The tables T_0 and $\tilde{T_0}$ are compatible. Now, the brown subtable of $\tilde{T_0}$ is compatible with the table

$$T'' = \begin{bmatrix} 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 \end{bmatrix}.$$

Finally, we exchange them obtaining T_1. Then we have a sequence of tables $T_0 \rightsquigarrow \tilde{T_0} \rightsquigarrow T_1$. We started from a degree three binomial given by the pair T_0 and T_1, and we generated it using degree two binomials.

In order to show the finiteness of the phylogenetic complexity, we prove that $\phi(G, n)$ is eventually constant. Our task is to demonstrate that there exists n_0, such that for any $n > n_0$, any pair of tables of size $d \times n$ is generated by binomials of degree at most $\phi(G, n_0)$. The proof is based on an analysis of combinatorial features of the tables representing binomials in the ideal $I(X, K_{1,n})$. Given a $d \times n$ table T filled with elements of G, we restrict to a subtable T' where a chosen element g in G is one of the most frequent in all the columns. This is not a serious restriction, as n is very large and we work with a subtable with at least $n/|G|$ columns. We construct a subdivision into subtables, with certain properties, on the

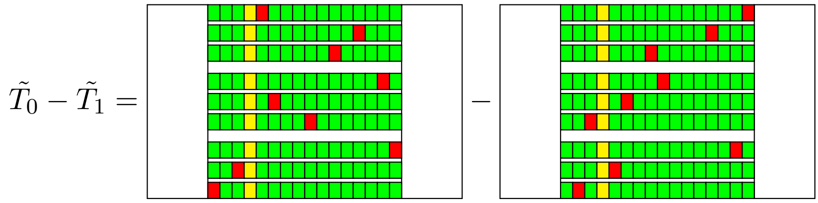

Figure 3.2. Vertical stripes

restrictions T'_0, T'_1 of a pair of tables T_0, T_1. An instance of a subdivision into subtables is depicted in Figure 3.2, where subtables are denoted by colored squares. The subdivision algorithm transforms the tables T_0, T_1 into suitable tables $\tilde{T}_0, \tilde{T}_1$ using only moves of degree two. The important feature is that this algorithm produces corresponding vertical stripes in $\tilde{T}_0$ and $\tilde{T}_1$ of subtables consisting of two columns, whose rows contain exactly the same elements row by row. An example of such a vertical stripe is drawn in yellow in Figure 3.2. During the process, there are subtables failing our requirements. The red squares in Figure 3.2 denote these subtables. A yellow vertical stripe needs to be chosen outside the red squares. Since in each step of the algorithm the number of red squares is very small compared to the total number of subtables, we can always choose a yellow vertical stripe. For technical details on this subdivision and its combinatorial structure, we refer to Paper IV.
After having produced such a pair of corresponding columns in the tables $\tilde{T}_0$ and $\tilde{T}_1$, we are able to use an inductive argument on the number of leaves n. Fix $n_0 \gg |G|$ sufficiently large and take $n > n_0$. We want to show that $\phi(G, n) \leq \phi(G, n-1)$. In other words, we want to prove that the phylogenetic complexity is eventually constant.

The first crucial step is to use the Hilbert basis theorem as basis for the induction. This theorem states that an ideal in a polynomial ring with finitely many variables is finitely generated. Once we fix n_0, the ideal $I(X(G, K_{1,n_0}))$ is in a polynomial ring with finitely many variables and so it is finitely generated. This means that the phylogenetic complexity $\phi(G, n_0)$ is finite.

The other crucial step is to use the subdivision algorithm above. By this algorithm, we may assume that the tables T_0 and T_1 have two pairs of columns whose corresponding elements are exactly the same row by row. Summing up these columns in both of the tables, we go from n leaves to

$n-1$ leaves. The key observation is that every move on $n-1$ leaves can be lifted to a move on n leaves, up to moves of degree two. In other words, we do not deal directly with large degree moves, but, instead, we use induction. This proves the finiteness of phylogenetic complexity, but it does not give an effective bound and it is not even close to the conjectural one, which is $|G|$ [143, Conjecture 29]. The issue is that we work with sufficiently large tables in order to device the subdivision.

The finiteness of the phylogenetic complexity sits in the setting of current reseach of finiteness results for models. Indeed, the result of Paper IV establishes the ideal-theoretic finiteness for group-based models. For equivariant models, which include the class of group-based models, the finiteness result on set-theoretic level was proved in [59, 62]. As a consequence, Paper IV can be regarded as a slightly stronger result, but for a smaller class. Finiteness plays also an increasingly important role in the context of infinite dimensional toric varieties [61]. There are two interesting long-standing conjectures for group-based models. The first is that the phylogenetic complexity of $G = \mathbb{Z}_2 \times \mathbb{Z}_2$ is four [143, Conjecture 30]. The second, already mentioned, is that the phylogenetic complexity of G is $|G|$ [143, Conjecture 29]. The first is already known to hold scheme-theoretically by the work of Michałek [102] and the second is known to be true on a Zariski open dense subset by Casanellas, Fernández-Sánchez, and Michałek [36]. More ideas are needed to solve these problems.

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