

Back to the roots: Solving polynomial systems with numerical linear algebra tools

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*In memory of Jan Willems
mentor, colleague, friend*

Abstract—In this presentation, we will develop a new approach based on numerical linear algebra to compute all the roots of a set of multivariate real polynomials. We explore several properties of the Macaulay matrix that is constructed with the coefficients of the monomials of these real polynomials, including the determination of the number of solutions via the calculation of a rank, and the computation of the roots via generalized eigenvalue problems, that derive from an nD-realization problem in the null space of the Macaulay matrix. We show how therefore polynomial optimization problems (such as e.g. Prediction Error Methods in system identification) boil down to solving a (large) eigenvalue problem.

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I. ROOTING MULTIVARIABLE POLYNOMIALS

Finding the real and complex roots of a set of multivariate polynomials with real coefficients, has numerous applications in geometry and optimization, systems and control theory, modeling and identification, statistics and bioinformatics, and many other scientific disciplines. It is an old yet fascinating problem, that has intrigued scientists through the ages, starting with the Greeks, over Fermat and Descartes, Newton, Leibniz, Bezout and many many others. It all started with trying to find the roots of a polynomial equation with real coefficients in one unknown. In the beginning of the 19-th century, formulas were known for the roots of polynomials up to degree 4, but it were Galois and Abel, who showed that no general formulas exist for degree 5 and higher. This implies that roots of polynomials of degree higher than 4 in general can only be found using (iterative) numerical algorithms. Soon thereafter, Sylvester and other contemporaries started research on how to find the roots of sets of multivariate polynomials. Sylvester derived an elimination algorithm, in which he eliminates variables one by one, ending up with a characteristic equation in one variable only. If one then has obtained the roots of this last equation, one can then back-substitute root-by-root into the other equations, and hence in principle find all roots. As a consequence, also the roots of multivariate polynomials have

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to be calculated numerically in general. Sylvester's algorithm is the equivalent of Gaussian elimination for linear equations, but more importantly, his results imply that, in general, finding the roots of a multivariate polynomial system, is an eigenvalue problem ! Sylvester's approach of resultants (which are the multivariate generalizations of determinants) was expanded on by many other mathematicians, including Macaulay. Later on, in the 20th century, there was a booming mathematical development, which gave birth to a discipline that today is called algebraic geometry, sometimes labeled as the queen of mathematics, with a fabulous rich history, to which famous mathematicians, such as Hilbert, but also many others, contributed. From the sixties on, it led to the machinery of Grobner bases and the like, which today are ubiquitous in books on and symbolic methods in algebraic geometry, with numerous applications in fields like geometric design, combinatorics and integer programming, coding theory, robotics, etc.

II. BACK TO THE ROOTS

In this presentation, we will not pursue the developments in algebraic geometry, and the symbolic approaches they have led to (e.g. Mathematica, Maple, etc.), but somehow return to Sylvester and Macaulay. Instead of using the classical algebraic tools of resultants and elimination approaches, we will rephrase the problem in the modern language of numerical linear algebra and realization theory for nD linear systems. Our talk will develop ideas on three complementary levels:

- *Geometric linear algebra* dealing with linear independency, column and row vector spaces of matrices, dimensions, orthogonality, null spaces, generalized eigenvalue problems.
- *Numerical linear algebra* dealing conceptually with tools like Gram-Schmidt orthogonalization, ranks, angles between subspaces, singular value decomposition.
- *Numerical algorithms* implementing the numerical linear algebra tools into an efficient and numerically robust method. Here we can exploit matrix structures (e.g. Toeplitz-like or sparsity), investigate variations of iterative methods (e.g. power methods) or try to speeden up convergence (e.g. by FFT).

Starting from a set of multivariate polynomials, we will show how, from the matrix of coefficients, we can construct a block-Toeplitz-like matrix, which is known as the Macaulay matrix. For two multivariate polynomial equations in two variables, $p(x, y) = 0$ and $q(x, y) = 0$, the Macaulay matrix is the matrix with as its rows the coefficients of consecutive monomials $1, x, y, x^2, xy, y^2, \dots$ of the given multivariate polynomials $p(x, y)$ and $q(x, y)$ and of monomial multiples of these polynomials, such as $x.p(x, y), x.q(x, y), y.p(x, y), y.q(x, y)$, etc. In this way the Macaulay matrix can be generated for any system of multivariate polynomials in any number of variables. We will analyse several interesting properties of this Macaulay matrix, as its number of rows and columns grow towards infinity:

- We will show how and when the Macaulay matrix gets overdetermined (i.e. number of rows larger than the number of columns).
- We will show how the Macaulay matrix is rank deficient (i.e. not of full column rank), and therefore has a nontrivial null space. The dimension of its null space is the corank of the Macaulay matrix, i.e. the number of columns minus the rank of the matrix.
- The corank reveals the dimension of the variety of roots of the set of multivariate polynomials. In particular, when there is a zero-dimensional variety (i.e. all roots are isolated points), we show how, as the dimensions of the Macaulay matrix grow, its rank increases, but its corank stabilizes. In the case that the dimension of the variety is larger than zero, we show how the corank increases polynomially, as the so-called Hilbert polynomial of the problem.
- We will discuss an interesting duality between the column space of the Macaulay matrix and its null space (in the 0-dimensional variety case):
 - We show how linear dependent columns in the Macaulay matrix correspond to so-called standard basis monomials (which correspond to minimal Grobner bases). In the null space, they correspond to linear independent rows.
 - The quasi-block-Toeplitz-like structure in the Macaulay matrix, generates a generalized Vandermonde-like structure in the null space, both for the affine (i.e. finite) zeros, as for the zeros at infinity. We will show that, as the dimensions of the Macaulay matrix grow, there are two groups of linearly independent columns in the Macaulay matrix (or linear independent rows in the null space), separated by an increasing gap in which the columns are all linearly dependent (mind-the-gap-phenomenon). This observation will reveal the so-called degree-of-regularity, and allows to count and separate the roots at infinity from the affine (finite) roots.
- We will show, using the Weierstrass Canonical Form, how the generalized Vandermonde-like structure (both for finite and infinite roots) of the null space can be modeled with nD-dimensional linear (possibly singular) systems. In doing so, we demonstrate that finding the roots of sets of multivariate polynomials, is equivalent to nD-realization theory, in which the roots can be derived from the generalized eigenvalue decomposition of the system matrices of the nD-system. This also allows us to understand and calculate multiplicities of finite and infinite roots. We will elaborate on these insights in some detail.

The duality between the column space of the Macaulay matrix and the row space of its kernel, basically leads to two approaches to find all roots of a set of multivariable polynomials:

- A *null space based algorithm* in which one first has to compute the null space of the Macaulay matrix, and then apply nD-realization theory after one can construct generalized eigenvalue problems from which the roots are obtained.
- A *data-driven algorithm* in which we directly operate with the Macaulay matrix, solve a set of linear equations using the QR-decomposition, and then obtain generalized eigenvalue problems in terms of certain blocks of the triangular factor R. Our main claim is, that in due time, we will have a numerical linear algebra based tool set (using the singular value decomposition, the QR-decomposition and algorithms to solve generalized eigenvalue problems) to efficiently and robustly find all roots of a set of multivariate polynomials.

III. EXAMPLES AND OPEN PROBLEMS

We will illustrate our results with some motivating examples, such as:

- How to find the minimizing root of polynomial optimization problems, i.e. optimization problems in which the objective function and constraints are multivariate polynomials. In particular, we will show that Prediction Error Methods in (linear) system identification, in principle solve an eigenvalue problem.
- Algebraic statistics, in which the maximum likelihood estimation of the parameters of discrete statistical models (such as in Bayesian networks or Hidden Markov Models), leads to finding the roots of a set of multivariate polynomials.
- Multi-way arrays of data or numerical tensors, which arise in statistics, biomedical data and signal processing, system identification, datamining etc. In particular, the problem of approximating a given data tensor in a least squares sense by one of lower multilinear rank, results in a set of multivariate polynomials, and hence is an eigenvalue problem.

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During the talk, we will comment on the connection between our linear algebra framework, and terminology that derives from algebraic geometry. Finally, we will briefly elaborate on some challenges of current research: how to parametrize the nD -system that models the null space of the Macaulay matrix, in the case where the dimension of the variety of zeros of the set of multivariate polynomials is larger than 0? How to effectively exploit the sparsity of the Macaulay matrix when calculating its null space ? How to come up with an iterative method that only calculates the roots that minimize the objective function in the case of a polynomial optimization problem?