What is Numerical Algebraic Geometry?

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Abstract

The foundation of algebraic geometry is the solving of systems of polynomial equations. When the equations to be considered are defined over a subfield of the complex numbers, numerical methods can be used to perform algebraic geometric computations forming the area of numerical algebraic geometry. This article provides a short introduction to numerical algebraic geometry with the subsequent articles in this special issue considering three current research topics: solving structured systems, certifying the results of numerical computations, and performing algebraic computations numerically via Macaulay dual spaces.

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Introduction

Numerical algebraic geometry is concerned with "numerical computations" of objects connected with algebraic sets defined over subfields of the complex numbers. Some examples of such objects include solution sets and irreducible decompositions [80], monodromy groups [56], and exceptional sets of an algebraic map [35, 89]. The term "numerical" refers to computations which are potentially inexact, e.g., floating-point arithmetic. Another approach to compute similar quantities is to use a symbolic approach, e.g., based on Gröbner basis computations over an algebraic number field or over a prime field of characteristic $p > 0$. There are

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advantages and disadvantages of each approach, e.g., see [5] for a comparison of approaches to compute irreducible decompositions. A near-term goal is to design hybrid symbolic-numeric methods that utilize advantages of both approaches.

Classically, the part of algebraic geometry defined over subfields of the complex numbers is called *transcendental algebraic geometry*. The sets that arise are highly structured and provide many of the basic objects inspiring complex analysis, differential geometry, algebraic topology, and homological algebra.

When floating-point computations are used, at a basic level, one has a finite approximation to all data. A disadvantage of this can be seen with the equation

$$z^2 - 2 = 0. \tag{1}$$

Numerically, a solution may be represented by a numerical approximation such as 1.412 or 1.414213562, neither of which is actually a solution to (1). Due to this, one needs a notion of what it means to numerically compute a solution to system of equations. For a polynomial system $f : \mathbb{C}^N \to \mathbb{C}^N$, suppose that $\xi \in \mathbb{C}^N$ is a nonsingular solution of $f = 0$, i.e., $f(\xi) = 0$ and $Jf(\xi)$ is invertible where $Jf(z)$ is the Jacobian matrix of f evaluated at z. One could use the notion of an *approximate solution* associated to ξ based on Newton's method [17, Chap. 8] as a definition for "numerically computing" ξ. In this case, there is an open neighborhood containing ξ, each point of which is an approximate solution of ξ, such that Newton's method is a quadratically convergent contraction mapping with ξ being a fixed point of this map. Quadratic convergence yields that ξ can be effectively approximated to any given accuracy starting from an approximate solution.

The two key aspects for defining what it means to "numerically compute" a solution are (1) compute a sufficiently accurate numerical approximation, and (2) have an algorithm that can effectively produce approximations of a true solution to any given accuracy starting from the numerical approximation. Here, "sufficiently accurate" is dependent on the algorithm used to refine the solution, e.g., inside the quadratic convergence basin of Newton's method. In situations related to computing solutions using homotopy continuation, the refining algorithm could be an endgame, e.g., [8, 49, 65, 66, 67], where the region of interest is called the endgame operating zone [88, § 3.3.1],[18]. Armed with this information, one is able to recover information about the solution, e.g., deciding reality [42] and recovering exact equations [6].

Disadvantages of not working with exact answers can be balanced by an increase in the number of computational methods, e.g., parallelization and typically less memory utilized due to rounding that avoids expression swell. Numerical methods also have the advantage of computing and manipulating individual points on an algebraic set.

One way to generate large systems of polynomial equations is to discretize a system of differential equations. This yields richly structured partially ordered sets of sparse polynomial systems. Such systems are an important part of transcendental algebraic geometry, to which numerical algebraic geometry naturally applies.

The remaining sections of this introductory article are as follows. Section 1 contains a brief history of numerical algebraic geometry (which is not meant to be exhaustive). Sections 2 and 3 provide a short summary of two main ideas used in this area: path tracking and witness sets, respectively. We conclude in Section 4 with a short summary of the articles in this special issue.

1. A Brief History

The foundational method which led to the development of numerical algebraic geometry is continuation (often called homotopy continuation). In practice, continuation is simply the ability to track along a solution path (see §2 below).

The first modern uses of continuation, e.g., [46, 52, 72], were used to find fixed points with the tracking schemes based on simplicial approximations of the spaces the paths went through. Continuation then evolved into a general method of finding roots of systems of equations, with a major focus in solving differential equations [28, 50, 70]. A brief overview of this early history, which we followed here, is given in the introduction of [1]. Allgower and Georg's book [4] and articles [2, 3] provide surveys of this theory with the important case of polynomial systems placed in the perspective of much more general systems.

Due to the special nature of polynomial systems, continuation has been an extremely effective method for computing isolated roots of polynomial systems. There was a flood of articles following [23, 30]. The book [64] and the survey [60] provide an overview of the area when computing isolated solutions was the focus with Shub and Smale addressing certification and yielding complexity estimates [73, 74, 75, 76, 77, 78] in the nonsingular isolated case (see also [13, 14, 15, 17, 19]).

The term *Numerical Algebraic Geometry* was coined in [87] which showed how techniques for finding isolated zeroes could be used to compute the dimension of an algebraic set and, in particular, decide if the solution set was empty. This article also provided an algorithm for finding a numerical version of general points. A better algorithm for carrying out the basic computations of [87] was given in [79]. This lead to a sequence of articles containing algorithms for computing the numerical version of the irreducible decomposition [80, 81, 82, 83] with related work in [29, 71]. During this period the concept of a *witness set*, which is the fundamental data structure used in numerical algebraic geometry to represent an algebraic set, was introduced and clarified (see §3 below). Algorithms for intersecting algebraic sets [84, 85] (see also [44]) led to a new class of algorithms

[40, 41, 86] for solving systems equation by equation as well as other notions of witness sets [38, 39].

One fundamental concern with numerical methods is the ability to handle singularities. Endgames, such as [8, 49, 65, 66, 67], are algorithms for computing the endpoint, which may be singular, of a solution path. Another important development to handle singularities was the deflation algorithm of Leykin, Verschelde, and Zhao [57] (see also [58]) that built on earlier work of [68, 69] (see also [53]). Leykin, Verschelde, and Zhao demonstrated an algorithm for regularizing isolated singular solutions thereby restoring the local quadratic convergence of Newton's method. This led to many refinements and extensions, e.g., [26, 31, 32, 37, 59, 63], and development related to nonisolated cases, e.g., [7, 43].

A picture of numerical algebraic geometry up to the end of 2004 is provided in the book [88]. The survey [61] from a year earlier is of particular interest due to its extensive description of polyhedral methods for solving polynomial systems (see also [47, 48, 91]). The book [10] surveys major developments up to 2013.

The are four main software packages associated with numerical algebraic geometry under ongoing development: `Bertini`™ [10], `HOM4PS-2.0 & HOM4PS-3` [54, 20, 21], `NAG4M2` [55], and `PHCpack` [90].

2. Path Tracking

Measured by either computer usage or the amount of numerical analysis used, numerically tracking the lift of a single path is the major computation of numerical algebraic geometry. To make this precise in a broad context, consider the map $\pi : X \to Y$ from a reduced quasiprojective algebraic set X to an irreducible reduced quasiprojective algebraic set Y. Let $x_1 \in X$ be a manifold point such that $y_1 := \pi(x_1)$ is a manifold point of Y and $\mathrm{d}\pi$ is an isomorphism from the tangent space of X at x_1 to the tangent space of Y at y_1. Suppose that $y_0 \in Y$ and $\phi : (0,1] \to Y$ is a smooth map with $\phi(1) = y_1$ and $\lim_{t\to 0^+} \phi(t) = y_0$. With this setup, one aims to compute the smooth map $\widehat{\phi} : (0,1] \to X$ where $\widehat{\phi}(1) = x_1$ and $\pi \circ \widehat{\phi} = \phi$ assuming such a map $\widehat{\phi}$ exists. In relation to solving systems of equations, the particular focus is on computing the *endpoint* $\lim_{t\to 0^+} \widehat{\phi}(t)$.

By using appropriate genericity, the lifting $\widehat{\phi}$ of ϕ may be broadly guaranteed. One key maneuver in numerical algebraic geometry is to utilize a random number generator to make choices to achieve appropriate genericity. This maneuver combined with computations performed using appropriate precision yields speed and robustness at the cost of allowing some numerical error [9].

We consider an example to cement the ideas using a common type of problem in numerical algebraic geometry. Suppose that $z = (z_1, \ldots, z_N) \in \mathbb{C}^N$ and

$$f(z) := \begin{bmatrix} f_1(z) \\ \vdots \\ f_N(z) \end{bmatrix} \tag{2}$$

is a system of N polynomials on $\mathbb{C}^N$. That is, f is a called a *square system*. Let $d_i = \deg f_i$ and consider the polynomial system

$$g(z) := \begin{bmatrix} z_1^{d_1} - 1 \\ \vdots \\ z_N^{d_N} - 1 \end{bmatrix}. \tag{3}$$

For any nonzero complex number γ, consider the family of polynomial systems

$$H_\gamma(z, t) := (1 - t) \cdot f(z) + \gamma \cdot t \cdot g(z) \tag{4}$$

with solution set

$$\mathcal{V}(H_\gamma) := \left\{(z, t) \in \mathbb{C}^{N+1} \;\middle|\; H_\gamma(z, t) = 0\right\}.$$

For $X := \mathcal{V}(H_\gamma)$ and $Y := \mathbb{C}$, we take $\pi : X \to Y$ to be the projection map $\pi(z, t) = t$. Clearly, the solution set of $g = 0$, namely $\mathcal{V}(g)$, consists of $D = \prod_{i=1}^N d_i$ points where D is called the Bézout number of both f and g. The map π from a neighborhood of $\mathcal{V}(g) \times \{1\} \subset X$ to Y is a D-sheeted covering of a neighborhood of $1 \in Y$. For any $\gamma \in \mathbb{C}$ that does not lie on finitely many rays in $\mathbb{C}$, i.e., for a *random* γ, the path-lifting property holds with $\phi : (0, 1] \to \mathbb{C}$ given by $\phi(t) = t$ starting at every point in $\mathcal{V}(g)$. That is, for each $z^* \in \mathcal{V}(g)$, there is a smooth path $\widehat{\phi}_{z^*} : (0, 1] \to X$ with $\widehat{\phi}_{z^*}(1) = (z^*, 1)$ such that $\pi \circ \widehat{\phi}_{z^*} = \phi$. The set of finite endpoints of all the paths, namely

$$\left\{x^* \;\middle|\; z^* \in \mathcal{V}(g) \text{ and } \lim_{t \to 0^+} \widehat{\phi}_{z^*}(t) = (x^*, 0) \in \mathbb{C}^N\right\}$$

contains at least one point on every connected component of $\mathcal{V}(f)$. In particular, it is a classical result for each isolated point $x \in \mathcal{V}(f)$, the number of paths ending at x is equal to the multiplicity of x with respect to f, e.g. [88, Theorem A.14.1].

This example is called the total degree (or Bézout) homotopy. The numerical tracking along the path described by $\widehat{\phi}_{z^*}(t)$ reduces down to solving the Davidenko differential equation

$$\frac{\partial H_\gamma}{\partial z} \cdot \frac{\mathrm{d}z}{\mathrm{d}t} + \frac{\partial H_\gamma}{\partial t} = 0$$

with initial condition $\widehat{\phi}_{z^*}(1) = (z^*, 1)$. Since $H_\gamma\left(\widehat{\phi}_{z^*}(t)\right) \equiv 0$, the system H_γ consists of *first integrals* for the Davidenko differential equation and is used to control both the local and global error when numerically performing path tracking.

The following is a basic problem that deserves more study.

Problem 1. *Compute the probability of error given numerical parameters, random choices, and numerical algorithm.*

In practice, different checks and dynamically changing the number of digits used in the computations are made to reduce the probability of error in path tracking. If the path $\widehat{\phi}_{z^*}$ is smooth on $[0, 1]$, i.e., additionally at $t = 0$, then the path tracking can be certified using an *a priori*, e.g., [13, 14, 15, 17, 19, 33, 73, 74, 75, 76, 77, 78], or an *a posteriori* [36] certified tracking scheme.

3. Witness Sets

One key difference between numerical algebraic geometry and the use of symbolic approaches is the representation of algebraic sets. Typically, in symbolic approaches, an algebraic set is represented by a finite collection of polynomial equations whose solution set is the algebraic set of interest. In this way, computations performed by symbolic approaches arise as the manipulation of equations.

Witness sets are general linear slices of algebraic sets. The intellectual underpinning of this notion is the rich classical study of the close relation of algebraic sets and their linear sections [12]. Computations are performed on algebraic sets using witness sets by manipulating points. In particular, suppose that f is a polynomial system and X is a pure k-dimensional algebraic subset of $\mathcal{V}(f)$. A witness set for X is the triple

$$\{f, L, W\}$$

where L is a system of k general linear polynomials and $W = X \cap \mathcal{V}(L)$ is a set consisting of $\deg X$ points.

By using path tracking (see §2), given a witness set for X, it is computationally inexpensive to compute $X \cap \mathcal{V}(M)$ for any other system of k linear equations M provided that $|X \cap \mathcal{V}(M)| < \infty$. This idea, for example, can be used to sample points on X and decide membership in X, e.g., see [88, Chap. 15].

Various computations can be performed using witness sets, such as computing intersections [44, 84, 85], recovering exact defining equations [6], and describing the set of real points [16, 62]. Two other computations of interest are computing images of algebraic sets and deciding algebraic properties. In classical elimination theory, one aims to compute the closure of the image of an algebraic set under an algebraic map. This computation can be performed from a geometric perspective using numerical algebraic geometry [39]. Another computation with a more algebraic viewpoint that can be performed using a witness set is deciding if an algebraic set is a complete intersection, arithmetically Cohen-Macaulay, or arithmetically Gorenstein [24, 25].

4. Summary of Articles

The seven research articles included in this special issue focus on three topics: solving structured systems, certifying the results of numerical computations, and performing algebraic computations numerically via Macaulay dual spaces. The following provides a brief summary of these articles.

4.1. Solving structured systems

One way to increase efficiency of homotopy methods and numerical algebraic geometric algorithms in general is to exploit structure in the polynomial system which is to be solved. The first four articles in this special issue exploit structure in various ways, which we summarize briefly.

The first article [11] considers decomposing a large polynomial system into smaller subsystems that only depend on a decoupled subset of the variables.

The second article [21] describes computations related to exploiting the polyhedral structure of a polynomial system.

In the third article [22], the authors consider systems consisting of binomials, that is, systems consisting of polynomials having at most two terms.

The fourth article [27] considers exploiting the structure of polynomial systems arising in the computation of critical points.

4.2. Certifying results of numerical computations

As mentioned in the Introduction, one needs a notion of what it means to numerically compute a solution. When a system has the same number of equations as variables, a so-called *square system*, and the solution is nonsingular, one can consider computing approximate solutions based on Newton's method, e.g., Smale's α-theory as summarized in [17, Chap. 8] and implemented in [42]. The next two articles in this special issue consider aspects of certification in the square case.

In particular, the fifth article [34] considers the case of certifying numerical computations arising from square systems of polynomial-exponential equations.

The sixth article [45] considers problems in Schubert calculus, which are typically formulated as an overdetermined system. The authors show that these problems can be reformulated as a square system so that standard certification techniques based on Smale's α-theory can be employed.

4.3. Algebraic computations using Macaulay dual spaces

As described in §3, a witness set is a data structure built on the geometry of a solution set to a system of polynomial equations. For considering the algebraic structure of a systems of equations from a numerical point of view, one needs additional tools. The last article [51] in this special issue considers using Macaulay dual spaces to perform algebraic computations numerically.

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