Noname manuscript No.
(will be inserted by the editor)

Algebraic geometry in the interface of pure and applied mathematics

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Received: date / Accepted: date

Abstract In its simplest form, algebraic geometry is the study of geometric objects defined by (typically nonlinear) algebraic equations, i.e., multivariate polynomials. Many models in the sciences and engineering are expressed as sets of real solutions to such systems of polynomial equations. Algebraic geometry is good at counting (solutions, tangencies, obstructions, etc.), giving structure to interesting sets (varieties with special properties, moduli spaces, etc.) and, principally, understanding structure. Starting in the 80's with the development of Computer Algebra Systems (CAS), and increasingly over the last years, ideas and methods from algebraic geometry are being applied in a great number of new areas (both in mathematics and in other disciplines including biology, computer science, physics, chemistry, etc.). This article is a survey of some of these exciting developments.

Keywords algebraic geometry · systems biology · tensors · algebraic vision · geometric modeling · polynomial system solving

Mathematics Subject Classification (2000) 14 · 13 · 15 · 92

1 Introduction

The new era of applications of algebra and geometry started in the 1980's, with the availability of personal computers and the implementations of algorithms to compute Gröbner bases, introduced by B. Buchberger in his 1965 thesis written under the direction of W. Gröbner. Two of the free and open-source CAS for polynomial computations that started being developed in that period and are now widely used and still in active development, are Macaulay2 [34] and Singular [20]. Macaulay2 was designed and written by D. Grayson and M. Stillman, with the aim of supporting computation in research in algebraic geometry, commutative algebra, and related fields, including applications in biology, physics, and statistics. Singular has been developed under the direction of W. Decker, G.-M. Greuel, G. Pfister, and H. Schönemann, who head Singular's core development team within the Department of Mathematics of the University of Kaiserslautern. It has a special emphasis on commutative and non-commutative algebra, algebraic geometry, and singularity theory. Further functionality is obtained by combining Singular with third-party software; this includes tools for convex geometry, tropical geometry, and visualization. Another pioneer CAS is CoCoA, developed in the University of Genova [1]. One important aspect of these systems is that once computations of abstract objects are enabled, researchers often find major new theorems and applications of these objects by experimentation.

The book *Ideals, Varieties, and Algorithms* [13], written by D. Cox, J. Little, and D. O'Shea, first published in 1992, represented a timely vision that algebraic geometry and computational commutative algebra could be made accessible not just to mathematicians who were not experts in the area, but also to users of mathematics in engineering and computer science. It was followed by a graduate text by the same authors: *Using Algebraic Geometry* [14] first published in 1998, with the same accesible style which broadened the way we teach and use (computational) algebraic geometry.

The maturity of the subject led to the creation in 2016 of the SIAM Journal on Applied Algebra and

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Geometry (abbreviated: SIAGA). This journal offers a new home for exciting emerging applications using tools from algebra, geometry and topology. Its Editor in Chief is B. Sturmfels, the author of several fundamental books (in particular, [50, 51, 42]) and a large number of papers introducing techniques of algebraic geometry and combinatorics in many different areas of mathematics and applications.

In the following sections I will give a brief description of some of the application areas and the algebro-geometric concepts involved. Section 2 will be devoted to applications in biology and Section 3 will survey other important applications. In turn, these applications lead to interesting and basic theoretical questions; some of these questions have been answered along the way and some remain as directions of active research. Finally, Section 4 contains other pointers to software for polynomial system solving.

2 Biological applications

Systems biology's main goal is to understand the design principles of living systems. Algebraic geometry can be used to analyze the standard models in the field. In particular, in the realm of biochemical reaction networks, that is, chemical reaction networks in biochemistry, the usual mass-action kinetics modeling of the evolution of the concentrations of the different chemical species along time yields an autonomous system of polynomial ordinary differential equations $\frac{dx}{dt} = f_\kappa(x)$ in the unknown vector of concentrations x of the n species as functions of time This is indeed a *family* of polynomial differential systems associated to a labeled directed graph G of reactions. The monomial terms come from the labels of the nodes of G by complexes in the given species, the coefficients depend on the (positive) reaction rate constants κ that label the edges of G and the total production of each reaction (which is the difference of the labels of the target and source nodes). The n real polynomials $f_{\kappa,i}(x)$ carry a combinatorial structure inherited from G. Linear dependencies among these polynomials give linear conservation relations and the behavior of the system also depends on the values of the total amounts (the constant value of these invariant linear functions on the concentrations). In many cases, these linear invariants are easily predicted in terms of the biochemistry. Limits of trajectories are steady states of the system, that is, solutions to the algebraic system $f_\kappa(x) = 0$. Thus, questions about steady states in biochemical reaction networks under mass-action kinetics are fundamentally questions about nonnegative real solutions to parametrized polynomial ideals. We refer the reader to the survey article [21] for basic definitions and further references and we review here some advances developed after that article was published.

We introduced a general framework for biological systems called MESSI systems [43], that describe Modifications of type Enzyme-Substrate or Swap with Intermediates, and we proved general results based on the network structure. Many post-translational modification networks are MESSI systems. For example: the motifs in [29], sequential distributive multisite phosphorylation networks [44], sequential processive multisite phosphorylation networks, phosphorylation cascades, the bacterial EnvZ/ OmpR network in [47], many two component systems, and all linear networks. We showed that, under mass-action kinetics, MESSI systems are conservative, and we simplified the study of steady states of these systems by explicit elimination of intermediate complexes (inspired by [30, 55]).

A (bio)chemical reaction network is said to exhibit multistationarity if there exist at least two positive steady states with the same total amounts. Multistationarity provides a crucial mechanism for switching between different response states in cell signaling systems and enables multiple outcomes for cellular-decision making. We identified an important subclass of MESSI systems with toric steady states [44] and we gave in this case an easy algorithm to determine the capacity for multistationarity. It provides choices of rate constants for which multistationarity takes place, based on the theory of oriented matroids.

When a network has the capacity for multistationarity, the next question is how to predict (semialgebraic) regions in parameter space which give rise to multistationary systems. The nice recent article [11] deals with this question based on degree theory, allowing for the determination of both multistationarity and monostationarity conditions depending on the rate constants (while the conditions on the total amounts are not precised). A different approach using results from real algebraic geometry has been developed in [32], where we get only open sufficient conditions, but jointly on rate constants and total amounts. Other main problems in the area are to develop tools to find the maximal number of positive steady states and to find regions in parameter space with the predicted number of positive steady states, or at least where lower/upper bounds apply. Another important question is the characterization of networks that allow for stable oscillations, as in the Lotka-Volterra population model (which can be seen as arising from a directed graph under the mass-action kinetics modeling). There are many theoretical and computational tools in real algebraic geometry, but we need precise answers for systems of biological interest, usually with (too) many variables and (too) many parameters. The question is also difficult because in general, it is hard to find sparse real polynomial systems with many (positive) real roots (see for instance Theorem 1.2 in [24]).

Most of the different results to decide the capacity for multistationarity of a given reaction network have been summarized in Theorem 1.4 of [40]. A consequence of these results driven by applications is the first partial generalization of the classical Descartes' rule to guarantee the existence of at most one positive root in the multivariate setting (which was hidden in [19]). Classical Descartes' rule of signs was stated by Descartes in 1637 in "La Géometrie", an appendix to his "Discours de la Méthode". It gives a very simple bound for the number of positive real roots of a univariate real polynomial in terms of the number of sign variations of its coefficients. We were also able to find an analog of Descartes' rule of signs in the multivariate case in case the support of the polynomials in the system is a circuit [3] (with $n+2$ monomials in n variables). This study shows the difficulty to even state a conjectural complete generalization in the multivariate case, which is a widely open question. For other real questions, see [48].

In previous works, we developed in [15] the basic theory of toric dynamical systems (a.k.a. complex balanced systems) in the context of computational algebraic geometry and showed that the associated moduli space is also a toric variety. We proved this for detailed balancing systems whose invariant polyhedron is two-dimensional and bounded the simplest case of the main open conjecture that the unique complex balancing steady state is a global attractor of the trajectories. In [37], we presented an efficient procedure for calculating steady state invariants that are linear combinations of complexes and depend on selected variables. We showed how enzyme bifunctionality can lead to different forms of concentration control that are robust to changes in initial conditions or total amounts.

Discrete dynamical systems have been also increasingly successful in modeling biological networks and algebraic geometry provides powerful tools for their study. The literature is too vast to be cited in this survey, so we will just mention one sample recent article. Many problems in biomedicine and other areas of the life sciences can be characterized as control problems, with the goal of finding strategies to change a disease or otherwise undesirable state of a biological system into another, through an intervention, such as a drug or other therapeutic treatment. The paper [41] presents a method for the identification of potential intervention targets in Boolean molecular network models using algebraic techniques. The proposed control methods are useful and efficient for moderately large networks.

An important question in neuroscience is understanding the neural code and, in particular, how the collective activities of neurons represent information about the outside world. In many brain areas, the firing patterns of neurons have been shown to encode information about an animal's interaction with its environment, including sensory inputs and the animal's position in space. These experiments give clues about the intrinsic structure of neural codes, and how they encode various stimuli. In particular, it has been shown that the encoding of the maps connecting external inputs to neural responses are often given by an arrangement of convex receptive fields. Methods from algebraic geometry and combinatorics are now being used to analyze the intrinsic structure of neural codes [18, 17]. The combinatorial data can be represented algebraically via the neural ideal, much as simplicial complexes are algebraically encoded by Stanley–Reisner ideals. Moreover, ideas from topological data analysis have been used to show how such codes reflect the structure of the underlying stimulus space. In the case of hippocampal place cell codes, which are responsible for tracking the animal's position in space, these methods have been used to show that correlations in neural activity reflect the underlying topological and geometric properties of the environment [33]. We refer the reader to the survey [16].

Another area of interaction of algebraic geometry and biology is the study of phylogenetic invariants in evolution. Phylogenetic varieties contain the set of joint distributions at the leaves of a tree evolving under a Markov model of molecular evolution. These varieties are interesting from a biological point of view because they provide new tools of non-parametric inference of phylogenetic trees, and also pose interesting algebro-geometric challenges. We refer the reader to [9] and the references therein.

3 Other emerging applications

In recent years there has been a number of advances about tensors and their different notions of rank, which have applications in phylogenetics, algebraic statistics, signal processing, quantum information, convex algebraic aeometry, and combinatorial algebraic geometry. An elementary introduction to tensors focusing on some applications can be found in the article by P. Comon [10]; a standard textbook is [38] by J. Landsberg; B. Sturmfels wrote a nice recent survey [52]; for the spectral theory there is a recent book by L. Qi and Z. Luo [45]. There is a strong link between tensors and algebraic geometry. For instance, decomposable tensors have rank

1 and correspond to the Segre variety, symmetric tensors correspond to homogeneous polynomials, symmetric tensors which are powers of linear forms have rank 1 and correspond to the Veronese variety, tensors of rank bounded by k make a dense subset of the k-secant variety of the Segre variety, tensors of border rank bounded by k make exactly the k-secant variety of the Segre variety, etc.

For general varieties, the concept of Euclidean distance degree -introduced in [26]- counts the number of critical points of the squared distance to a general point outside the variety, appealing to classical intersection theory from the perspective of computational algebraic geometry. For Segre varieties these numbers have been computed in [31]. The nearest point map of a real algebraic variety with respect to Euclidean distance is an algebraic function (for instance, for varieties of low rank matrices, the Eckart-Young Theorem states that this map is given by the singular value decomposition), which is of importance in control theory, geometric modeling, computer vision, and low rank matrix completion.

Algebraic geometry and polynomial optimization techniques have been used to formulate and solve a number of problems in computer vision since long [28]. Visibility computations with moving viewpoints lead to interesting and difficult problems in real algebraic geometry, even for simple classes of objects (such as balls and polytopes) [54]. The emerging field of algebraic vision attemps to introduce new ideas from moduli theory, representation theory, as well as numerical, real, and combinatorial algebraic geometry into computer vision, also driving new ideas back into algebraic geometry (see for instance [39]). There is a lot of recent activity in multi-view geometry, the sub-discipline of computer vision that studies 3D scene reconstructions from images, and which has deep foundations in projective geometry and linear algebra.

One of the earliest successes of applied algebraic geometry has been to the area of geometric modeling. In 1995, Sederberg and Chen introduced a method for the study of implicitization problems in geometric modeling, that they termed as *moving curves and surfaces* [46]. D. Cox realized that underlying their work was the algebraic notion of syzygies [12], which opened up a fruitful area of research. In 2002, L. Busé and J.-P. Jouanolou abstracted and generalized on a sound basis the method of Sederberg–Chen [7] via approximation complexes, a tool in homological commutative algebra that had been developed by J. Herzog, A. Simis and W. Vasconcelos [35,36]. They later produced other interesting articles on the subject jointly with M. Chardin. In [6] we unveiled in concrete terms the general machinery of the syzygy-based algorithms for the implicitization of rational surfaces in terms of the monomials in the polynomials defining the parametrization. The theoretical justification is not naive and requires a good command of techniques of (homological) commutative algebra. However, the algorithms do not require a heavy background and are easy to explain.

The relation between nonnegative real forms and multivariate polynomials that can be written as a sum of squares is of great interest because of the active area of research on sum of squares optimization, which has applications in many areas, notably control theory. The nice article [5] substantially extends Hilbert's celebrated characterization of equality between nonnegative forms and sums of squares, giving geometric insight to the different cases via the relation with projective varieties of minimal degree. In the more recent work [4], they extend their study from irreducible varieties to reduced schemes. Their results have applications to the positive semidefinite matrix completion problem and to the truncated moment problem on projective varieties.

Frame theory studies special vector arrangements which arise in numerous signal processing applications. Over the last decade, the need for frame-theoretic research has grown alongside the emergence of new methods in signal processing. Interestingly, modern advances in frame theory involve techniques from algebraic geometry, semidefinite programming, algebraic and geometric combinatorics, and representation theory (see for instance [8]).

Finally, we refer to the forthcoming book [53], to be published by the American Mathematical Society, for a good account of the basics of the active area of algebraic statistics. This is an introductory graduate text book which includes a fair amount of background on probability, algebra and algebraic geometry, statistics, and convex geometry.

4 Back to software

Applications require the solution to other problems in computational algebraic geometry. For example, in recent and ongoing research of A. Braun, C. Long, L. McAllister, M. Stillman, and B. Sung, it has been necessary to find many (possibly singular) rigid divisors (defined in terms of sheaf cohomologies) on a Calabi-Yau 3-fold. In cosmological solutions of string theory, if there are suitable rigid divisors then one might see a bright signal in cosmic microwave background experiments. D. Eisenbud, M. Mustata and M. Stillman had found algorithms for computing the required sheaf cohomolgies. These were implemented in Macaulay2 by G. G. Smith. Unfortunately, the implemented algorithms cannot compute the cohomologies needed. Stillman and his co-authors found a method to compute the cohomologies of a large (but finite) class of divisors, which often works by hand. The physics implications of the results of these computational algebraic geometric methods is still a work in progress.

Symbolic computation allows in principle to make computations with parametric systems of polynomials, that is, with families of algebraic varieties. F. Rouillier and M. Safey El Din have implemented and constantly improved certified computations with real polynomials and real solutions, which were used in manifold applications, for example, in the study of the structural stability of n-dimensional systems in control theory, or in the discovery or preclusion of geometrical structures in certain 3D manifolds [27].

The inherent complexity of most nonlinear algebraic computations has lead to the development of software for polynomial system solving based on *numerical algebraic geometry*. The numerical solution of systems of polynomial equations is based on well tuned algorithms for homotopy continuation. A. Leykin has been instrumental in adding numerical algebraic geometry methods to Macaulay2. Other two useful free software for the numeric solution of polynomial systems are Bertini [2] and PHCPack [56]. Bertini is a general-purpose solver, that was created for research about polynomial continuation, designed and written in C by D. Bates, J. Hauenstein, A Sommese and C. Wampler. There are many applications of Bertini to questions in robotics, see e.g. [25]. PHCpack is an open source software created and maintained by J. Verschelde. It was originally designed to implement polynomial homotopies exploiting structure in order to better approximate all isolated solutions. The package also exports the numerical irreducible decomposition, and can compute all positive dimensional solution sets of a system. There is currently a PHCpack Web Interface to solve polynomial systems.

The basics of symbolic-numeric methods for polynomial system solving, including resultants, discriminants, solving equations via algebras, residues and duality, primary decomposition, border bases, and numerical algebraic geometry can be found in the book [23]. See also [22] for applications of multidimensional polynomial residues.

Acknowledgements I am grateful to Eduardo Cattani, Giorgio Ottaviani and Bernd Sturmfels for their generous input to improve this survey.

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