

ALGORITHMS, APPLICATIONS AND CERTIFICATION IN NONLINEAR ALGEBRA

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My research interests are in applied algebraic geometry which is also called nonlinear algebra. One of the basic problems in algebraic geometry studies solutions of polynomial equations. The word ‘applied’ means that its methods are not only applied but also combined with methods from other fields of mathematics such as numerical and complex analysis, combinatorics, and topology. Algorithms for realizing theories, the applications associated with other fields, and certification for checking their correctness are aspects of nonlinear algebra that incite my interest.

Solving polynomial systems via methods of symbolic computation often involves costly Gröbner bases computation. Numerical algebraic geometry, on the other hand, involves approximates that may produce results faster but may require verification. Our work in [7] approaches this problem numerically using homotopy continuation and monodromy group action. We focus on the monodromy action induced from a generic choice which permutes the solutions of the system to deal with a polynomial system chosen generically from a parametrized space of polynomial systems. Our paper [15] implements algorithms for finding real roots of polynomial systems using the polyhedral homotopy continuation. Both papers show how algorithms in nonlinear algebra can be effective on solving various kinds of systems of equations.

Advances in algorithms allow the use of algebraic geometry in many applications involving polynomial system solving. Good examples are my papers [16] and [17]. The first paper demonstrates numerical algebraic geometry approaches to the problem of analytic combinatorics in several variables. The second paper deals with the generalized Nash equilibrium problem using the polyhedral homotopy continuation. Two problems both can be translated into a problem of solving a polynomial system and similar numerical techniques are successful in these seemingly distant applications.

My research also focuses on certifying the output of such numerical algorithms. Numerical methods with floating point arithmetic have a problem that their outputs are not guaranteed to be correct. Our paper [4] devises a general framework for certifying a nonsingular root of a system with analytic equations using Krawczyk method and Smale’s α -theory. The paper [14] demonstrates a Macaulay2 package `NumericalCertification` implementing this framework for certifying solutions of polynomial systems. As a further expansion, my ongoing work with Burr and Leykin deals with singular root certification using certified cluster isolation via the method of inflation.

Besides numerical algebraic geometry, my research extends to the field of combinatorics, real algebraic geometry, and tropical geometry. Our work in [1] considers a real symmetric matrix low-rank completion problem, i.e. completing a given generic partial real symmetric matrix to get the lowest possible rank which is called a typical rank. My ongoing project with Cai, Hill and Yu relates this problem with the space of matrices of tropical symmetric rank 2 from the perspective of tropical convexity.

I have briefly described above the projects in various stages of completion. What follows is the detailed explanation of the projects and related future directions.

ALGORITHMS FOR SOLVING A SYSTEM OF EQUATIONS

We discuss a series of projects about algorithms for solving a system of equations. The performance of finding numerical solutions using the homotopy continuation is greatly influenced by the choice of a start system. A naive choice of a start system may result in expensive computation or

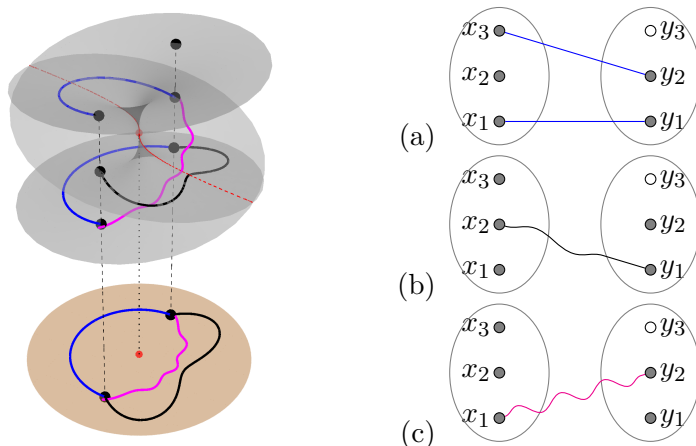


FIGURE 1. 3 edges connect 2 vertices in the base space. The picture on the left shows that 3 edges also connect the fibers. The picture on the right shows its correspondence. For example, in (a) x_1 uses the blue edge to get y_1 , and in (b) y_1 uses the black edge to get x_2 and so on.

producing too many uninterested solutions. It can be remedied by devising an algorithm working for a specific family of systems of equations or special situations.

Solving polynomial systems via monodromy. The project started in 2016 [7] establishes a numerical method that uses monodromy group and homotopy continuation. We first consider a base space B isomorphic to \mathbb{C}^m which parametrizes a space of polynomial systems linearly. We exclude the set of irregular loci D and to each point $p \in B \setminus D$ consider a polynomial system F_p . Each F_p in the family shares the same monomials but has different coefficients represented by p . A generic choice of regular p induces the *monodromy action* which permutes the solutions of the system F_p . We would like to find all solutions of F_p under assumptions that the monodromy action is transitive and the number of solutions is finite.

Our idea is to construct an undirected multigraph $G = (V, E)$ on B chosen by users. The graph G is for recording data of found solutions. Edges of G correspond to homotopies between polynomial systems, and vertices of G are known solutions of the system. As we track an edge of G , we obtain new solutions on each fiber in the covering space. Each vertex records these known solutions and the new solutions, and it tracks edges of G until we find all solutions. Figure 1 displays an example of how this algorithm actually works.

The algorithm is implemented as Macaulay2 [9] package **MonodromySolver**. Our implementation shows more effective performance than existing softwares especially when the system is more complicated than a sparse system. Examples from chemical reaction networks and the degree of the special orthogonal group are used to demonstrate the capabilities of our framework. The additional considerations for probabilistic analysis and parallelization were done in [2].

The polyhedral homotopy for finding real roots. In joint work [15] with Lindberg and Rodriguez, we implement the polyhedral homotopy method for finding real roots. The theory for the real polyhedral homotopy was established in [8] which combines the polyhedral homotopy [13] and Viro's patchworking for complete intersections [21]. It notes the fact that the number of real roots doesn't change if a homotopy path doesn't cross the discriminant locus. Considering a $\log |C|$ -lifting of each monomial, we obtain a homotopy whose paths don't cross the amoeba of the discriminant locus. The $\log |C|$ -lifting induces a collection of binomial systems whose real solutions

can be found readily by linear algebra. For a family of polynomial systems passing a certain process of certification, it is guaranteed to find all real solutions using the homotopy obtained.

Our implementation is released as a Julia package `RealPolyhedralHomotopy.jl`. Our paper foreshadows further study on effective real polyhedral homotopy algorithm. I pose the following question for an extension of the research.

Question 1. *The current algorithm checks all binomial start systems at once if the homotopy paths cross the discriminant locus. Can we check this for each binomial system separately? It will give more flexibility in applying the real polyhedral homotopy.*

SOLVING A SYSTEM OF EQUATIONS AND ITS APPLICATIONS

I am interested in discovering a useful aspect of numerical algebraic geometry as a tool for approaching problems in other areas. Capturing a geometric description of a problem and transitioning it into a polynomial system make this discovery possible. In this section, we discuss how techniques in numerical algebraic geometry provide approaches to problems in combinatorics and game theory.

Homotopy techniques for analytic combinatorics in several variables. The project started in 2021 [16] establishes a numerical method for problems in analytic combinatorics in several variables. Let $(f_n)_{n \in \mathbb{N}}$ be a sequence of complex numbers with generating function $F(z) = \sum_{n \geq 0} f_n z^n$. The field of analytic combinatorics studies the asymptotic behavior of f_n through an analytic property of $F(z)$. Recently, a theory of analytic combinatorics in several variables arises for studying the analytic properties of a multivariate rational function

$$F(\mathbf{z}) = \sum_{\mathbf{i} \in \mathbb{N}^d} f_{\mathbf{i}} z^{\mathbf{i}} = \sum_{\mathbf{i} \in \mathbb{N}^d} f_{i_1, \dots, i_d} z_1^{i_1} \cdots z_d^{i_d}$$

from the asymptotic behavior of its coefficient sequence $(f_{\mathbf{i}})_{\mathbf{i} \in \mathbb{N}^d}$. The asymptotic behavior is determined by the behavior of F at minimal critical points which are singularities close to the origin coordinate-wisely. As critical points satisfy a square polynomial system called a system of critical point equations, the techniques for solving polynomial systems become relevant.

For a rational function $F(\mathbf{z}) = \frac{G(\mathbf{z})}{H(\mathbf{z})}$, it is called combinatorial when its power series coefficients are all nonnegative. The paper [20] of Melczer and Salvy derived polynomial systems for finding minimal critical points for combinatorial and non-combinatorial cases. In combinatorial case, a point $\mathbf{w} \in \mathbb{R}_{>0}^d$ is a minimal critical point of F if and only if the system

$$\begin{aligned} H(\mathbf{z}) &= H(tz_1, \dots, tz_d) = 0 \\ z_1 H_{z_1}(\mathbf{z}) - r_1 \lambda &= \cdots = z_d H_{z_d}(\mathbf{z}) - r_d \lambda = 0 \end{aligned} \tag{1}$$

has a solution $(\mathbf{z}, \lambda, t) \in \mathbb{R}^{d+2}$ with $\mathbf{z} = \mathbf{w}$ and $t = 1$, and no solution $\mathbf{z} = \mathbf{w}$ and $0 < t < 1$. If F is not combinatorial, checking minimality with only critical points with positive real coordinates are not enough. Therefore, we consider the real and imaginary decomposition of the polynomial $H(\mathbf{x} + i\mathbf{y}) = H^R(\mathbf{x}, \mathbf{y}) + iH^I(\mathbf{x}, \mathbf{y})$. Hence, we obtain the system of polynomial equations

$$\begin{aligned} H^R(\mathbf{a}, \mathbf{b}) &= H^I(\mathbf{a}, \mathbf{b}) = 0 \\ a_j H_{x_j}^R(\mathbf{a}, \mathbf{b}) + b_j H_{y_j}^R(\mathbf{a}, \mathbf{b}) - r_j \lambda_R &= 0 \\ a_j H_{x_j}^I(\mathbf{a}, \mathbf{b}) + b_j H_{y_j}^I(\mathbf{a}, \mathbf{b}) - r_j \lambda_I &= 0 \\ x_j^2 + y_j^2 - t(a_j^2 + b_j^2) &= 0 \\ (\nu_1 y_j - \nu_2 x_j) H_{x_j}^R(\mathbf{x}, \mathbf{y}) - (\nu_1 x_j + \nu_2 y_j) H_{y_j}^R(\mathbf{x}, \mathbf{y}) &= 0 \end{aligned} \tag{2}$$

for finding minimal critical points. A point $\mathbf{p} + i\mathbf{q}$ is a minimal critical point if there is a solution $(\mathbf{a}, \mathbf{b}, \mathbf{x}, \mathbf{y}, \boldsymbol{\lambda}, \boldsymbol{\nu}, t)$ of the system with $(\mathbf{a}, \mathbf{b}) = (\mathbf{p}, \mathbf{q})$ but none of the has $0 < t < 1$. We solve the system for the combinatorial case using the polyhedral homotopy and the system for the non-combinatorial case using the polyhedral homotopy and monodromy.

We implement the algorithm as a Julia package `ACSVHomotopy.jl`. Our implementation shows more effective performance than existing software for the combinatorial case especially when the denominator of F has higher degree or random coefficients. Also, it is the first known software for dealing with the non-combinatorial case. I pose the following question for further research in this direction.

Question 2. *A further study on the geometric properties of the system (2) could help make numerical approaches more powerful. What can we say about a zero set of (2)? What is a degree? How many irreducible components it has?*

The polyhedral homotopy method for generalized Nash equilibrium problems. The generalized Nash equilibrium problem (GNEP) is a family of games to find strategies for a group of players such that every player's objective function is optimized. A GNEP for N -player game can be considered as a problem for finding a generalized Nash equilibrium (GNE) $u = (u_1, \dots, u_N)$ such that for given $u_{-i} = (u_1, \dots, u_{i-1}, u_{i+1}, \dots, u_N)$, each $u_i \in \mathbb{R}^{n_i}$ is a minimizer for

$$\begin{cases} \min_{x_i \in \mathbb{R}^{n_i}} & f_i(x_i, u_{-i}) \\ \text{s.t} & x_i \in X_i(u_{-i}) \end{cases}$$

where $X_i = \{x_i \in \mathbb{R}^{n_i} \mid g_{i,j}(x_i, x_{-i}) = 0 \text{ for } j \in \mathcal{E}_i, g_{i,j}(x_i, x_{-i}) \geq 0 \text{ for } j \in \mathcal{I}_i\}$ is a feasible set consists of polynomial equality and inequality constraints. The project started in 2020 [17] studies the polyhedral homotopy approach on GNEP. Under some constraint qualifications, each GNE satisfies the KKT conditions

$$\begin{cases} \nabla_{x_i} f_i(x) - \sum_{j=1}^{m_i} \lambda_{i,j} \nabla_{x_i} g_{i,j}(x) = 0, & (i \in \{1, \dots, N\}) \\ \lambda_{i,j} g_{i,j}(x) = 0, \quad g_{i,j}(x) = 0, & (i \in \{1, \dots, N\}, j \in \mathcal{E}_i) \\ \lambda_{i,j} \geq 0, \quad g_{i,j}(x) \geq 0, & (i \in \{1, \dots, N\}, j \in \mathcal{I}_i). \end{cases}$$

for some Lagrange multiplier vectors $\lambda_i, \dots, \lambda_N$. It gives a set of polynomials

$$F_i(x, \lambda_i) \begin{cases} \nabla_{x_i} f_i(x) - \sum_{j=1}^{m_i} \lambda_{i,j} \nabla_{x_i} g_{i,j}(x) = 0 \\ \lambda_{i,j} g_{i,j}(x) = 0 & \text{for } j \in \mathcal{E}_i \\ g_{i,j}(x) \geq 0 & \text{for } j \in \mathcal{I}_i \end{cases}$$

From each F_i , we define the KKT system $F(x, \lambda_1, \dots, \lambda_N) = \bigcup_{i=1}^N F_i(x, \lambda_i)$ which is a square system. One of our main contributions is theoretical proof that the polyhedral homotopy can be optimal for solving this system.

Theorem 3. *Suppose all f_i and $g_{i,j}$ are generic dense polynomials in $\mathbb{C}[x]_{d_{i,0}}$ and $\mathbb{C}[x]_{d_{i,j}}$ respectively. Then, the KKT system has the mixed volume many isolated solutions over the torus $\mathbb{C} \setminus \{0\}$.*

Using the polyhedral homotopy, we devise the algorithm for solving GNEPs. When, the polyhedral homotopy finds the mixed volume many solutions for the KKT system, then all GNEs can be found or we can detect the non-existence of GNEs. Our algorithm shows more effective performance than existing methods especially when the feasible sets X_i are non-convex. Moreover, we find GNEs of some benchmark examples that were never detected from other optimization-based algorithms.

Numerical algorithms for solving systems of equations mostly rely on heuristic. Therefore, certification for checking its correctness is required. For given a compact region I in \mathbb{C}^n (or \mathbb{R}^n) and a square system $F : \mathbb{C}^n \rightarrow \mathbb{C}^n$, we apply algorithms to check the existence and uniqueness of a solution of F in I . Here are explanations of my works related to certification for numerical solutions.

Macaulay2 package NumericalCertification. The paper [14] introduces a Macaulay2 package `NumericalCertification`. It implements Smale's α -theory and Krawczyk method [4] for regular solution certification and a deflation method [18] for soft verification of a singular solution. It is the first internal Macaulay2 package for root certification. When users solve the system numerically via Macaulay2, solutions can be certified inside Macaulay2 without using other external solvers. Also, it provides two methods which have different advantages and disadvantages. The Krawczyk method allows more crude input than α -theory, but α -theory has a better rate of convergence. Users can choose an appropriate method depending on their problems. Lastly, it provides a Macaulay2 interface of `alphaCertified` [12]. It runs with inputs internally obtained from Macaulay2 so that makes easier use of `alphaCertified` possible. These features surpass the limitation of `HomotopyContinuation.jl` [3] and `alphaCertified` in several applications.

Certified cluster isolation via inflation. When a system of equations is solved by a numerical solver, numerical approximations of a singular solution form a cluster. Isolating this cluster gives an idea for certifying a singular solution. In [6], the authors considered this for a root with multiplicity 2. In [5], the authors considered the method of inflation to extend the idea. The ongoing project started in 2021 generalizes the idea of inflation.

For a given square system $F : \mathbb{C}^n \rightarrow \mathbb{C}^n$ of analytic functions, the cluster isolation computes regions $R_0, R_1 \in \mathbb{C}^n$ and a natural number k such that (1) $\overline{R_0} \subset R_1^c$, (2) R_0 has k solutions of F and (3) there is no zero of F in $R_1 \setminus R_0$. For a given system F , applying a suitable change of coordinates, we may assume that a singular solution is located at the origin. The inflation is the map $S(x_i) = x_i^{d_i}$ with a proper positive integer d_i making the initial forms of $F \circ S$ doesn't vanish on the unit sphere and has the same total degree d . For the inflated system $F \circ S$, we find a lower bound M on the norm of the initial forms of $F \circ S$ on the unit sphere. Then, bound all variables in non-initial forms of the system by ε , and find values of ε until the lower bound on the initial form $M\varepsilon^d$ dominates the upper bound of non-initial forms. These values of ε determine the regions R_0 and R_1 . Lastly, applying Rouché's theorem, we have the number of roots k of the system $F \circ S$ in the unit sphere.

The inflation method provides more geometric information about the cluster than previously known works [6],[11]. We also provide a way to isolate the cluster for systems of equations that the inflation is not available.

Here is the question we desire to answer in research of this direction.

Question 4. *Characterize systems of equations that the inflation method is applicable.*

REAL SYMMETRIC MATRIX COMPLETION

In this section we describe the low-rank real symmetric matrix completion problem. Given a partially specified symmetric matrix, we complete the matrix with real numbers in a way that we achieve the lowest possible rank. Real symmetric matrix completion was considered in [10], and the authors also found its application to the *maximum likelihood threshold* of a Gaussian graphical model. Our work [1] deals with this problem by encoding a symmetric matrix M with a semisimple graph $G = (V, E)$, i.e. a simple graph that allows a loop on its vertices, such that entries $M_{ij} = M_{ji}$ of M are specified if $(i, j) \in E$ for the corresponding graph. We prove which semisimple graphs

have the largest possible rank and characterize semisimple graphs with relatively small completion ranks.

The ongoing joint work with Cai, Hill and Yu studies this problem for tropical symmetric rank from the viewpoint of tropical convexity. For a given $n \times n$ matrix of tropical rank 2, the tropical convex hull of the column vectors is of dimension 1, hence it is a tree. In [19], the authors construct a metric tree on $2n$ leaves with labels $1, 2, \dots, n, 1', 2', \dots, n'$ as follows. Label a leaf labeled i at the i -th column vector of the matrix. Attaching infinite rays in coordinate directions, consider the convex hull as a balanced 1-dimensional polyhedral complex. Label a leaf labeled j' at the j -th coordinate direction. The leaves with labels are considered to have infinite length while the internal edges have finite length induced from the matrix. We call these trees as bicolored trees.

If we consider an $n \times n$ symmetric matrix of tropical rank 2, then its bicolored tree has symmetry. We study the combinatorics of the symmetric bicolored trees to understand the space of symmetric matrices with tropical rank 2. We have the following conjecture.

Conjecture 5. *The space of symmetric matrices with tropical rank 2 has simplicial complex structure as symmetric bicolored trees.*

Furthermore, by restricting matrices with tropical symmetric rank 2, we may consider additional characterization.

Conjecture 6. *A real symmetric matrix $M \in \mathbb{R}^{n \times n}$ has tropical symmetric rank 2 if and only if its corresponding symmetric bicolored tree has an embedding in \mathbb{R}^2 and is symmetry about a line.*

We are interested in how the space of real matrices with tropical symmetric rank 2 can be understood from the point of view of the matrix completion problem. I pose the following question to extend the research.

Question 7. *For an $n \times n$ real symmetric matrix, to achieve tropical symmetric rank 2, what entries can be chosen independently? Can we describe the patterns of entries using symmetric bicolored trees?*

REFERENCES

- [1] D. I. Bernstein, G. Blekherman, and K. Lee. Typical ranks in symmetric matrix completion. *Journal of Pure and Applied Algebra*, 225(7):106603, 2021.
- [2] N. Bliss, T. Duff, A. Leykin, and J. Sommars. Monodromy solver: Sequential and parallel. In *Proceedings of the 2018 ACM International Symposium on Symbolic and Algebraic Computation*, ISSAC '18, pages 87–94, New York, NY, USA, 2018. ACM.
- [3] P. Breiding and S. Timme. HomotopyContinuation.jl: A package for homotopy continuation in Julia. In *International Congress on Mathematical Software*, pages 458–465. Springer, 2018.
- [4] M. Burr, K. Lee, and A. Leykin. Effective certification of approximate solutions to systems of equations involving analytic functions. In *Proceedings of the 2019 on International Symposium on Symbolic and Algebraic Computation*, ISSAC '19, pages 267–274, New York, NY, USA, 2019. ACM.
- [5] M. Burr and A. Leykin. Inflation of poorly conditioned zeros of systems of analytic functions. *Arnold Mathematical Journal*, 7(3):431–440, 2021.
- [6] J. P. Dedieu and M. Shub. On simple double zeros and badly conditioned zeros of analytic functions of n variables. *Mathematics of computation*, pages 319–327, 2001.
- [7] T. Duff, C. Hill, A. Jensen, K. Lee, A. Leykin, and J. Sommars. Solving polynomial systems via homotopy continuation and monodromy. *IMA Journal of Numerical Analysis*, 04 2018.
- [8] A. A. Ergür and T. de Wolff. A polyhedral homotopy algorithm for real zeros. *arXiv preprint arXiv:1910.01957*, 2019.
- [9] D. R. Grayson and M. E. Stillman. Macaulay2, a software system for research in algebraic geometry. Available at <http://www.math.uiuc.edu/Macaulay2/>.
- [10] E. Gross and S. Sullivant. The maximum likelihood threshold of a graph. *Bernoulli*, 24(1):386–407, 2018.
- [11] Z. Hao, W. Jiang, N. Li, and L. Zhi. On isolation of simple multiple zeros and clusters of zeros of polynomial systems. *Mathematics of Computation*, 2019.

- [12] J. D. Hauenstein and F. Sottile. alphaCertified: Software for certifying numerical solutions to polynomial equations. *Available at math.tamu.edu/~sottile/research/stories/alphaCertified*, 2011.
- [13] B. Huber and B. Sturmfels. A polyhedral method for solving sparse polynomial systems. *Mathematics of computation*, 64(212):1541–1555, 1995.
- [14] K. Lee. The NumericalCertification package in Macaulay2. *arXiv preprint arXiv:2208.01784*, 2022.
- [15] K. Lee, J. Lindberg, and J. I. Rodriguez. Implementing real polyhedral homotopy. *arXiv preprint arXiv:2207.05323*, 2022.
- [16] K. Lee, S. Melczer, and J. Smolčić. Homotopy techniques for analytic combinatorics in several variables. *arXiv preprint arXiv:2208.04490*, 2022.
- [17] K. Lee and X. Tang. On the polyhedral homotopy method for solving generalized Nash equilibrium problems of polynomials. *arXiv preprint arXiv:2208.03931*, 2022.
- [18] A. Leykin, J. Verschelde, and A. Zhao. Newton’s method with deflation for isolated singularities of polynomial systems. *Theoretical Computer Science*, 359(1-3):111–122, 2006.
- [19] H. Markwig and J. Yu. The space of tropically collinear points is shellable. *Collect. Math.*, 60(1):63–77, 2009.
- [20] S. Melczer and B. Salvy. Effective coefficient asymptotics of multivariate rational functions via semi-numerical algorithms for polynomial systems. *Journal of Symbolic Computation*, 103:234–279, 2021.
- [21] B. Sturmfels. Viro’s theorem for complete intersections. *Annali della Scuola Normale Superiore di Pisa-Classe di Scienze*, 21(3):377–386, 1994.