Certification using Newton-invariant subspaces

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Abstract. For a square system of analytic equations, a Newton-invariant subspace is a set which contains the resulting point of a Newton iteration applied to each point in the subspace. For example, if the equations have real coefficients, then the set of real points form a Newton-invariant subspace. Starting with any point for which Newton's method quadratically converges to a solution, this article uses Smale's α-theory to certifiably determine if the corresponding solution lies in a given Newton-invariant subspace or its complement. This approach generalizes the method developed in collaboration with F. Sottile for deciding the reality of the solution in the special case that the Newton iteration defines a real map. A description of the implementation in `alphaCertified` is presented along with examples.
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1 Introduction

The increased computing capability has lead to a wide-spread use of computers to study and solve a variety of problems in algebraic geometry and related areas. One topic of particular interest in computational algebraic geometry, especially when numerical computations are utilized, is the ability to develop certificates of the computed result. Smale's α-theory [17] provides a method for certifying the quadratic convergence of Newton's method using data computed at one point. Since Newton's method is a foundational tool for numerically solving polynomial systems, the α-theoretic certificates provide a way to rigorously prove results following numerical computations. For example, the implementation of α-theory in `alphaCertified` [9,10] has been used to prove results in various applications, such as enumerative geometry [4,7,9] and potential energy landscapes arising in a physical or chemical system [13]. In these applications, which is common in many applications, one is interested in certifying the reality or nonreality of solutions. It was shown in [9] that certifying reality or nonreality is possible when the map corresponding to a Newton iteration is a real map, that is, maps real points to real points.

Two open problems related to α-theory are the ability to certify that an overdetermined system of analytic equations has a solution and to certify a singular solution for a square system of analytic equations. One can prove quadratic convergence of overdetermined Newton's method to critical points of the nonlinear least squares problem [5], some of which need need not be solutions. By randomizing down to square systems, points which do not solve the overdetermined system can be certifiably identified [9]. For singular solutions, the behavior of Newton's method nearby can vary drastically (e.g., convergence, repulsion, and attracting cycles). Theorem 4 and Corollary 1 make progress towards these open problems via Newton-invariant subspaces.

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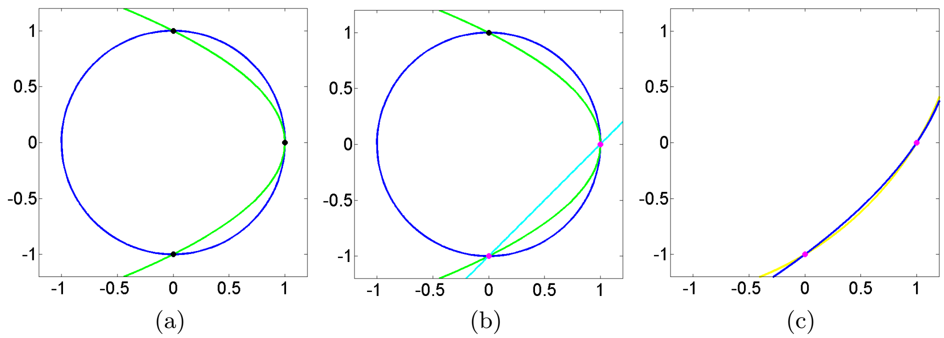

Fig. 1. Plots for (a) $f(x, y)$, (b) $G(x, y)$, and (c) $G_S(x, y)$ in (1)

To illustrate the results presented in Theorem 4 and Corollary 1 with Lemma 1, consider

$$f(x,y) = \begin{bmatrix} x^2+y^2-1 \\ x+y^2-1 \end{bmatrix},\ G(x,y) = \begin{bmatrix} f(x,y) \\ x-y-1 \end{bmatrix},\ \text{and } G_S(x,y) = \begin{bmatrix} 1 & 0 & 3 \\ 0 & 1 & 2 \end{bmatrix} \cdot G(x,y) \quad (1)$$

which are plotted in Figure 1. Example 1 shows that the set defined by $y = x - 1$ is Newton-invariant with respect to f. That is, if the input of Newton's method applied to f is a point on the line $y = x - 1$, the resulting point will also be on the line $y = x - 1$. Even though G_S is a randomized square system, G is overdetermined, and one of the two solutions of $G = 0$ is singular with respect to f, Theorem 4 and Corollary 1 together with Lemma 1 show that G_S and G can be used to prove the quadratic convergence of Newton's method to solutions of $f = 0$.

Newton-invariant sets can be considered as "side conditions." The algorithm **Certify** described in Section 3 certifiably decides if a point ξ which is a solution of a square system $f = 0$ is contained in a Newton-invariant set V or in its complement $\mathbb{C}^n \setminus V$ using α-theory applied to a given numerical approximation of ξ. The "side conditions" could be defined via analytic equations, such as $y = x - 1$. Another naturally arising case is deciding "reality" of solutions in various coordinate systems. As mentioned above, the approach of [9] focuses on reality of solutions in Cartesian coordinates. When the map defined by a Newton iteration is a real map, the set of real points is a Newton-invariant subspace that is not defined by analytic equations. For Cartesian coordinates, Remark 1 shows that **Certify** reduces to the real certification approach of [9]. However, even though the two approaches may appear similar, the use of certifying "side conditions" as well as certifying "reality" in other coordinate systems show that this generalization is useful in a wide variety of applications. For example, consider a harmonic univariate polynomial $h(z)$ [12]. That is, $h(z) = p(z) + q(\text{conj}(z))$ where p and q are univariate polynomials and $\text{conj}(z)$ is the complex conjugate of z. One can compute the solutions of $h = 0$ by letting z and $\overline{z}$ be independent variables and solving the system

$$F(z, \overline{z}) = \begin{bmatrix} p(z) + q(\overline{z}) \\ \overline{p}(\overline{z}) + \overline{q}(z) \end{bmatrix} = 0$$

where $\overline{p}$ and $\overline{q}$ are univariate polynomials obtained by conjugating each coefficient of p and q, respectively. In particular, the solutions of $h = 0$ correspond to the solutions of $F = 0$ lying on the Newton-invariant set $\{(t, \text{conj}(t)) \mid t \in \mathbb{C}\}$. Such isotropic coordinates also arise naturally in algebraic kinematics [19].

The remainder of this section summarizes Smale's α-theory. Section 2 considers Newton invariant sets with Section 3 describing the algorithm **Certify**. The main theoretical results are presented in Section 4 with Section 5 describing the implementation in `alphaCertified` along with examples.

1.1 Smale's α-theory

For an analytic map $f : \mathbb{C}^n \to \mathbb{C}^n$, the map $N_f : \mathbb{C}^n \to \mathbb{C}^n$ defined by

$$N_f(x) := \begin{cases} x - Df(x)^{-1}f(x) & \text{if } Df(x) \text{ is invertible,} \\ x & \text{otherwise,} \end{cases}$$

is a Newton iteration of f at x where $Df(x)$ is the Jacobian matrix of f at x. With this definition, N_f is globally defined with the set of fixed points being

$$\{x \in \mathbb{C}^n \mid f(x) = 0 \text{ or rank } Df(x) < n\}.$$

Therefore, if $Df(x)$ is invertible, $N_f(x) = x$ if and only if $f(x) = 0$.

For each $k \geq 1$, define

$$N_f^k(x) := \underbrace{N_f \circ \cdots \circ N_f}_{k \text{ times}}(x).$$

A point $x \in \mathbb{C}^n$ is said to be an *approximate solution* of $f = 0$ if there is a point $\xi \in \mathbb{C}^n$ such that $f(\xi) = 0$ and

$$\|N_f^k(x) - \xi\| \leq \left(\frac{1}{2}\right)^{2^k-1} \|x - \xi\| \tag{2}$$

for each $k \geq 1$ where $\|\cdot\|$ is the Euclidean norm on $\mathbb{C}^n$. In this case, the point ξ is called the *associated solution* to x and the sequence $\{N_f^k(x)\}_{k\geq 1}$ converges quadratically to ξ.

Smale's α-theory describes sufficient conditions using data computable from f and x for certifying that x is an approximate solution of $f = 0$. The algorithm presented in Section 3 will be based on the following theorem, which follows from results presented in [3, Ch. 8].

Theorem 1. *Let $f : \mathbb{C}^n \to \mathbb{C}^n$ be analytic and $x, y \in \mathbb{C}^n$ such that $Df(x)$ and $Df(y)$ are invertible. Define*

$$\alpha(f, x) := \beta(f, x) \cdot \gamma(f, x),$$

$$\beta(f, x) := \|x - N_f(x)\| = \|Df(x)^{-1}f(x)\|, \text{ and}$$

$$\gamma(f, x) := \sup_{k\geq 2} \left\| \frac{Df(x)^{-1}D^kf(x)}{k!} \right\|^{\frac{1}{k-1}}.$$

1. *If x is an approximate solution of $f = 0$ with associated solution ξ, then $N_f(x)$ is also an approximate solution with associated solution ξ and $\|x - \xi\| \leq 2\beta(f, x) = 2\|x - N_f(x)\|$.*
2. *If $4 \cdot \alpha(f, x) < 13 - 3\sqrt{17}$, then x is an approximate solution of $f = 0$.*
3. *If $\alpha(f, x) < 0.03$ and $\|x - y\| \cdot \gamma(f, x) < 0.05$, then x and y are approximate solutions of $f = 0$ with the same associated solution.*

The value $\beta(f, x)$ is called the *Newton residual*. In the definition of $\gamma(f, x)$, $D^kf(x)$ is the k^{th} derivative of f [11, Ch. 5]. That is, $D^kf(x)$ is a symmetric tensor that one may view as a linear map from $S^k\mathbb{C}^n$, the k-fold symmetric power of $\mathbb{C}^n$, to $\mathbb{C}^n$ whose entries are all of the partial derivatives of f of order k. When restricting to polynomial systems, $D^kf(x) = 0$ for all sufficiently large k so that $\gamma(f, x)$ is a maximum over finitely many terms. That is, $\gamma(f, x)$ could be computed algorithmically. However, due to the possibly large-scale nature of this computation, a commonly used upper bound for $\gamma(f, x)$ for a polynomial system f is described in [16]. A similar upper bound for polynomial-exponential systems is presented in [8].

2 Newton-invariant sets

A set $V \subset \mathbb{C}^n$ is *Newton-invariant* with respect to an analytic system $f : \mathbb{C}^n \to \mathbb{C}^n$ if

1. $N_f(x) \subset V$ for every $x \in V$ and
2. $\lim_{k\to\infty} N_f^k(x) \in V$ for every $x \in V$ such that $\lim_{k\to\infty} N_f^k(x)$ exists.

Clearly, if $N_f(x) \in \mathbb{R}^n$ for every $x \in \mathbb{R}^n$, then $\mathbb{R}^n$ is Newton-invariant with respect to f. Additionally, the set of solutions of $f = 0$ is also Newton-invariant. The following two examples show other cases of Newton-invariant sets.

Example 1. Let $f : \mathbb{C}^2 \to \mathbb{C}^2$ be the system defined in (1). Since f has real coefficients, N_f is a real map so that $V_1 := \mathbb{R}^2$ is trivially a Newton-invariant set for f. Consider the sets

$$V_2 := \{(0, y) \mid y \in \mathbb{C}\}, \quad V_3 := V_2 \cap \mathbb{R}^2, \quad V_4 := \{(1, y) \mid y \in \mathbb{C}\}, \quad V_5 := V_4 \cap \mathbb{R}^2,$$

$$V_6 := \{(x, x-1) \mid x \in \mathbb{C}\}, \quad V_7 := V_6 \cap \mathbb{R}^2, \quad V_8 := \{(x, 1-x) \mid x \in \mathbb{C}\}, \quad \text{and} \quad V_9 := V_8 \cap \mathbb{R}^2.$$

One can show that $V_2, \ldots, V_9$ are also Newton-invariant sets for f as follows. Symbolically, $N_f(x, y) = (x + \Delta x, y + \Delta y)$ where

$$\Delta x = \frac{x(x-1)}{2x-1} \quad \text{and} \quad \Delta y = \frac{y}{2} + \frac{(x-1)^2}{2y(2x-1)} \tag{3}$$

assuming that $x \neq 1/2$ and $y \neq 0$. For these special cases, $\Delta x = \Delta y = 0$ so they are not a concern when showing Newton-invariance. The Newton-invariance of $V_2, \ldots, V_5$ follows directly from the fact that $\Delta x = 0$ when either $x = 0$ and $x = 1$, and that N_f is a real map. If $y = x - 1$, it is easy to verify that $\Delta x = \Delta y$ which yields the Newton-invariance of V_6 and V_7. Finally, the Newton-invariance of V_8 and V_9 follows from the fact that $\Delta x = -\Delta y$ when $y = 1 - x$.

Example 2. The inverse kinematics problem of an RR dyad is the computation of the required angles θ_1 and θ_2 of the revolute joints needed to position the end effector at the point $(p_x, p_y) \in \mathbb{R}^2$ given that the RR dyad is anchored at $(0, 0)$ with fixed leg lengths $\ell_1 > 0$ and $\ell_2 > 0$. In short, this corresponds to solving the equations

$$\ell_1 \cos\theta_1 + \ell_2 \cos\theta_2 - p_x = \ell_1 \sin\theta_1 + \ell_2 \sin\theta_2 - p_y = 0. \tag{4}$$

Following a commonly used technique in algebraic kinematics [19], we will transform these equations into a polynomial system based on isotropic coordinates. Let $i = \sqrt{-1}$ and define

$$z_j := \cos\theta_j + i \cdot \sin\theta_j, \quad \overline{z}_j := \cos\theta_j - i \cdot \sin\theta_j, \quad \text{and} \quad p = p_x + i \cdot p_y.$$

After substitution into (4), simplification, and addition of Pythagorean identities, the resulting polynomial system is

$$F(z_1, \overline{z}_1, z_2, \overline{z}_2) = \begin{bmatrix} \ell_1 z_1 + \ell_2 z_2 - p \\ \ell_1 \overline{z}_1 + \ell_2 \overline{z}_2 - \mathrm{conj}(p) \\ z_1 \overline{z}_1 - 1 \\ z_2 \overline{z}_2 - 1 \end{bmatrix}$$

where conj() denotes complex conjugation. In the isotropic coordinates $(z_1, \overline{z}_1, z_2, \overline{z}_2)$, the corresponding set of "real" points is

$$V := \{(z_1, \mathrm{conj}(z_1), z_2, \mathrm{conj}(z_2)) \mid z_j \in \mathbb{C}\}.$$

Since each $\ell_j > 0$, it is easy to verify that V is Newton-invariant with respect to F.

2.1 Finding Newton-invariant sets

In Example 1, Newton-invariant sets where determined by performing a Newton iteration involving $f : \mathbb{C}^n \to \mathbb{C}^n$. That is, one first symbolically performs a Newton iteration for f to compute $\Delta x = Df(x)^{-1} f(x)$. Then, for example, the linear Newton-invariant spaces are found by computing matrices A and vectors b such that $Ax + b = 0$ and $A\Delta x = 0$. One may also parameterize the linear space and find the parameterizations which hold for x and $x + \Delta x$. The following reconsiders Example 1 to highlight this procedure followed by a polynomial system considered by Griewank and Osborne [6].

Example 3. Consider lines in $\mathbb{C}^2$ which are invariant with respect to (3). That is, we aim to find $(m_1, m_2) \in \mathbb{P}^1$ and $b \in \mathbb{C}$ such that $m_1 \Delta x = m_2 \Delta y$ whenever $m_2 y = m_1 x + b$.

If $m_2 = 0$, then we take $m_1 = -1$ and aim to find $b \in \mathbb{C}$ such that $\Delta x = 0$ whenever $x = b$. From (3), it is clear that $b = 0$ or $b = 1$. These lines correspond with $V_2, \ldots, V_5$ in Ex. 1.

If $m_2 \neq 0$, then we take $m_2 = 1$ and aim to find $m_1, b \in \mathbb{C}$ such that $\Delta y = m_1 \Delta x$ whenever $y = m_1 x + b$. Upon substitution and simplification, this requirement is equivalent to solving

$$m_1^2 + 2bm_1 + 1 = b^2 - 1 = 0$$

which yields $(m_1, b) = (1, -1)$ or $(-1, 1)$. These lines correspond with $V_6, \ldots, V_9$ in Ex. 1.

Example 4. Consider computing all linear Newton-invariant sets of a polynomial system first considered in [6], namely

$$G(x, y) = \begin{bmatrix} 29x^3/16 - 2xy \\ y - x^2 \end{bmatrix}. \tag{5}$$

For this system, which has a multiplicity 3 root at the origin, Griewank and Osborne showed that Newton's method diverges to infinity for almost all initial points. We have

$$\Delta x = \frac{3x^3}{32y - 23x^2} \quad \text{and} \quad \Delta y = \frac{29x^4 - 55x^2 y + 32y^2}{32y - 23x^2}. \tag{6}$$

From (6), it is easy to verify that the vertical line $x = 0$ (over $\mathbb{C}$ and over $\mathbb{R}$) defines the only linear Newton-invariant set for G. We revisit this example in Section 5.3.

For larger polynomial systems f, it may be challenging to symbolically perform a Newton iteration for f, e.g., computing $\Delta x = Df(x)^{-1} f(x)$, thereby making it difficult to find all (linear) Newton-invariant sets for f. However, for particular applications, one often knows which Newton-invariant sets are of interest. Moreover, one can construct systems having a particular Newton-invariant set, as shown in the following.

Theorem 2. *Let n_1 and n_2 be positive integers with $n = n_1 + n_2$. Let $g : \mathbb{C}^{n_1} \to \mathbb{C}^n$ such that $g(0) = 0$, $A : \mathbb{C}^{n_1} \to \mathbb{C}^{n \times n_2}$, and $h : \mathbb{C}^{n_2} \to \mathbb{C}^{n_2}$ all be analytic. Then, $V := \{0\} \times \mathbb{C}^{n_2} \subset \mathbb{C}^n$ is a Newton-invariant set with respect to the square analytic system $F : \mathbb{C}^n \to \mathbb{C}^n$ defined by*

$$F(x, y) = g(x) + A(x) \cdot h(y).$$

Moreover, if N_h is a real map, then $V_{\mathbb{R}} := V \cap \mathbb{R}^n$ is Newton-invariant with respect to F.

Proof. Suppose that $y^* \in \mathbb{C}^{n_2}$ such that $DF(0, y^*)$ is invertible. Thus, $A(0) \cdot Dh(y^*)$ is an $n \times n_2$ matrix of rank n_2 so that $Dh(y^*)$ is invertible. It is easy to verify that $\Delta x = 0$ and $\Delta y = Dh(y^*)^{-1} h(y^*)$ is the unique solution of

$$DF(0, y^*) \begin{bmatrix} \Delta x \\ \Delta y \end{bmatrix} = F(0, y^*)$$

showing that V is Newton-invariant with respect to F. The remaining statement follows immediately from the fact that Δy is real whenever N_h is a real map.

By using a change of coordinates, it follows that every linear subspace of $\mathbb{C}^n$ and $\mathbb{R}^n$ is a Newton-invariant set for some square system.

3 Certification algorithm for square systems

Let $f : \mathbb{C}^n \to \mathbb{C}^n$ be analytic and $V \subset \mathbb{C}^n$ be Newton-invariant with respect to f. Given an approximate solution $x \in \mathbb{C}^n$ of $f = 0$, this section develops an algorithm which certifiably decides if $\xi \in V$ or $\xi \in \mathbb{C}^n \setminus V$ where ξ is the associated solution of x. This algorithm depends on a function which measures the distance between a given point and V, say $\delta_V : \mathbb{C}^n \to \mathbb{R}$ where

$$\delta_V(z) = \inf_{v \in V} \|z - v\|. \tag{7}$$

For example, $\delta_{\mathbb{R}^n}(z) = \|z - \mathrm{conj}(z)\|/2$ with Remark 1 showing how the following algorithm generalizes the test for determining if $\xi \in \mathbb{R}^n$ proposed in [9] when N_f is a real map. Additionally, if computing $\delta_V(z)$ exactly is difficult, note that the following algorithm can be easily modified to use upper and lower bounds on $\delta_V(z)$ such that the upper bound limits to zero as z approaches V and the lower bound becomes positive as z limits to a solution ρ of $f = 0$ provided $\delta_V(\rho) > 0$.

The following procedure is shown to be a correct algorithm by Theorem 3.

Procedure $b =$ **Certify**(f, x, δ_V)

Input A square analytic system $f : \mathbb{C}^n \to \mathbb{C}^n$ such that $\gamma(f, \cdot)$ can be computed (or bounded above) algorithmically, a point $x \in \mathbb{C}^n$ which is an approximate solution of $f = 0$ with associated solution ξ such that $Df(\xi)^{-1}$ exists, and a function $\delta_V : \mathbb{C}^n \to \mathbb{R}$ defined by (7) for some Newton-invariant subspace V which can be computed algorithmically.

Output A boolean b which is `true` if $\xi \in V$ and `false` if $\xi \notin V$.

Begin

1. Compute $\beta := \beta(f, x)$, $\gamma := \gamma(f, x)$, and $\alpha := \beta \cdot \gamma$.
2. If $\delta_V(x) > 2\beta$, **Return** `false`.
3. If $\alpha < 0.03$ and $\delta_V(x) < 0.05\gamma^{-1}$, **Return** `true`.
4. Update $x := N_f(x)$ and go to Step 1.

Theorem 3. *Procedure* **Certify** *is an algorithm, i.e., terminates after finitely many steps, and develops a certificate of the correct answer.*

Proof. Consider the setup described in **Certify**. To prove the theorem, we will first show that if **Certify** returns in Step 2 or in Step 3, then the return value is correct. Afterwards, we will show that **Certify** must terminate in finitely many steps. Since each step in **Certify** is algorithmic, this shows that **Certify** is an algorithm.

Suppose that **Certify** returned through Step 2. For every $v \in V$, the triangle inequality and Item 1 of Theorem 1 yields

$$\delta_V(x) \leq \|x - v\| \leq \|x - \xi\| + \|\xi - v\| \leq 2\beta(f, x) + \|\xi - v\|.$$

Therefore,

$$0 < \delta_V(x) - 2\beta(f, x) \leq \inf_{v \in V} \|\xi - v\| = \delta_V(\xi)$$

yielding $\xi \notin V$ since $\delta_V(\xi) > 0$.

Similarly, suppose that **Certify** returned through Step 3. Then, since

$$\delta_V(x) = \inf_{v \in V} \|x - v\| < 0.05\gamma^{-1},$$

there must exist $v^* \in V$ such that $\|x - v^*\| < 0.05\gamma^{-1}$. By Item 3 of Theorem 1, both x and v^* are approximate solutions of $f = 0$ with the same associated solution ξ. Since $v^* \in V$ and V is Newton-invariant, it follows that $\xi \in V$.

To show termination of **Certify**, suppose that $\xi \notin V$. Define $\delta := \delta_V(\xi) > 0$ and consider

$$B(\xi, \delta/8) = \{y \in \mathbb{C}^n \mid \|y - \xi\| \leq \delta/8\}.$$

Since $N_f^k(x) \to \xi$ as $k \to \infty$, there exists some integer k_0 such that $N_f^k(x) \in B(\xi, \delta/8)$ for all $k \geq k_0$. It immediately follows from the triangle inequality that $\delta_V(N_f^{k_0}(x)) \geq 7\delta/8$ and $\beta(f, N_f^{k_0}(x)) = \|N_f^{k_0}(x) - N_f^{k_0+1}(x)\| \leq \delta/4$. Thus,

$$\delta_V(N_f^{k_0}(x)) \geq 7\delta/8 > 2\beta(f, N_f^{k_0}(x))$$

showing that Step 2 will force **Certify** to return after at most k_0 loops.

Similarly, suppose that $\xi \in V$. Then, since $Df(\xi)^{-1}$ exists, $\gamma(f, z)$ is bounded in a neighborhood W of ξ, say by B. Thus, there exists an integer k_0 such that $N_f^k(x) \in W$ for all $k \geq k_0$ so that $\gamma(f, N_f^k(x)) \leq B$ for all $k \geq k_0$. Since $\beta(f, N_f^k(x)) \to 0$ as $k \to \infty$, we know that $\alpha(f, N_f^k(x)) \to 0$ as $k \to \infty$. Hence, there must exist some integer k_1 such that $\alpha(f, N_f^k(x)) < 0.025$ for all $k \geq k_1$. Since $\xi \in V$, Item 1 of Theorem 1 yields

$$\delta_V(z) \leq \|z - \xi\| \leq 2\beta(f, z) = 2\alpha(f, z)\gamma(f, z)^{-1} < 0.05\gamma(f, z)^{-1}$$

where $z := N_f^{k_1}(x)$. Therefore, Step 3 will force **Certify** to return after at most k_1 loops.

Remark 1. When N_f is a real map, $\mathbb{R}^n$ is an Newton-invariant subspace with respect to f. For $z \in \mathbb{C}^n$, let $\pi_{\mathbb{R}}(z) \in \mathbb{R}^n$ be the real part of z, i.e., $\pi_{\mathbb{R}}(z) = (z + \mathrm{conj}(z))/2$. Hence,

$$\delta_{\mathbb{R}^n}(z) = \|z - \mathrm{conj}(z)\|/2 = \|z - \pi_{\mathbb{R}}(z)\|.$$

Thus, **Certify** reduces to the algorithm **CertifyRealSoln** described in [9] in this case.

4 Systems constructed from Newton-invariant sets

In algorithm **Certify**, Newton iterations were performed on the square system and used to test if a solution was contained in a given Newton-invariant set or its complement, even if the Newton-invariant set was not defined by analytic equations (complex conjugation is not analytic). In this section, we investigate overdetermined systems constructed from a linear Newton-invariant set and randomized square subsystems. In particular, Theorem 4 and Corollary 1 show that if Newton's method applied to such systems quadratically converges, then the limit point is a solution of the original square system, even if it is singular with respect to the original system. That is, the additional equations could turn a singular solution of the square system into a nonsingular solution of an overdetermined and randomized square subsystem with certifiable quadratic convergence. See Sections 5.3 and 5.4 for examples involving traditional benchmarks.

The statements of Theorem 4 and Corollary 1 rely upon the following two definitions. For an analytic system $f : \mathbb{C}^n \to \mathbb{C}^n$, define

$$\mathrm{Sing}_f := \{x \in \mathbb{C}^n \mid Df(x) \text{ is not invertible}\}.$$

Overdetermined Newton's method for an analytic system $g : \mathbb{C}^n \to \mathbb{C}^N$ (i.e., $n < N$) is

$$N_g(x) := x - Dg(x)^\dagger g(x)$$

where $Dg(x)^\dagger$ is the Moore-Penrose pseudoinverse of $Dg(x)$.

Unlike square systems, the fixed points of N_g need not be solutions of $g = 0$ and the fixed points for which the Jacobian is full rank need not be attracting. For the former, consider

$$g(x) = \begin{bmatrix} x \\ x - 4 \end{bmatrix}.$$

Clearly, $g = 0$ has no solutions but $x = 2$ is a fixed point of N_g and minimizes $\|g\|_2$. For the latter, consider the system adapted from [5]:

$$h(x) = \begin{bmatrix} x \\ x^2 + 1 \end{bmatrix}.$$

Clearly, $h = 0$ has no solutions but N_h has a fixed point at $x = 0$. It is shown in [5] that $x = 0$ is a repulsive point for Newton's method near the origin.

From a certification viewpoint, one can use the α-theoretic approach of [5] to prove quadratic convergence to fixed points of N_g. The fixed points of N_g which do not solve $g = 0$ can be certifiably identified using randomization via the approach of [9]. The following provides an approach for certifiably showing that a given fixed point of N_g is indeed a solution of $g = 0$ when g is constructed via Newton-invariant sets. As mentioned above, this fixed point may be a singular solution of the original square system used to construct such an overdetermined system g.

Since linear Newton-invariant sets for a system are invariant under a linear change of coordinates, we simplify the presentation of our results based on systems having a coordinate subspace as a Newton-invariant set.

Lemma 1. *Let $0 < m < n$ and $f : \mathbb{C}^m \times \mathbb{C}^{n-m} \to \mathbb{C}^n$ be an analytic system such that $V := \{0\} \times \mathbb{C}^{n-m} \subset \mathbb{C}^n$ is Newton-invariant with respect to f and $V \not\subset \mathrm{Sing}_f$. Let $g(y) = f(0, y)$ and $G(x, y) = \{f(x, y), x\}$. If $z \in \mathbb{C}^{n-m}$ such that $(0, z) \in V \setminus \mathrm{Sing}_f$, $R \in \mathbb{C}^{(n-m)\times n}$, and $S \in \mathbb{C}^{n\times(n+m)}$ such that* rank $Dg_R(y) = n - m$ *and* rank $DG_S(0, z) = n$ *where $g_R(y) = R \cdot g(y)$ and $G_S(x, y) = S \cdot G(x, y)$, then $N_{G_S}(0, z) = N_G(0, z) = N_f(0, z) = (0, N_{g_R}(z)) = (0, N_g(z))$.*

Proof. Let $\Delta := Df(0, z)^{-1} \cdot f(0, z)$. Since $(0, z) \in V$, $\Delta_i = 0$ for $i = 1, \ldots, m$. Let $\Delta z \in \mathbb{C}^{n-m}$ such that $\Delta = (0, \Delta z)$. Since $Dg_R(z)$ and $DG_S(0, z)$ have full column rank, the same is true for $Dg(z)$ and $DG_S(0, z)$. Thus, the statement follows since

$$DG(0, z) \cdot \Delta = G(0, z), \quad DG_R(0, z) \cdot \Delta = G_R(0, z), \quad Dg(z) \cdot \Delta z = g(z), \quad Dg_R(z) \cdot \Delta z = g_R(z).$$

Following the notation of Lemma 1, for simplicity, the following relate the square system f, the overdetermined system g, and the randomized square subsystem g_R. These can be trivially extended via Lemma 1 to the overdetermined system G and randomized square system G_S.

Theorem 4. *Let* $0 < m < n$ *and* $f : \mathbb{C}^m \times \mathbb{C}^{n-m} \to \mathbb{C}^n$ *be an analytic system such that* $V := \{0\} \times \mathbb{C}^{n-m} \subset \mathbb{C}^n$ *is Newton-invariant with respect to* f *and* $V \not\subset \mathrm{Sing}_f$. *Let* $g(y) = f(0, y)$. *If* $(0, z) \in V \setminus \mathrm{Sing}_f$ *and* $R \in \mathbb{C}^{(n-m)\times n}$ *such that* $\{N_{g_R}^k(z)\}_{k\geq 1}$ *quadratically converges to* $\xi \in \mathbb{C}^{n-m}$ *with* rank $Dg_R(\xi) = n - m$ *where* $g_R(y) = R \cdot g(y)$, *then* $g(\xi) = f(0, \xi) = 0$.

Proof. Since g_R is a square system with $N_{g_R}(\xi) = \xi$ and rank $Dg_R(\xi) = n - m$, we know $g_R(\xi) = 0$, $\alpha(g_R, \xi) = 0$, and $\gamma(g_R, \xi) < \infty$. Thus, Theorem 1(3) shows that, for the ball $B \subset \mathbb{C}^{n-m}$ centered at ξ with radius $0.05/\gamma(g_R, \xi) > 0$, Newton's method for g_R starting at any point in B is an approximate solution of $g_R = 0$ with associated solution ξ. Define $W_f := \{y \mid (0, y) \in V \setminus \mathrm{Sing}_f\} \subset \mathbb{C}^{n-m}$. Since V is not contained in Sing_f, it follows that $B \cap W_f$ is dense in B. Therefore, we can construct $\{z_\ell\}_{\ell\geq 1} \subset B \cap W_f$ such that $0 < \|z_\ell - \xi\| < \ell^{-1}$. In particular, this construction yields rank $Df(0, z_\ell) = n$ and rank $Dg_R(z_\ell) = n - m$ for all $\ell \geq 1$.

For each $\ell \geq 1$, let $\Delta z_\ell := Dg_R(z_\ell)^{-1} g_R(z_\ell) = z_\ell - N_{g_R}(z_\ell)$. By Lemma 1, we know $(0, \Delta z_\ell) = (0, z_\ell) - N_f(0, z_\ell) = Df(0, z_\ell)^{-1} f(0, z_\ell)$. If we assume that $\|\Delta z_\ell\| \leq 2 \cdot \ell^{-1}$, then

$$\|g(z_\ell)\| = \|f(0, z_\ell)\| = \|Df(0, z_\ell) \cdot (0, \Delta z_\ell)\| \leq 2 \cdot \|Df(0, z_\ell)\| \cdot \ell^{-1}.$$

By continuity, $g(z_\ell) = f(0, z_\ell) \to g(\xi) = f(0, \xi)$ and $Df(0, z_\ell) \to Df(0, \xi)$. Since $Df(0, \xi)$ is an $n \times n$ matrix with complex entries, we know $\|Df(0, \xi)\| < \infty$. Taking limits, we have $\|g(\xi)\| = \|f(0, \xi)\| = 0$. Hence, $g(\xi) = f(0, \xi) = 0$.

Therefore, all that remains is to show $\|\Delta z_\ell\| \leq 2 \cdot \ell^{-1}$ for all $\ell \geq 1$. To reach a contradiction, we assume that $\ell \geq 1$ such that $\|\Delta z_\ell\| > 2 \cdot \ell^{-1}$. By construction, $\ell^{-1} > \|z_\ell - \xi\| > 0$ so that

$$\|z_\ell - N_{g_R}(z_\ell)\| = \|\Delta z_\ell\| > 2 \cdot \|z_\ell - \xi\| > 0.$$

The triangle inequality yields

$$\|z_\ell - \xi\| + \|N_{g_R}(z_\ell) - \xi\| \geq \|z_\ell - N_{g_R}(z_\ell)\| = \|\Delta z_\ell\| > 2 \cdot \|z_\ell - \xi\| > 0$$

providing $\|N_{g_R}(z_\ell) - \xi\| > \|z_\ell - \xi\| > 0$. However, since $z_\ell \in B$, i.e., z_ℓ is an approximate solution of $g_R = 0$ with associated solution ξ, (2) yields the impossible statement

$$\frac{1}{2}\|z_\ell - \xi\| \geq \|N_{g_R}(z_\ell) - \xi\| > \|z_\ell - \xi\| > 0.$$

Corollary 1. *Let* $0 < m < n$ *and* $f : \mathbb{C}^m \times \mathbb{C}^{n-m} \to \mathbb{C}^n$ *be an analytic system such that* $V := \{0\} \times \mathbb{C}^{n-m} \subset \mathbb{C}^n$ *is Newton-invariant with respect to* f *and* $V \not\subset \mathrm{Sing}_f$. *Suppose that* $g(y) = f(0, y)$. *If* $(0, z) \in V \setminus \mathrm{Sing}_f$ *such that* $\{N_g^k(z)\}_{k\geq 1}$ *quadratically converges to* $\xi \in \mathbb{C}^{n-m}$ *with* rank $Df(0, N_g^k(z)) = n$ *for all* $k \geq 1$ *and* rank $Dg(\xi) = n - m$, *then* $g(\xi) = f(0, \xi) = 0$.

Proof. Since rank $Dg(\xi) = n - m$, there is a Zariski open and dense $\mathcal{U} \subset \mathbb{C}^{(n-m)\times n}$ such that, for all $R \in \mathcal{U}$, rank $Dg_R(\xi) = n$ where $g_R(x) = R \cdot g(x)$. Fix $R \in \mathcal{U}$. By Theorem 1(3), Newton's method for g_R starting at any point in the ball B centered at ξ with radius $0.05/\gamma(g_R, \xi) > 0$ quadratically converges to ξ. Since $N_g^k(z) \to \xi$, let $k_0 \geq 1$ such that $\{N_g^k(z)\}_{k\geq k_0} \subset B$. Since Dg_R is full rank on B, Lemma 1 yields $N_g^k(z) = N_{g_R}^k(z)$ for all $k \geq k_0$. The statement now follows immediately from Theorem 4.

Example 5. Let $f : \mathbb{C}^2 \to \mathbb{C}^2$ be the polynomial system defined in (1). Example 1 showed the complex line $V_6 := \{(x, x-1) \mid x \in \mathbb{C}\}$, which is defined by $x - y - 1 = 0$, is Newton-invariant with respect to f. Restricting to V_6, $f = 0$ has two solutions, namely $\xi_1 = (0, -1)$ and $\xi_2 = (1, 0)$. One can verify that $Df(\xi_1)$ is invertible while ξ_2 is a singular solution of $f = 0$. The overdetermined polynomial system

$$G(x, y) = \begin{bmatrix} x + y^2 - 1 \\ x^2 + y^2 - 1 \\ x - y - 1 \end{bmatrix}$$

has rank $DG(\xi_1) = \text{rank } DG(\xi_2) = 2$, i.e., ξ_1 is nonsingular with respect to both f and G, but ξ_2 is singular with respect to f and nonsingular with respect to G. Using `alphaCertified` [10] with the points $z_1 = (1/250, -249/250)$ and $z_2 = (251/250, -1/250)$, and square subsystem

$$G_S(x, y) = \begin{bmatrix} x + y^2 - 1 + 3(x - y - 1) \\ x^2 + y^2 - 1 + 2(x - y - 1) \end{bmatrix},$$

we know that $\{N_G^k(z_j)\}_{k\geq 1} = \{N_{G_S}^k(z_j)\}_{k\geq 1}$ quadratically converges for $j = 1, 2$. Theorem 4 and Corollary 1 together with Lemma 1 yield that the corresponding limit points, ξ_j, are indeed solutions of $f = 0$.

5 Implementation details and examples

Before demonstrating the developed techniques on several examples, we first briefly summarize its implementation in `alphaCertified` [10].

5.1 Implementation in `alphaCertified`

The software program `alphaCertified` can perform α-theoretic computations in exact rational or arbitrary precision floating point arithmetic. When rational computations are utilized, the internal computations are certifiable. The analytic system f must either be a polynomial system or a polynomial-exponential system and presented with constants that are rational complex numbers, i.e., in $\mathbb{Q}[i]$. The value of $\gamma(f, x)$ is bounded above using [16] or [8], respectively.

The algorithm **Certify** is implemented in version 1.3 of `alphaCertified` as follows. For a Newton-invariant set $V \subset \mathbb{C}^n$, the function δ_V defined by (7) is assumed to be of the form

$$\delta_V(z) = \|z - (P \cdot z_{\mathbb{R}} + i \cdot Q \cdot z_{\mathbb{I}} + r)\| \tag{8}$$

for $n \times n$ matrices P and Q and n vector r with rational complex entries where

$$z_{\mathbb{R}} = (z + \text{conj}(z))/2 \quad \text{and} \quad z_{\mathbb{I}} = i \cdot (\text{conj}(z) - z)/2.$$

For example, if $V = \mathbb{R}^n$, then $P = I_n$, $Q = 0$, and $r = 0$ where I_n is the $n \times n$ identity matrix. Additionally, if $V = \{(x, \text{conj}(x)) \mid x \in \mathbb{C}\} \subset \mathbb{C}^2$, one can easily verify that

$$P = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \quad Q = \frac{1}{2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}, \quad \text{and} \quad r = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

5.2 A basic example

Reconsider the system f defined in (1) with the real Newton-invariant sets (see Example 1)

$$V_1 := \mathbb{R}^2, \quad V_3 := \{(0, y) \mid y \in \mathbb{R}\}, \quad V_5 := \{(1, y) \mid y \in \mathbb{R}\},$$
$$V_7 := \{(x, x - 1) \mid x \in \mathbb{R}\}, \quad \text{and} \quad V_9 := \{(x, 1 - x) \mid x \in \mathbb{R}\}.$$

It is easy to verify that each δ_{V_j} can be presented in the form (8). Let P_j, Q_j, and r_j be the corresponding elements. Since each $V_j \subset \mathbb{R}^2$, we have $Q_j = 0$. Additionally, since the origin is contained in V_1 and V_3, we also have $r_1 = r_3 = 0$. The remaining elements are:

$$P_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, P_3 = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, P_5 = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, P_7 = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, P_9 = \frac{1}{2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix},$$

$$r_5 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \ r_7 = \begin{bmatrix} 1/2 \\ -1/2 \end{bmatrix}, \ r_9 = \begin{bmatrix} 1/2 \\ 1/2 \end{bmatrix}.$$

Since the singular solution $(1, 0)$ of $f = 0$ was considered in Example 5, we now consider the two nonsingular solutions, namely $(0, \pm 1)$. Clearly, both of $(0, \pm 1)$ lie in V_1 and V_3, with one in V_7 and the other in V_9. Algorithm **Certify** in `alphaCertified` using exact rational arithmetic promptly proves the proceeding statement starting with the approximations

$$(1/1502 - i/3203, 1256/1255 + i/1842) \ \text{ and } \ (-1/2934 + i/8472, -1483/1482 - i/2384).$$

5.3 An example from Griewank and Osborne

Reconsider the polynomial system G from [6] defined in (5) for which the vertical line $x = 0$ is a Newton-invariant set. For any $y \neq 0$, $N_G(0, y) = (0, 0)$ so that Newton's method converges to the only solution of $G = 0$ in one iteration.

We now consider applying Newton's method to the point $P = (10^{-16}, 1)$. Figure 2 plots the Newton residual, i.e., β, for the first 200 iterations of Newton's method starting at P computed using `alphaCertified`. As suggested by this plot, Newton's method diverges to infinity. However, one can easily verify that for the system

$$H(x, y) = \begin{bmatrix} G(x, y) \\ x \end{bmatrix}$$

as well as for a randomization of H down to a square system, Newton's method starting at P immediately quadratically converges to the origin in stark contrast to the results of [6].

5.4 A system with embedded points

Consider the system defining the cyclic 4-roots [2], namely

$$F_4(x_1, x_2, x_3, x_4) = \begin{bmatrix} x_1 + x_2 + x_3 + x_4 \\ x_1x_2 + x_2x_3 + x_3x_4 + x_4x_1 \\ x_1x_2x_3 + x_2x_3x_4 + x_3x_4x_1 + x_4x_1x_2 \\ x_1x_2x_3x_4 - 1 \end{bmatrix}.$$

The solution set defined by $F_4 = 0$ has two irreducible curves while the ideal generated by F_4 in $\mathbb{C}[x_1, \ldots, x_4]$ also has 8 embedded points. It is easy to verify that the line $\{(-t, -t, t, t) \mid t \in \mathbb{C}\}$ is Newton-invariant with respect to F_4 and contains 4 of the embedded points, namely when $t = \pm 1, \pm\sqrt{-1}$. For the overdetermined system G_4 constructed by appending the linear polynomials $x_1 - x_2$, $x_1 + x_3$, and $x_1 + x_4$ to the system F_4, each of these four embedded points are nonsingular solutions of $G_4 = 0$. For a general randomization of G_4, `Bertini` [1] computed numerical approximations of its 20 nonsingular solutions. Using the approach of [9], we are able to use `alphaCertified` to certifiably determine 16 of these solutions do not solve $F_4 = 0$. With Theorem 4, we can now use `alphaCertified` to certifiably show the other 4 solve $F_4 = 0$.

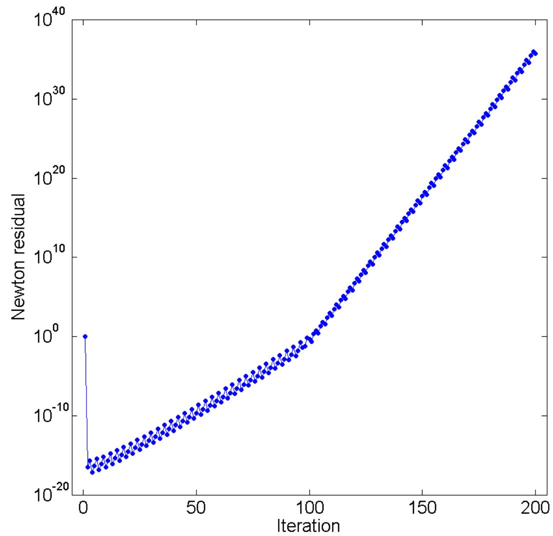

Fig. 2. Plot of the Newton residual for 200 iterations starting at P

5.5 Four-bar linkages using isotropic coordinates

A general four-bar linkage moves in a one-dimensional motion curve when the joints are permitted to rotate. The nine-point path synthesis problem asks to compute the one-dimensional motion curves of four-bar linkages that pass through nine given points. In [18], which showed there were 1442 motion curves passing through nine points in general position, the formulation of this problem used isotropic coordinates. Naturally, one may rewrite this system using Cartesian coordinates, which was used in the formulation of the problem in [15] and certification of real solutions in [9]. However, with **Certify**, one can certify directly using the isotropic formulation.

Let $\mathcal{P} = \{P_0, \ldots, P_8\} \subset \mathbb{C}^2$ be a collection of nine points written using isotropic coordinates. The polynomial system $f_{\mathcal{P}} : \mathbb{C}^{12} \to \mathbb{C}^{12}$ corresponding to the isotropic formulation of the nine-point path synthesis problem derived in [18] depends upon the variables

$$\{x, \overline{x}, a, \overline{a}, n, \overline{n}, y, \overline{y}, b, \overline{b}, m, \overline{m}\}$$

and is constructed as follows. The first four polynomials are

$$f_1 = n - a\overline{x}, \quad f_2 = \overline{n} - \overline{a}x, \quad f_3 = m - b\overline{y}, \quad \text{and} \quad f_4 = \overline{m} - \overline{b}y.$$

The remaining eight polynomials arise from the displacement from P_0 to the other points P_j. Define $Q_j := (\delta_j, \overline{\delta}_j) = P_j - P_0$, which is written via isotropic coordinates. Then, for $j = 1, \ldots, 8$,

$$f_{4+j} = \gamma_j \overline{\gamma}_j + \gamma_j \gamma_j^0 + \overline{\gamma}_j \gamma_j^0$$

where

$$\gamma_j = q_j^x r_j^y - q_j^y r_j^x, \quad \overline{\gamma}_j = r_j^x p_j^y - r_j^y p_j^x, \quad \gamma_j^0 = p_j^x q_j^y - p_j^y q_j^x$$

and

$$p_j^x = \overline{n} - \overline{\delta}_j x, \quad q_j^x = n - \delta_j \overline{x}, \quad r_j^x = \delta_j(\overline{a} - \overline{x}) + \overline{\delta}_j(a - x) - \delta_j \overline{\delta}_j,$$
$$p_j^y = \overline{m} - \overline{\delta}_j y, \quad q_j^y = m - \delta_j \overline{y}, \quad r_j^y = \delta_j(\overline{b} - \overline{y}) + \overline{\delta}_j(b - y) - \delta_j \overline{\delta}_j.$$

When $\mathcal{P}$ consists of points in general position, there is a six-to-one map from the solution set of $f_{\mathcal{P}} = 0$ to four-bar motion curves which pass through the points $\mathcal{P}$ arising from a two-fold symmetry and Roberts cognates. Moreover, when $\mathcal{P}$ consists of 9 points that are "real" in isotropic coordinates, then $\overline{\delta}_j = \text{conj}(\delta_j)$ and

$$V := \{(x, \text{conj}(x), a, \text{conj}(a), n, \text{conj}(n), y, \text{conj}(y), b, \text{conj}(b), m, \text{conj}(m)) \mid x, a, n, y, b, m \in \mathbb{C}\}$$

is Newton-invariant with respect to $f_{\mathcal{P}}$.

As a demonstration of the algorithm **Certify**, we certify the solution to two sets of real points. The first, called Problem 3 in Table 2 of [18], was also considered in [9] using Cartesian coordinates. The corresponding δ_j are

$$\begin{array}{l}\delta_1 = 0.27 + 0.1i, \quad \delta_2 = 0.55 + 0.7i, \delta_3 = 0.95 + i, \quad \delta_4 = 1.15 + 1.3i, \\ \delta_5 = 0.85 + 1.48i, \delta_6 = 0.45 + 1.4i, \delta_7 = -0.05 + i, \delta_8 = -0.23 + 0.4i\end{array}$$

with $\overline{\delta}_j = \text{conj}(\delta_j)$. We used **Certify** implemented in `alphaCertified` to certify the approximations of the solutions obtained by `Bertini` [1]. Confirming previous computations in [9,18], this showed that 64 of the 1442 motion curves through the corresponding nine points were real.

The second set of real points is modeled after Problem 4 in Table 2 of [18] which took points on the ellipse $x^2 + y^2/4 = 1$. Since that collection of nine points was contained in the discriminant locus, we took a collection of nine points on this ellipse and perturbed them. For example, consider the following δ_j, with $\overline{\delta}_j = \text{conj}(\delta_j)$, constructing in this fashion:

$$\begin{array}{l}\delta_1 = 0.25 + 1.33i, \delta_2 = 0.5 + 1.74i, \delta_3 = 0.75 + 1.93i, \delta_4 = 1 + 2.01i, \\ \delta_5 = 1.25 + 1.95i, \delta_6 = 1.5 + 1.73i, \delta_7 = 1.75 + 1.33i, \delta_8 = 2 - 0.007i.\end{array}$$

After using `Bertini` to generate approximations to the solutions, **Certify** showed that 51 of the 1442 motion curves through the corresponding nine points were real.

6 Discussion and summary

Newton-invariant sets naturally arise when considering "real" solutions in other coordinate systems. They could also arise in other situations, such as "side conditions" for solution sets. Theorem 4 and Corollary 1 provide conditions in which the limit of Newton's method applied to an overdetermined system or a randomized square subsystem converges to a true solution. This article also described the algorithm **Certify** which, from an approximation of a solution, can certifiably determine if the corresponding solution is contained in a particular Newton-invariant set or its complement. This approach adds to the certifiable toolbox of methods that can be applied to various problems in computational algebraic geometry.

The algorithm **Certify** is implemented in `alphaCertified` using both exact rational and arbitrary precision floating point arithmetic. All computations are completely rigorous when using rational arithmetic. If floating point arithmetic is used, the current implementation does not fully control roundoff errors. One could, for example, use interval arithmetic [14] to bound the errors and produce certifiable computations in this case.

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