Applications of numerically solving polynomial systems*

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Abstract. The problem of solving systems of polynomial equations is ubiquitous throughout science and engineering. The mathematical subject of numerical algebraic geometry consists of a collection of approaches for numerically solving polynomial systems with one foundational technique being homotopy continuation. This short manuscript summarizes using homotopy continuation on two different problems. In the first problem, homotopy continuation is used to approximate a critical parameter value where two solutions of a parameterized differential equation merge together. In the second problem, homotopy continuation is used to compute critical points of a sum of squares best fit function for given data.

Keywords: numerical algebraic geometry · applied algebraic geometry · homotopy continuation · sum of squares best fit.

1 Introduction

Computing and analyzing the solution set of a system of nonlinear polynomial equations is a classical problem forming the foundation of the mathematical subject of algebraic geometry. Since systems of polynomial equations are ubiquitous throughout science and engineering, there are many applications of solving polynomial systems such as biology [13,32], chemistry [1,10,12,20,30], dynamical systems [11,17,22,27], physics [16,18,23], kinematics [7,14,15,26,28,33,34], and control [9,24,29] to list a few. For solving univariate polynomials equations of degree at most 4, there exists formulas for expressing the solutions in radicals in terms of the coefficients, such as the quadratic formula

$$ax^2 + bx + c = 0 \qquad \Longrightarrow \qquad x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}. \tag{1}$$

The impossibility of having similar explicit formulas for arbitrary univarite polynomials of degree at least 5, let alone for multivariate systems, has necessitated the development of numerical approaches for approximating solutions. For example, Newton's method is widely used to numerically approximate a solution since it is locally quadratically convergent near nonsingular solutions. That is, if

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one has a reasonably good guess of a nonsingular solution, then one can obtain highly accurate approximations in relatively few Newton iterations. In essence, the problem of solving is transformed into finding reasonably good guesses.

The mathematical subject of numerical algebraic geometry, e.g., see [6,31], consists of a collection of approaches for numerically computing and analyzing solution sets to systems of polynomial equations. One of the foundational techniques in numerical algebraic geometry is homotopy continuation which turns the problem of solving into path tracking. Path tracking traditionally consists of applying a predictor-corrector scheme. The predictor is often based on numerically approximating a solution to an initial value problem which yields a reasonably good guess to utilize a corrector, e.g., Newton's method, to remove local error and obtain accurate approximations.

The rest of this paper applies homotopy continuation to polynomial systems arising in various applications. In Section 2, homotopy continuation is used to identify a parameter value where two distinct solutions merge together for a parameterized polynomial system arsing from discretizing an ordinary differential equation. In Section 3, critical points of an objective function obtained via a sum of squares best fit of given data are computed using homotopy continuation.

2 Merging solutions

Homotopies are typically constructed to "end" at the system of interest so that efficient algorithms called endgames, e.g., see [6, Chap. 3] for an overview, can be used to accurately approximate the endpoints. An an illustration of using homotopy continuation, consider the following parameterized two-point boundary value problem for $\lambda > 0$ from [2, Sec. 3.2]:

$$\begin{aligned} y''(t) &= -\lambda(1 + y(t)^2) \quad \text{for } 0 < t < 1, \\ y(0) &= 0, \\ y(1) &= 0. \end{aligned} \tag{2}$$

It is known [2,19] that there exists $\lambda^* > 0$ such that (2) has two solutions for $\lambda \in (0, \lambda^*)$, unique solution for $\lambda = \lambda^*$, and no solutions for $\lambda \in (\lambda^*, \infty)$. Figure 1 plots the two solutions for $\lambda = 3$ and $\lambda = 4$.

One approach for computing λ^* is to construct a homotopy that forces the two solutions, say $y_{\lambda,1}(t)$ and $y_{\lambda,2}(t)$, corresponding to the same value of λ to merge together. Hence, by treating λ as a variable, the two solutions will merge together precisely when λ is equal to λ^*. In particular, for $\lambda_0 = 4$, let $y_{\lambda_0,1}$ and $y_{\lambda_0,2}$ be the two solutions depicted in Fig. 1(b) so that, at $s = 1$, $(y_{\lambda_0,1}, y_{\lambda_0,2}, \lambda)$ is the

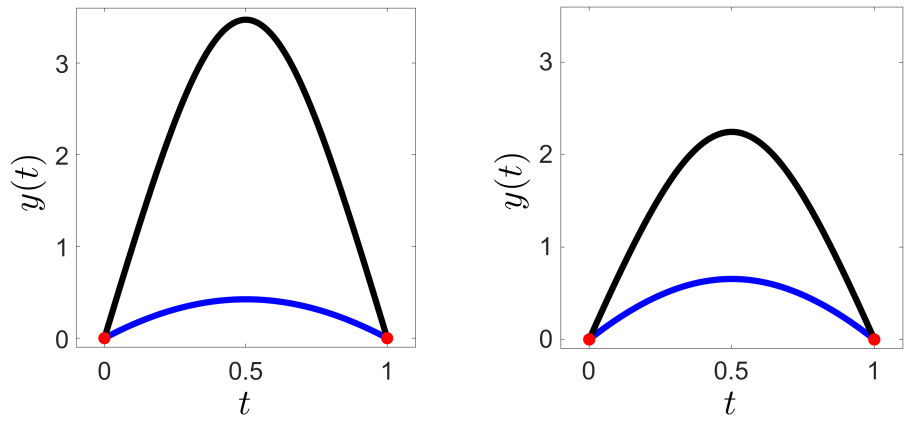

Fig. 1. Plot of the two solutions to (2) for (a) $\lambda = 3$ and (b) $\lambda = 4$.

start point of the following homotopy:

$$H(y_{\lambda,1}, y_{\lambda,2}, \lambda; s) = \left[\begin{array}{c} y''_{\lambda,1}(t) + \lambda(1 + y_{\lambda,1}(t)^2) \quad \text{for } 0 < t < 1 \\ y_{\lambda,1}(0) \\ y_{\lambda,1}(1) \\ \hline y''_{\lambda,2}(t) + \lambda(1 + y_{\lambda,2}(t)^2) \quad \text{for } 0 < t < 1 \\ y_{\lambda,2}(0) \\ y_{\lambda,2}(1) \\ \hline \|y_{\lambda,1} - y_{\lambda,2}\|_2^2 - s \cdot \|y_{\lambda_0,1} - y_{\lambda_0,2}\|_2^2 \end{array}\right] = 0.$$

Therefore, when $s = 0$, this homotopy "ends" with $\lambda = \lambda^*$ and $y_{\lambda,1} = y_{\lambda,2}$. Since this homotopy is formulated in terms of differential equations, we can approximate via polynomial equations, for example, by discretizing using equally spaced grid points and applying a second order central difference scheme. Hence, one can treat $y_{\lambda,1}$ and $y_{\lambda,2}$ as vectors so that the last equation in the homotopy simply corresponds with the square of the standard Euclidean norm of vectors. Utilizing `Bertini` [5], Table 1, which matches [8, Table 1], compares the grid spacing Δt with the computed value of λ^* showing that $\lambda^* \approx 4.755$.

3 Critical points from sum of squares best fit

A classical problem is to compute the best fit line of the form $y = mx + b$ to a collection of data points (x_i, y_i) for $i = 1, \ldots, N$ where N is sufficiently large. Thus, one is aiming to compute m and b which minimizes

$$F(m, b) = \sum_{i=1}^{N} (mx_i + b - y_i)^2.$$

Δt	λ^*
1/10	4.734384294
1/20	4.749878424
1/40	4.753696808
1/80	4.754647901
1/160	4.754885455
1/320	4.754944829
1/640	4.754959672
1/1280	4.754963383
1/2560	4.754964310

Table 1. Comparison of grid spacing Δt and corresponding value of λ^*.

Since the gradient vector ∇F with respect to m and b is a full rank linear system, there is a unique line of best fit for generic data corresponding with the unique solution of $\nabla F = 0$. The following considers more general problems of best fit.

Suppose that $f(x;p)$ is a polynomial in $x \in \mathbb{R}^n$ and $p \in \mathbb{R}^k$. Then, given a collection of data $(x_i, y_i) \in \mathbb{R}^n \times \mathbb{R}$ and weights $w_i \in \mathbb{R}_{>0}$ for $i = 1, \ldots, N$ where N is sufficiently large, consider the weighted sum of squares best fit function

$$F(p) = \sum_{i=1}^{N} w_i \cdot (f(x_i;p) - y_i)^2.$$

The set of critical points of $F(p)$ satisfy $\nabla F(p) = 0$ which is a system of k polynomials in k variables. Hence, there is a generic number of isolated nonsingular solutions to $\nabla F(p) = 0$ which we denote as SOSdegree(f).

Example 1. For $f(x;p) = p_1 x + p_2$ associated with constructing the best fit line, SOSdegree(f) $= 1$. In fact, by viewing this polynomial as a linear span of the monomials x and 1, this can be generalized to any linear span of distinct multivariate monomials. For example, suppose that $x^{\alpha_1}, \ldots, x^{\alpha_k}$ is a list of multivariate monomials with $\alpha_i \neq \alpha_j$ for $i \neq j$ and

$$f(x;p) = \sum_{j=1}^{k} p_j x^{\alpha_j},$$

then SOSdegree(f) $= 1$.

One can compute SOSdegree(f), for example, by counting the number of solutions to the polynomial system $\nabla F = 0$ obtained using homotopy continuation for generic data. Then, one can utilize a parameter homotopy [25] to deform from the generic data to the given data tracking SOSdegree(f) number of paths. This approach has already been used, for example, in approximate kinematics synthesis of mechanisms [3,4], and machine learning [21]. We conclude with an illustration of this approach on some data points in the plane.

Example 2. Consider the 50 data points shown in Fig. 2 and

$$f(x;p) = p_1(x_1 - p_2)^2 + p_3(x_2 - p_4)^2.$$

First, consider computing the critical parameters p of the sum of squares best fit with equal weights, i.e., $w_i = 1$, such that $y_i = 0.65^2 = 0.4225$ on the stars and $y_i = 1.15^2 = 1.3225$ on the dots from Fig. 2(a). To accomplish this, we first compute SOSdegree$(f) = 33$ using homotopy continuation in `Bertini` [5] and then perform a parameter homotopy which deforms from the generically selected data to this given data yielding 33 critical points of the sum of squares best fit. Of these, 11 are real and, by analyzing the Hessian matrix, there are 3 that are local minima. The one which is the global minimum is shown in Fig. 2(a).

For the second problem, on the same set of 50 data points, consider computing the critical parameters p of the sum of squares best fit with equal weights, i.e., $w_i = 1$, and equal output, i.e., $y_i = 1$. Performing a parameter homotopy to this special case results in 25 critical points which is less than the generic count. Of these, 9 are real and, by analyzing the Hessian matrix, there is a unique local minimum which is the global minimum that is shown in Fig. 2(b).

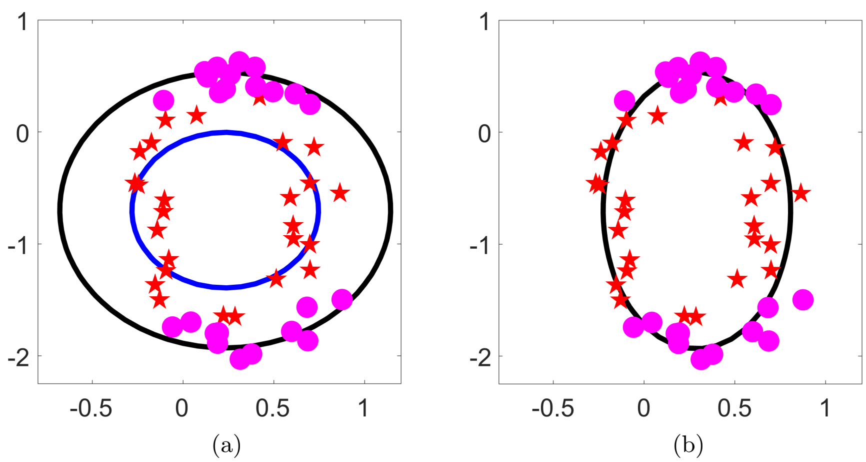

Fig. 2. Computing sum of squares best fit for the same 50 data points using (a) two ellipses and (b) one ellipse.

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