Singular Algebraic Equations with Empirical Data

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Abstract

Singular equations with rank-deficient Jacobians arise frequently in algebraic computing applications. As shown in case studies in this paper, direct and intuitive modeling of algebraic problems often results in nonisolated singular solutions. The challenges become formidable when the problems need to be solved from empirical data of limited accuracy. A newly discovered low-rank Newton’s iteration emerges as an effective regularization mechanism that enables solving singular equations accurately with an error bound in the same order as the data error. This paper elaborates applications of new methods on solving singular algebraic equations such as singular linear systems, polynomial GCD and factorizations as well as matrix defective eigenvalue problems.

1 Introduction

Algebraic equations can have singular solutions at which the Jacobians are rank-deficient. Those singular solutions can be isolated or in a form of varieties of positive dimensions. Such singular equations pose formidable challenges in scientific computing especially when the data are given from measurement with limited accuracy or processed with necessary round-off. Direct attempt of solving singular equations from empirical data may not achieve accurate solutions since the solutions can be altered substantially or even disappear. Common iterative methods such as Newton’s iteration are not guaranteed to converge at singular solutions. Those difficulties are well-documented in the literature such as [1, 10, 12, 6, 19, 24]. Even for linear equations whose singular solutions are elementary in linear algebra, the textbook advice is still to avoid solving singular equations with any perturbation [17] pp 217-218. Theories and computational methodologies appear to be inadequate on singular algebraic equations particularly with empirical data.

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Newton’s iteration is tremendously effective in solving regular equations. However, its textbook formulation is only a special case and finding nonsingular solutions is merely a fraction of its capabilities. Extending Newton’s iteration to solving singular equations has been studied in many works over the years such as [2, 3, 7, 18]. By a simple modification, a low-rank Newton’s iteration emerges as an effective method in solving singular equations for nonisolated solutions [29] and maintains quadratic convergence. More importantly, it serves as a regularization mechanism so that singular solutions can be solved accurately from perturbed data and the solution accuracy is bounded by a multiple the data error.

A generic class of singular equations that possess semiregular solutions are emphasized in this paper as opposed to ultrasingular ones, and we shall elaborate the low-rank Newton’s iteration on such equations. We shall establish semiregularity of some fundamental singular equations such as polynomial GCD/factorization and defective eigenvalue equations as applications of the low-rank Newton’s iteration and demonstrate its effectiveness in their accurate solutions. We shall also briefly elaborate experimental results of solving ultrasingular equations using the depth-deflation method.

We restrict our elaboration to solving singular equations as zero-finding for holomorphic mappings in complex domains. The same theories and computing methods apply to singular zeros of real mappings that are twice continuously differentiable.

2 Preliminaries

The space of $n$-dimensional vectors of complex numbers is denoted by $\mathbb{C}^n$ with the Euclidean norm $\| \cdot \|_2$. Matrices of $m \times n$ form the vector space $\mathbb{C}^{m \times n}$ with the Frobenius norm $\| \cdot \|_F$. Matrices are denoted by upper-case letters with $(\cdot)^H$ being the Hermitian transpose of any matrix $(\cdot)$. A zero matrix is denoted by $O$ whose the sizes are derived from the context.

Finite-dimensional normed vector spaces are denoted by, say $\mathcal{V}$, $\mathcal{W}$ etc, in which vectors are denoted by boldface lower-case letters with $\mathbf{0}$ being the zero vector. For any vector $\mathbf{v}$, the norm $\| \mathbf{v} \|$ is understood as the norm in the space where $\mathbf{v}$ belongs.

For any linear map $L : \mathcal{V} \to \mathcal{W}$, its norm is the operator norm

$$\|L\| := \max_{\mathbf{v} \in \mathcal{V}, \| \mathbf{v} \|=1} \|L(\mathbf{v})\|$$

derived from the norms of its domain $\mathcal{V}$ and codomain $\mathcal{W}$. A vector space $\mathcal{V}$ can be isomorphic to $\mathbb{C}^n$ where $n = \dim(\mathcal{V})$, the dimension of $\mathcal{V}$. Throughout this paper, the norm of a product space $\mathcal{V} \times \mathcal{W}$ is

$$\|(\mathbf{v}, \mathbf{w})\| := \sqrt{\|\mathbf{v}\|^2 + \|\mathbf{w}\|^2} \quad \text{for} \quad (\mathbf{v}, \mathbf{w}) \in \mathcal{V} \times \mathcal{W}.$$
For a holomorphic mapping $F : \Omega \subset \mathbb{C}^n \to \mathbb{C}^m$, we can designate a variable name, say $z$, and denote $F$ as $z \mapsto F(z)$. Then the Jacobian of $F$ at any $z_0 \in \Omega$ is the matrix denoted by $F_z(z_0)$. Let $V$ and $W$ be normed vector spaces isomorphic to $\mathbb{C}^n$ and $\mathbb{C}^m$ respectively via isomorphisms $\psi_V : V \to \mathbb{C}^n$ and $\psi_W : W \to \mathbb{C}^m$. Assume $v \mapsto g(v)$ is a mapping from an open subset $\Sigma$ of $V$ with a representation $z \mapsto G(z)$ where $G : \psi_V(\Sigma) \subset \mathbb{C}^n \to \mathbb{C}^m$ such that $g = \psi_W^{-1} \circ G \circ \psi_V$ that makes the following diagram commute

$$
\begin{array}{ccc}
\Sigma & \xrightarrow{g} & W \\
\psi_V \downarrow & & \psi_W^{-1} \\
\psi_V(\Sigma) & \xrightarrow{G} & \mathbb{C}^m.
\end{array}
$$

We say $g$ is holomorphic in $\Sigma$ if $G$ is holomorphic in $\psi_V(\Sigma)$. The Jacobian of $g$ at any $v_0 \in \Sigma$ is defined as the linear map $g(v_0)$ in the form of

$$
g_v(v_0) : V \longrightarrow W \\
v \longmapsto \psi_W^{-1} \circ G_z(z_0) \circ \psi_V(v)
$$

(1)

where $z_0 = \psi_V(v_0)$. The Jacobian $g_v(v_0)$ as a linear map is invariant under change of bases. Let $G_z(z_0)^\dagger$ be the Moore-Penrose inverse of the Jacobian matrix $G_z(z_0)$. If we further assume the isomorphisms $\psi_V$ and $\psi_W$ are isometric, namely

$$
\|\psi_V(v)\|_2 = \|v\| \quad \text{and} \quad \|\psi_W(w)\|_2 = \|w\| \quad \text{for all} \quad v \in V \quad \text{and} \quad w \in W,
$$

then $g_v(v_0)^\dagger$ is well-defined as

$$
g_v(v_0)^\dagger = \psi_V^{-1} \circ G_z(z_0)^\dagger \circ \psi_W
$$

that is invariant under isometric isomorphisms.

For any matrix $A \in \mathbb{C}^{m \times n}$, we denote $A_{\text{rank-}r}$ as the rank-$r$ projection of $A$. Namely $A_{\text{rank-}r}$ is the rank-$r$ matrix with the smallest distance $\|A - A_{\text{rank-}r}\|_F$ to $A$. The rank-$r$ projection is also called the rank-$r$ approximation and rank-$r$ truncated SVD in the literature. For a holomorphic mapping $v \mapsto g(v)$ with its Jacobian $g_v(v_0)$ defined in (1), its rank-$r$ projection $g_v(v_0)_{\text{rank-}r}$ is defined as the linear map

$$
g_v(v_0)_{\text{rank-}r} : v \longmapsto \psi_V^{-1} \circ G_z(z_0)_{\text{rank-}r} \circ \psi_V(v)
$$

where $z_0 = \psi_V(v_0)$ and $G_z(z_0)_{\text{rank-}r}$ is the rank-$r$ projection of the Jacobian matrix $G_z(z_0)$. The notation $g_v(v_0)^\dagger_{\text{rank-}r} := (g_v(v_0)_{\text{rank-}r})^\dagger$.

For multivariate mappings, say $(u, v, w) \mapsto f(u, v, w)$, its Jacobian at $(u_0, v_0, w_0)$ is denoted by $f_{uvw}(u_0, v_0, w_0)$, and the notation such as $f_{uw}(u_0, v_0, w_0)$ denotes the partial Jacobian with respect to $(u, w)$.

### 3 Semiregular and ultrasingular zeros

An equation $f(x) = 0$ is *singular* if the Jacobian $f_x(x_*)$ is rank-deficient so that $\text{nullity}(f_x(x_*)) > 0$ at the desired solution $x_*$. A solution $x_*$ is *isolated* if there is an
open neighborhood \( \Delta \) such that \( \Delta \cap f^{-1}(0) = \{x_*\} \). The Jacobian \( f_x(x_*) \) with nullity zero always implies \( x_* \) is isolated, and \( x_* \) is a regular zero. A nonisolated solution is singular and may be a point on a curve, a surface etc.

For a holomorphic mapping \( f: \Omega \subset \mathcal{V} \to \mathcal{W} \), we say the dimension of its zero \( x_* \) is \( k \) if there is an open neighborhood \( \Delta \subset \Omega \) of \( x_* \) in \( \mathcal{V} \) such that \( \Delta \cap f^{-1}(0) = \phi(\Lambda) \) where \( z \mapsto \phi(z) \) is a holomorphic injective mapping defined in a connected open set \( \Lambda \) in \( \mathbb{C}^k \) for \( k > 0 \) with \( \phi(z_*') = x_* \) and \( rank(\phi_z(z_*')) = k \). As a special case, an isolated zero is of dimension 0. A singular zero \( x_* \) of \( f \) is said to be semiregular if its dimension is identical to \( nullity(f_x(x_*)) \). A zero is ultrasingular if it is not semiregular. We say an equation is semiregular or ultrasingular if the intended solutions are.

The identity \( f(\phi(z)) \equiv 0 \) for \( z \) in the domain of \( \phi \) implies \( f_x(x_*) \phi_z(z_*) \) is a zero mapping and thus \( nullity(f_x(x_*)) \geq k \) since \( \phi_z(z_*) \) is of rank \( k \). A simple approach to establish semiregularity of a \( k \)-dimensional solution is to append a linear mapping \( L \) to \( f \) from the same domain as \( f \) to a codomain of dimension \( k \). A \( k \)-dimensional zero \( x_* \) is semiregular if Jacobian of the stacked mapping \( x \mapsto (f(x), L(x)) \) is injective so that \( nullity(f_x(x_*)) \) \( \leq k \) and must equal to \( k \). We shall apply this technique repeatedly in the sample applications.

Because tiny perturbations can only reduce nullities, semiregularity \( nullity(f_x(x_*)) = k \) is generic among singular solutions. Extra singularity is required to increase the nullity further and moves away from semiregularity. As a special case, a regular zero is semiregular with dimension 0.

Semiregular equations enjoy the stationary point property \footnote{29} [Lemma 4]: At any \( \bar{x} \) close to a semiregular zero \( x_* \) of a mapping \( x \mapsto f(x) \), the point \( \bar{x} \) satisfies the \( f_x(\bar{x}) \tens{rank-r} f(\bar{x}) = 0 \) if and only if \( f(\bar{x}) = 0 \). Consequently, the stationary equation \( f_x(x) \tens{rank-r} f(x) = 0 \) does not produce extraneous zeros of \( f \) near any semiregular zero.

### 4 The low-rank Newton’s iteration

It may come as a surprise that Newton’s iteration we have known is only a special case and finding regular isolated solutions is a small portion of its capabilities. The Simpson’s formulation

\[
    x_{j+1} = x_j - f_x(x_j)^{-1}f(x_j) \quad \text{for} \quad j = 0, 1, \ldots \tag{2}
\]

is the most widely applied method for finding zeros of a mapping \( f: \Omega \subset \mathcal{V} \to \mathcal{W} \) if the equation \( f(x) = 0 \) is square (i.e. \( \dim(\mathcal{V}) = \dim(\mathcal{W}) \)) and the Jacobian is invertible at the solution. Newton’s iteration in the form of \( \tens{[2]} \) is not suitable for computing singular solutions. Even if it converges to a singular solution, the rate of convergence is usually slow and the attainable accuracy is poor.

A recently discovered rank-r Newton’s iteration \footnote{29}

\[
    x_{j+1} = x_j - f_x(x_j)^t_{\tens{rank-r}} f(x_j) \quad \text{for} \quad j = 0, 1, \ldots \tag{3}
\]
not only retains all the features of the version \((2)\) but also expands the capability to equations of all three shapes (square, underdetermined and over determined) and to the mapping \(f\) whose Jacobian can be any rank \(r\) at the solution. Here in \((3)\) the notation \(f_x(x_j)^\dagger_{\text{rank}-r}\) represents the Moore-Penrose inverse of the rank-\(r\) projection of the Jacobian \(f_x(x_j)\). The conventional Newton’s iteration \((2)\) and the Gauss-Newton iteration are special cases of the rank-\(r\) Newton’s iteration when \(r\) is the full column rank of the Jacobian. This extension of Newton’s method appears to be the first general purpose iteration for computing nonisolated solutions of the equation \(f(x) = 0\). The following lemma can be considered a universal convergence theorem of Newton’s iteration.

**Lemma 1 (Convergence of Newton’s Iteration)\[29\]** Let \(f\) be a mapping twice continuously differentiable in an open domain with a rank \(r\) Jacobian \(f_x(x_*)\) at a semiregular zero \(x_*\). For every open neighborhood \(\Omega_1\) of \(x_*\), there is a neighborhood \(\Omega_0\) of \(x_*\) such that, from every initial iterate \(x_0 \in \Omega_0\), the rank-\(r\) Newton’s iteration \((3)\) converges quadratically to a zero \(\hat{x} \in \Omega_1\) of \(f\) in the same branch as \(x_*\).

Lemma 1 can be narrated in simpler terms: Assume an \(m \times n\) equation \(f(x) = 0\) has a \(k\)-dimensional solution set. Setting \(r = n - k\), the rank-\(r\) Newton’s iteration \((3)\) locally quadratically converges to a solution in the solution set if the solution set is semiregular. The geometric interpretation in \[29\] shows the iteration \((3)\) asymptotically follows a normal line of the solution set and approximately converges to the solution nearest to the initial iterate \(x_0\).

In practical applications, equations are often given through empirical data with limited accuracy. On the other hand, singular solutions are highly sensitive and may even disappear when data are perturbed. Those applications can be modeled as an equation

\[
f(x, y) = 0 \text{ for } x \in \Omega
\]

at a fixed parameter value \(y\) representing the data where \((x, y) \mapsto f(x, y)\) is a smooth mapping defined on a certain domain. Assume the equation \((4)\) has a semiregular solution \(x = x_*\) at a data point \(y = y_*\) but \(y_*\) is known only through empirical data \(\tilde{y} \approx y_*\). We can compute a semiregular zero of the mapping \(x \mapsto f(x, y_*)\) near \(x_*\) through the perturbed rank-\(r\) Newton’s iteration

\[
x_{k+1} = x_k - f_x(x_k, \tilde{y})^\dagger_{\text{rank}-r} f(x_k, \tilde{y}), \quad k = 0, 1, \ldots.
\]

If it converges, the iteration \((5)\) approaches a stationary point \(\tilde{x}\) where

\[
f_x(\tilde{x}, \tilde{y})^\dagger_{\text{rank}-r} f(\tilde{x}, \tilde{y}) = 0.
\]

but generally \(f(\tilde{x}, \tilde{y}) \neq 0\). The following lemma ensures that the stationary point approximates an exact solution \(\hat{x}\) of the equation \((4)\) at the exact data \(y = y_*\).

**Lemma 2 (Convergence of Newton’s iteration on Perturbed Data)\[29\]** Let a mapping \((x, y) \mapsto f(x, y)\) be twice continuously differentiable in an open domain. Assume \(x_*\) is a semiregular zero of the mapping \(x \mapsto f(x, y_*)\) at a fixed \(y_*\) with
\( \text{rank}(f_x(x_\ast, y_\ast)) = r > 0 \) and \( \|f_y(x_\ast, y_\ast)\| > 0 \). Then there exist a neighborhood \( \Omega_\ast \times \Sigma_\ast \) of \((x_\ast, y_\ast)\), a neighborhood \( \Omega_0 \) of \(x_\ast\) and a constant \( h \) with \( 0 < h < 1 \) such that, at every fixed \( \tilde{y} \in \Sigma_\ast \) serving as empirical data for \( y_\ast \) and from any initial iterate \( x_0 \in \Omega_0 \), the iteration (5) converges to a stationary point \( \tilde{x} \in \Omega_\ast \) at which \( f_x(\tilde{x}, \tilde{y})\)\(_{\text{rank}-r}\) \(f(\tilde{x}, \tilde{y}) = 0 \) with an error bound

\[
\|\tilde{x} - \hat{x}\| \leq \frac{8}{1 - h} \|f_x(x_\ast, y_\ast)\| \|f_y(x_\ast, y_\ast)\| \|\tilde{y} - y_\ast\| + O(\|\tilde{y} - y_\ast\|^2) \quad (6)
\]

to a semiregular zero \( \hat{x} \) of \( x \mapsto f(x, y_\ast) \) in the same branch of \( x_\ast \). The convergence rate is quadratic if \( \tilde{y} = y_\ast \).

In other words, the rank-\( r \) Newton’s iteration (5) is a de facto regularization method that solves the exact equation (4) at \( y = y_\ast \) approximately from perturbed data \( y = \tilde{y} \). Even though the solution of the system \( f(x, \tilde{y}) = 0 \) is substantially altered by the data perturbation or disappears altogether, the iteration (5) still converges to a stationary point \( \tilde{x} \) satisfying \( f_x(\tilde{x}, \tilde{y})\)\(_{\text{rank}-r}\) \(f(\tilde{x}, \tilde{y}) = 0 \) and \( \tilde{x} \) is an accurate solution to the underlying equation \( f(x, y_\ast) = 0 \) we intend to solve. The accuracy of the approximate solution \( \tilde{x} \) is guaranteed by the error bound (6) that is asymptotically proportional to the data error. Furthermore, the error bound (6) leads to a sensitivity

\[
\left\{ \begin{array}{ll}
\|f_x(x_\ast, y_\ast)\|_2 \|f_y(x_\ast, y_\ast)\|_2 & \text{if } x_\ast \text{ is semiregular} \\
\infty & \text{otherwise.}
\end{array} \right. \quad (7)
\]

that serves as the condition number of the singular solution \( x_\ast \). As a result, the singular zero-finding problem for \( x \mapsto f(x, y_\ast) \) at empirical data \( \tilde{y} \) is regularized as a well-posed problem of finding a stationary point \( \tilde{x} \) with an accuracy in the same order as the data.

Remark (On identifying the projection rank) Applying the iterations (5) and (3) requires identifying the rank of the Jacobian at the zero without knowing the exact location of the zero or exact data of the problem. We shall show in case studies that this rank can be determined analytically as a part of the modeling process. Finding the rank of a matrix from empirical data is a subject in numerical linear algebra as the rank-revealing problem (see, e.g. [8, 16, 13, 14]).

5 Singular linear equations

Solving linear systems in the matrix-vector form \( Ax = b \) is one of the most fundamental tasks in scientific computing but singular systems are rarely mentioned in the literature beyond elementary linear algebra. That is an entire class of linear equations missing in discussion. The textbook advise [17, pp 217-218] is to “avoid floating-point solutions of singular systems” altogether because it is well-known that the system becomes nominally nonsingular but highly ill-conditioned under infinitesimal data perturbations. As a result, the convention is to define the condition number as infinity for singular linear systems. In reality, however, the hypersensitivity of singular linear system is “notable for exaggerated fears” [20].
From exact data, the solution of a singular linear equation \( A \mathbf{x} = \mathbf{b} \) is known to be either the empty set or an affine subspace

\[
A^\dagger \mathbf{b} + \text{Kernel} (A) := \{ A^\dagger \mathbf{b} + \mathbf{z} \mid A \mathbf{z} = \mathbf{0} \}
\]  

(8)

assuming \( \mathbf{b} \in \text{Range}(A) \). Solving singular linear systems in exact sense is an ill-posed problem since the solution generically dissipates to an empty set under arbitrary perturbations. On the other hand, every vector in the affine subspace is a semiregular zero of the mapping \( \mathbf{x} \mapsto A \mathbf{x} - \mathbf{b} \) since the dimension of the affine subspace is identical to nullity \( (A) \). Consider the holomorphic mapping

\[
f : \mathbb{C}^n \times \mathbb{C}^{m \times n} \times \mathbb{C}^m \longrightarrow \mathbb{C}^n
\]

\[
(x, G, z) \mapsto G x - z.
\]

At exact data \( G = A \) of rank \( r \) and \( z = \mathbf{b} \), the zeros of \( x \mapsto f(x, A, \mathbf{b}) \) form the affine subspace \( (8) \). If exact \( A \) and \( \mathbf{b} \) are unknown but given through empirical data \( G = \tilde{A} \) and \( z = \tilde{\mathbf{b}} \), the one-step rank-\( r \) Newton’s iteration \( (9) \) from a initial iterate \( \mathbf{x}_0 \) produces

\[
\mathbf{x} = \mathbf{x}_0 + \tilde{A}_\text{rank-}r^\dagger (\tilde{A} \mathbf{x}_0 - \tilde{\mathbf{b}}) = \tilde{A}_\text{rank-}r^\dagger \tilde{\mathbf{b}} + (I - \tilde{A}_\text{rank-}r^\dagger \tilde{A}) \mathbf{x}_0 \tag{9}
\]

that accurately approximates the exact solution

\[
\mathbf{x} = A^\dagger \mathbf{b} + (I - A^\dagger A) \mathbf{x}_0 \tag{10}
\]

of the underlying equation \( A \mathbf{x} = \mathbf{b} \) we intend to solve. Moreover, the particular exact solution \( \mathbf{x} \) is the nearest point in the affine subspace \( (8) \) to the initial iterate \( \mathbf{x}_0 \). The condition number \( (7) \) is a moderate multiple of \( \| A^\dagger \|_2 \) that is finitely bounded and can even be small in applications. The “fear” of singularity is indeed “exaggerated”.

In a recent paper \[28\], this author elaborates the sensitivity of singular linear systems from a different perspective: The general solution of a singular system \( A \mathbf{x} = \mathbf{b} \) is a unique point in an affine Grassmannian in which the sensitivity \( \| A \|_2 \| A^\dagger \|_2 \) is bounded. A properly formulated approximage solution from empirical data within an error tolerance uniquely exists in the same affine Grassmannian, enjoys Lipschitz continuity and accurately approximates the exact solution with an accuracy in the same order of the data. Furthermore, one can solve the perturbed system \( \tilde{A} \mathbf{x} = \tilde{\mathbf{b}} \) using any method as long as it is backward stable. The resulting solution accurately approximates one of the infinitely many (vector) solutions. The perceived “errors” are actually a part of the solution and not error at all. Those results are summarized below.

**Theorem 1 (Regularization of Singular Linear Systems)** Let \( A \in \mathbb{C}^{m \times n} \) of rank \( r \) and \( \mathbf{b} \in \text{Range}(A) \). Assume the empirical data \( (\tilde{A}, \tilde{\mathbf{b}}) \) of \( (A, \mathbf{b}) \) is accurate so that \( \| \tilde{A} - A \|_2 < 0.46 \| A^\dagger \|_2^{-1} \). Then the following assertions hold.
(i) [28, Theorem 8] Any backward accurate solution \( \tilde{x} \) of the data system \( \tilde{A}x = \tilde{b} \) is an accurate approximation to a solution \( x_* \) of the underlying system \( Ax = b \) with an error bound
\[
\frac{\| \tilde{x} - x_* \|_2}{\| x_* \|_2} \leq \frac{\| A\|_2 \| A^\dagger \|_2}{1 - \| A^\dagger \|_2 \| \Delta A \|_2} \left( 2 \sqrt{2} \frac{\| \Delta A \|_2}{\| A \|_2} + \frac{\| \Delta b + e \|_2}{\| b \|_2} \right)
\]
where \( \Delta A = \tilde{A} - A \), \( \Delta b = \tilde{b} - b \) and \( e = \tilde{A} \tilde{x} - \tilde{b} \).

(ii) For any given \( x_0 \in \mathbb{C}^n \), the vector \( \tilde{x} \) in (9) is an accurate approximation to \( \hat{x} \) in (10) that is the solution of \( A\hat{x} = b \) nearest to \( x_0 \) with an error bound
\[
\| \tilde{x} - \hat{x} \|_2 \leq \alpha \| A^\dagger \|_2 (\| \tilde{A} - A \|_2 + \| \tilde{b} - b \|_2) + \text{h.o.t.}
\]
where \( \alpha > 0 \) is a constant of moderate magnitude and h.o.t. represents higher order terms of data error.

(iii) [28, Corollary 7] The affine subspace \( \tilde{A}_{\text{rank-}r}^\dagger \tilde{b} + \text{Ker}(\tilde{A}_{\text{rank-}r}) \) accurately approximates the general solution (8) with an error bound
\[
\max \left\{ \| \tilde{A}_{\text{rank-}r}^\dagger \tilde{b} - A^\dagger b \|_2, \text{dist} \left( \text{Ker}(\tilde{A}_{\text{rank-}r}), \text{Ker}(A) \right) \right\} \\
\leq \| A \|_2 \| A^\dagger \|_2 \frac{\sqrt{4 \| A^\dagger b \|_2^2 + 1}}{\| A \|_2^2 - \| A^\dagger b \|_2^2} \| (\tilde{A}, \tilde{b}) - (A, b) \|
\]

For a comprehensive discussion on solving singular linear systems from empirical data and error analyses, see [28].

6 Software implementation

The methods in this paper are implemented in the software package NACLAB [30] on the MATLAB platform along with an intuitive interface [27] for solving linear and nonlinear system of equations directly as zero-finding for mappings, bypassing the process of representing the system in multivariate or matrix forms.

Solving general linear equation \( L(x) = b \) for any linear mapping \( L \), including singular and homogeneous cases, is implemented as the module LinearSolve with an optional input item to set the error tolerance \( \theta > 0 \) so that the module attempts to solve the linear equation \( L_\theta(x) = b_\theta \) where \( L_\theta \) is the mapping the nearest to \( L \) with the smallest rank of all mappings within \( \theta \) of \( L \) and \( b_\theta \) is the orthogonal projection of \( b \) on \( \text{Range}(L_\theta) \).

The general Newton’s iteration including the Gauss-Newton and low-rank Newton’s iterations for solving equations in the form of \( f(x) = 0 \) is implemented as the module Newton with the projection rank \( r \) of the Jacobian as an optional input.

Both modules accept mappings \( L \) and \( f \) directly as in-line MATLAB anonymous functions with no need to write subroutines in most cases. Matrix representations for \( L \) and the Jacobian \( f_\xi(x_0) \) are generated automatically as internal process so users can avoid the tedious and error-prone tasks of constructing such matrices. We shall present several computing demos in this paper.
7 Application: Numerical Algebraic Geometry with empirical data

Numerical algebraic geometry and its application in kinematics heavily involve computing solutions of positive dimensions of polynomial systems [1] [21, 22]. Mechanisms have been developed in solving those systems including adding auxiliary equations to isolate witness points on the solution sets.

When the system is given through empirical data, however, the nonisolated solutions generally dissipates into isolated points. The low-rank Newton’s iteration can serve as a regularization mechanism and recover the lost solutions of the underlying system.

Example 1 (Recovering lost solutions of positive dimensions) Consider the given mapping $\tilde{f} : \mathbb{C}^3 \longrightarrow \mathbb{C}^3$ defined as

$$\tilde{f} : (x, y, z) \longmapsto (4.899 x^3 y - 5.6568 x^2 - 8.4852 x^3 y^2 - 2.8284 x^3 z^2 + 4 x^4 + 6 x^2 g^2 + 2 x^2 z^2 + 7.3485 x y^3 - 2 x^2$$

$$+ 2.4495 x y z + 2.8284 x^3 y - 5.1963 y^3 - 1.7321 y z^2 - 2.4495 x y + 1.7321 y,$$

$$8.4852 x^3 y^2 - 9.798 x^2 y - 14.697 x^3 y^2 + 4.899 x^3 z^2 + 5.6568 x^3 + 2.8284 x^3 z^2 + 4.899 x^3 y$$

$$+ 3.4642 x^2 y z + 5.1963 y^3 + 1.7321 y z^3 - 2.8284 x^3 - 2 x^2 z^2 - z^3 - 1.7321 y z + z - 3 y z^2,$$

$$5.6568 x^2 z^2 - 5.6568 x^2 z + 5.1963 y^3 z^2 + 1.7321 y z^4 + 16.97 x^3 y^2 z + 3.4642 x^2 y z^2 + 5.6568 x^2 z$$

$$+ 2 x^2 z^2 - 11.314 x^2 - 4 x^2 z^2 - 2 x^2 z^4 + 2 x^2 z^3 + 11.314 x^2 z^2 - 5.6568 x^2 z^2 - 16.97 x^3 y^2$$

$$- 1.7321 y z^3 - 4.899 x^3 y z + 4.899 x^3 y z - 9.798 x^3 y z - 6 x^2 y^2 z^2 + 3.4642 x^2 y z^2 + 5.6568 x^2 z$$

$$+ 9.798 x^2 y + 14.697 x^3 y^2 - 5.1963 y^3 z^2 - 1.7321 y z^4 + 1.7321 y z + 4.899 x^3 y z^2 - 3.4642 x^2 y z + 4 x^2 z)$$

as empirical data for the equation $f(x, y, z) = (0, 0, 0)$ that is a variation of the system given in [1, p. 143] by replacing $x$ and $y$ with $\sqrt{2}x$ and $\sqrt{3}y$. The underlying mapping $\tilde{f}$ has zero sets

$$\{\sqrt{3}y = x^2, z = 2\sqrt{2}x^3\}, \{\sqrt{2}x = \pm 1, \sqrt{3}y = 1\}, \{\sqrt{2}x = 1, z = 1\}, \text{and } \{2x^2 + 3y^2 + z^2 = 1\}$$

that are semiregular except at intersection points. We experiment solving this system from the data mapping $\tilde{f}$ obtained by rounding the polynomial coefficients in five digits.

The solutions of dimension 1 and 2 disappear from rounding errors in coefficients. An attempt to solve the data system directly by Maple using rational coefficients did not receive results in several hours. The homotopy method (implemented in NACLAB as the module psolve) terminates in seconds but results in different number (35-43) of isolated solutions with many of them ill-conditioned. Bertini [1] produced 36 regular solutions using hardware precision and 77 with adaptive multiple precision. The solution varieties of dimension 1 and 2 are lost by data perturbation even if the precision is extended in floating point arithmetic. Accurate recovery of those solutions from the given system becomes the problem of solving (underlying) singular system from empirical data.

By setting the projection rank $r = 1$ or $r = 2$, the rank-$r$ Newton’s iteration on $\tilde{f}$ locally converges to solutions of dimension $3 - r = 2$ or 1 respectively. For instance, we proactively seek a solution of dimension 2 by setting $r = 1$ from a random initial
iterate. The following is a NACLab demo of the MATLAB command-line process that is intuitive without the need to write a single subroutine.

\[
\begin{align*}
&\text{>> } P = \{('4.899' \times '3 y - 8.4852' \times '3y^2, ...' \}; \quad \% \text{ enter polyn. as character strings} \\
&\text{>> } v = \{'x';'y';'z'; \}; \quad \% \text{ enter cell array of variable names} \\
&\text{>> } J = \text{PolynomialJacobian}(P,v); \quad \% \text{ Jacobian of } P \text{ w.r.t. the variable names in } v \\
&\text{>> } f = \text{PolynomialEvaluate}(P,v,x); \quad \% \text{ function handle for evaluating } P \text{ at } v \\
&\text{>> } \text{Jjac} = \text{PolynomialEvaluate}(J,v,x0)*x; \quad \% \text{ func. evaluating } J \text{ at } v \\
&\text{>> } \text{domain} = \text{ones}(3,1); \text{param} = \{P,J,v\}; \quad \% \text{ domain (3x1 vectors) and parameters} \\
&\text{>> } z0 = [\text{-}0.25518; \text{-}0.60376; \text{-}0.020624]; \quad \% \text{ random initial iterate} \\
&\text{>> } \{z,\text{res},\text{fcond}\} = \text{Newton}(\{f,domain,param\},\{\text{Jjac},1\},z0,1); \quad \% \text{ rank-1 Newton iteration from } z0 \text{ using display type 1} \\
\end{align*}
\]

Notice that the residual can only reduce to \(6.93 \times 10^{-8}\). Namely the limit \((\tilde{x}, \tilde{y}, \tilde{z})\) is not a zero of \(\tilde{f}\) but a stationary point as a solution to \(\tilde{f}_{xyz}(\tilde{x}, \tilde{y}, \tilde{z})^\dagger \tilde{f}(\tilde{x}, \tilde{y}, \tilde{z}) = 0\). as indicated by the shifts

\[\left\| (x_j + 1, y_j + 1, z_j + 1) - (x_j, y_j, z_j) \right\|_2, \quad j = 0, 1, \ldots\]

approaching hardware zero. The stationary equation regularizes the singular equation \(f(x, y, z) = 0\). The iteration terminates in 6 steps at

\[(\tilde{x}, \tilde{y}, \tilde{z}) = (-0.234036969240715 - 0.544684891672585 - 0.020211408075956)\]

that accurately approximates a point \((\tilde{x}, \tilde{y}, \tilde{z})\) in the solution set \(\{2x^2 + 3y^2 + z^2 = 1\}\) with 10 correct digits.

8 Application: the GCD equation

An intuitive model for computing the greatest common divisor (GCD) of a polynomial pair \(p\) and \(q\) is solving the GCD equation

\[(u \, v - p, \, u \, w - q) = (0, 0) \quad (14)\]

for \((u, v, w) = (u_s, v_s, w_s)\) where \(u_s\) is a constant multiple of the GCD and \((v_s, w_s)\) is a pair of co-factors. However, the equation \((14)\) is obviously singular with the 1-dimensional solution set

\[\{(t \, u_s, \frac{1}{t} v_s, \frac{1}{t} w_s) \mid t \in \mathbb{C} \setminus \{0\}\}. \quad (15)\]

The model \((14)\) is viable only if we can accurately solve for its singular solutions, or after adding unnatural auxiliary constraints. Furthermore, the solution set \((15)\) is infinitely sensitive and generically reduces to the trivial set \(\{(t, p/t, q/t) \mid t \in \mathbb{C} \setminus \{0\}\}\)
under arbitrary data perturbations. As a result, solving the equation (14) has been
an ill-posed problem with empirical data. On the other hand, the emergence of
the low-rank Newton’s iteration enables solving the GCD equation (14) directly and
accurately even if the data are perturbed and the nontrivial GCD disappears.

Let \( P_l \) denote the vector space of polynomials with degrees up to \( l \) with a norm \( \| u \| \)
defined as the 2-norm of the coefficient vector of \( u \in P_l \) so that \( P_l \) is isometrically
isomorphic to \( \mathbb{C}^{l+1} \). Assume \((p,q) \in P_m \times P_n\) of degrees \( m \) and \( n \), respectively, with
the GCD degree \( k \). We define the holomorphic mapping

\[
f : P_k \times P_{m-k} \times P_{n-k} \times P_m \times P_n \longrightarrow P_m \times P_n
\]

\[
(u,v,w,f,g) \longmapsto (uv - f, uw - g)
\]

The following lemma establishes the semiregularity of the solution set (15).

**Lemma 3 (Semiregularity of the GCD Equation)** Let \( f \) be defined in (16). Assume \((p,q) \in P_m \times P_n\) of degrees \( m \) and \( n \), respectively, with the GCD degree \( k \). Then any zero \((\hat{u},\hat{v},\hat{w})\) of the mapping \( g : (u,v,w) \mapsto f(u,v,w,p,q) \) at the fixed
parameter value \((f,g) = (p,q)\) with \( \deg(\hat{u}) = k \) is semiregular. 

**Proof.** Let \((u_*,v_*,w_*)\) be a particular zero of \( g \) with \( \deg(u_*) = k \). Then (15)
is the zero set \( g^{-1}(0) \) of dimension one. Consequently \( \text{nullity}(g_{uvw}(\hat{u},\hat{v},\hat{w})) \geq 1 \). By [25, Lemma 4.1], appending one extra linear equation to \( g(u,v,w) = 0 \) makes the Jacobian of the left side injective at \((\hat{u},\hat{v},\hat{w})\). Namely \( \text{nullity}(g_{uvw}(\hat{u},\hat{v},\hat{w})) \leq 1 \). As
a result, the zero \((\hat{u},\hat{v},\hat{w})\) is semiregular since the nullity of \( g_{uvw}(\hat{u},\hat{v},\hat{w}) \) is 1 and identical to the dimension of (15).

Since the zero set (15) of \( g \) is of dimension 1 and semiregular, the rank of the Jacobian
at any particular solution is

\[ r = \dim (P_k \times P_{m-k} \times P_{n-k}) - 1 = m + n - k + 2 \]

and the rank-\( r \) Newton’s iteration with \( r \) as in (17)

\[
(u_{j+1},v_{j+1},w_{j+1}) = (u_j,v_j,w_j) - f_{uvw}(u_j,v_j,w_j,\tilde{p},\tilde{q})_{\text{rank}-r}^\dagger f(u_j,v_j,w_j,\tilde{p},\tilde{q})
\]

for \( j = 0,1,\ldots \) at empirical data \((f,g) = (\tilde{p},\tilde{q})\) locally converges to a GCD triple
\((\hat{u},\hat{v},\hat{w})\) that accurately approximates an exact GCD triple \((\tilde{u},\tilde{v},\tilde{w})\) of the underlying
data \((p,q)\) in the zero set (15). Consequently, the iteration (18) serves as an effective
regularization mechanism for the singular GCD equation (14) so that the GCD can
be accurately computed from empirical data, as asserted in the following theorem.

**Theorem 2 (Regularization of GCD)** Let \((p,q)\) be a polynomial pair of degrees
\( m \) and \( n \) respectively with a GCD degree \( k \). Assume the data \((\tilde{p},\tilde{q})\) is sufficiently close
to \((p,q)\) and the initial iterate \((u_0,v_0,w_0)\) is sufficiently close to a zero \((\hat{u},\hat{v},\hat{w})\) of
the mapping $g : (u,v,w) \mapsto f(u,v,w,p,q)$. Setting $r = m + n - k + 2$, the rank-$r$
Newton’s iteration \([18]\) at the data $(\tilde{p}, \tilde{q})$ converges to $(\tilde{u}, \tilde{v}, \tilde{w})$ with an error bound
\[
\|(\tilde{u}, \tilde{v}, \tilde{w}) - (\bar{u}, \bar{v}, \bar{w})\| \leq c \|f_{uvw}(\bar{u}, \bar{v}, \bar{w}, p, q)^{r\text{rank}}\| \cdot \|\|p, q\| + h.o.t. \tag{19}
\]
where $(\tilde{u}, \tilde{v}, \tilde{w}) \in g^{-1}(0)$ is an exact GCD triple of $(p, q)$ and $c > 0$ is a constant of
moderate magnitude. The convergence rate is quadratic if data $(\tilde{p}, \tilde{q}) = (p, q)$. The
GCD condition number can be defined as $\|f_{uvw}(\tilde{u}, \tilde{v}, \tilde{w}, p, q)^{r\text{rank}}\|$ at the polynomial
pair $(p, q)$

**Proof.** A straightforward verification based on Lemma 2 and Lemma 3.

The GCD model \([14]\) is not restricted to the univariate GCD problem. Multivariate
GCD’s can be computed by solving the same equation from proper domains of polynomial spaces using the same iteration \([18]\) except that the projection rank $r$ needs to be adjusted to one less than the dimension of the corresponding domain.

### 9 Application: Factoring polynomials

A straightforward and intuitive model for factoring a multivariate polynomial $p$ is to solve the factorization equation
\[
u_0 u_1^{\ell_1} \cdots u_k^{\ell_k} - p = 0 \tag{20}
\]
for an irreducible factor array $(u_0, \ldots, u_k) = (\hat{u}_0, \ldots, \hat{u}_k)$ where $\ell_1, \ldots, \ell_k > 0$ are integers. For convenience, we assume $\hat{u}_0 \in \mathbb{C}$; $\ell_0 = 1$ and $\hat{u}_1, \ldots, \hat{u}_k$ are nontrivial.

The equation \((20)\) is singular with a solution set of dimension $k$ in the form of
\[
\{(t_0\hat{u}_0, t_1\hat{u}_1, \ldots, t_k\hat{u}_k) \mid t_1, \ldots, t_k \in \mathbb{C} \setminus \{0\}, t_0 = t_1^{-\ell_1} \cdots t_k^{-\ell_k}\} \tag{21}
\]
which is hypersensitive and the exact nontrivial factorization is generally impossible if $p$ is known only through empirical data $\tilde{p}$.

Let $U_0 = \mathbb{C}$ and $U_1, \ldots, U_k$ be vector spaces of polynomials containing $\hat{u}_0, \ldots, \hat{u}_k$ respectively. For $j = 0, 1, \ldots, k$, assume every $U_j$ is a proper hosting space of $\hat{u}_j$ in the
sense that $s \hat{u}_j \in U_j$ implies $s$ is a constant. Let $\mathcal{P}$ be a vector space of polynomials
containing $p$, $\tilde{p}$ and all the products $u_0u_1 \cdots u_k$ for $u_j \in U_j$, $j = 0, 1, \ldots, k$. Define the
holomorphic mapping
\[
f : U_0 \times U_1 \times \cdots \times U_k \times \mathcal{P} \longrightarrow \mathcal{P}
\]
\[(u_0, u_1, \ldots, u_k, f) \longmapsto u_0 u_1^{\ell_1} \cdots u_k^{\ell_k} - f \tag{22}\]

The following lemma establishes the crucial semiregularity of \((21)\).

**Lemma 4 (Semiregularity of Polynomial Factorization)** Let $f$ be defined in \([22]\) and $p \in \mathcal{P}$ with an irreducible factorization $\hat{u}_0 \hat{u}_1^{\ell_1} \cdots \hat{u}_k^{\ell_k}$ where $\hat{u}_j$ belongs to
a proper hosting space $U_j$ for $j = 0, 1, \ldots, k$. Then every zero $(\tilde{u}_0, \ldots, \tilde{u}_k)$ of the
mapping $g : (u_0, \ldots, u_k) \mapsto f(u_0, \ldots, u_k, p)$ at $f = p$ is semiregular and
\[
\text{rank}(g_{u_0 \ldots u_k}(\tilde{u}_0, \ldots, \tilde{u}_k)) = \dim(U_0 \times \cdots \times U_k) - k \tag{23}
\]
Proof. The Jacobian $g_{u_0 \cdots u_k}(\tilde{u}_0, \ldots, \tilde{u}_k)$ is the linear map

$$(u_0, \ldots, u_k) \mapsto \sum_{i=0}^{k} u_i (\ell_i \tilde{u}_i^{\ell_i-1} \prod_{j \neq i} \tilde{u}_j^{\ell_j})$$

whose nullity is at least $k$ since the zero set (21) of $g$ is of dimension $k$. Let $\phi_j : U_j \to \mathbb{C}$ be a linear functional with $\phi_j(\tilde{u}_j) = \beta_j \neq 0$ for $j = 1, \ldots, k$. Consider the mapping

$$h : (u_0, \ldots, u_k) \mapsto (f(u_0, \ldots, u_k, p), \phi_1(u_1) - \beta_1, \ldots, \phi_k(u_k) - \beta_k)$$

and we claim its Jacobian at $(\tilde{u}_0, \ldots, \tilde{u}_k)$ is injective. In fact, setting

$$h_{\tilde{u}_0 \cdots \tilde{u}_k}(\tilde{u}_0, \ldots, \tilde{u}_k)(u_0, \ldots, u_k) = 0$$

yields, for any $i \in \{0, \ldots, k\}$,

$$u_i(\ell_i \prod_{j \neq i} \tilde{u}_j^{\ell_j}) = -\tilde{u}_i \left( \sum_{l \neq i} u_l (\ell_l \tilde{u}_l^{\ell_l-1} \prod_{j \neq l, i} \tilde{u}_j^{\ell_j}) \right)$$

implying $u_i = s \tilde{u}_i$ and $s$ must be a constant. As a result, we have $\phi_i(s \tilde{u}) = s \phi_i(\tilde{u}) = 0$, leading to $s = 0$. Thus $u_i = 0$ for all $i = 0, \ldots, k$ so the Jacobian of $h$ is injective at $(\tilde{u}_0, \ldots, \tilde{u}_k)$. Since appending $k$ linear functionals to $g_{u_0 \cdots u_k}(\tilde{u}_0, \ldots, \tilde{u}_k)$ reduces its nullity to zero, its nullity is no more than $k$, leading to the semiregularity of $(\tilde{u}_0, \ldots, \tilde{u}_k)$ and (23) holds.

Setting $r$ as (23) by Lemma 4 the rank-$r$ Newton’s iteration

$$(u_0^{(j+1)}, \ldots, u_k^{(j+1)}) = (u_0^{(j)}, \ldots, u_k^{(j)}) - f_{u_0 \cdots u_k}(u_0^{(j)}, \ldots, u_k^{(j)}, \tilde{p})_{\text{rank-}r}^{-1} f(u_0^{(j)}, \ldots, u_k^{(j)}, \tilde{p})$$

regularizes the factorization problem as asserted in the following theorem.

**Theorem 3 (Regularization of Polynomial Factorization)** Let $p = \hat{u}_0 \hat{u}_1^{\ell_1} \cdots \hat{u}_k^{\ell_k}$ be an irreducible polynomial factorization where $\hat{u}_j$ belongs to a proper hosting space $U_j$ for $j = 0, \ldots, k$ and $U_0 = \mathbb{C}$. Let $\mathcal{P} \ni p$ be a vector space containing all products $u_0 u_1^{\ell_1} \cdots u_k^{\ell_k}$ for $u_j \in U_j$, $j = 0, \ldots, k$ and set $r$ to be (23). Then, for any $\tilde{p} \in \mathcal{P}$ sufficiently close to $p$ as empirical data and from any initial iterate $(u_0^{(0)}, \ldots, u_k^{(0)}) \in U_0 \times \cdots \times U_k$ near $(\hat{u}_0, \ldots, \hat{u}_k)$, the rank-$r$ Newton’s iteration (25) converges to a $(\tilde{u}_0, \ldots, \tilde{u}_k) \in U_0 \times \cdots \times U_k$ with an error bound

$$\left\| (\tilde{u}_0, \ldots, \tilde{u}_k) - (\hat{u}_0, \ldots, \hat{u}_k) \right\|_2 \leq \alpha \|f_{u_0 \cdots u_k}(\hat{u}_0, \ldots, \hat{u}_k, \tilde{p})_{\text{rank-}r}^{-1} \| \|\tilde{p} - p\| + O(\|\tilde{p} - p\|)^2)$$

where $(\tilde{u}_0, \ldots, \tilde{u}_k)$ an exact factor array of $p$ in (21) and $\alpha > 0$ is a constant of moderate size. The convergence is quadratic if $\tilde{p} = p$. The norm $\|f_{u_0 \cdots u_k}(\hat{u}_0, \ldots, \hat{u}_k, p)_{\text{rank-}r}^{-1}\|$ can be defined as the factorization condition number of $p$. 
Proof. The assertions follow from a straightforward verification using Lemma 2 and Lemma 4. ■

Regularizing the singular factorization problem by taking advantage of the semiregularity and the low-rank Newton’s iteration in [5] substantially improves the existing results in [23] theoretically and computationally by eliminating the unnatural auxiliary components \( \phi_j(u_j) - \beta_j \) for \( j = 1, \ldots, k \) in (24) from the model.

Example 2 (Factoring a polynomial from empirical data) The data for the polynomial \( p = (\frac{4}{5}y^2 + \frac{1}{2}x^2z^6)^3(-1 + \frac{4}{5}yz + x^3) \) is given in

\[
\begin{align*}
\tilde{p} &= 0.296296y^9 - 0.269360y^10z^2 + 0.0612182y^{11}z^2 + 0.466545y^{10}x^5 + 0.888889y^9x^{10} + 1.14286y^6x^5 + 1.038696y^7x^5 + 3.958966y^8x^5 + 0.2301268y^9x^5 + 1.799534y^7x^7 + 3.42857y^8x^7 + 1.46939y^9x^7 - 1.33581y^8x^8 - 5.09911y^9x^8 + 0.303556y^{10}x^8 + 2.31639y^9x^9 + 4.08681y^{10}x^9 + 6.29738y^{11}x^{12} - 0.572489x^6 + 6y^{13}y - 2.18148x^{11}z^{12} + 0.130111x^{12}y^2 + 0.991580x^{11}z^3 + 1.88921x^{16}z^{12} \\
\end{align*}
\]

From the data polynomial \( \tilde{p} \), the factorization structure of \( p \) can be identified by the methods elaborated in [23] along with initial approximation of factors. Applying Proposition 3 with \( k = 2 \), \( \ell_1 = 3 \), \( \ell_2 = 2 \) along with fewnomial spaces \( U_1 = \text{span}\{y^3, x^2z^4\} \) and \( U_2 = \text{span}\{1, yz, x^5\} \), we can carry out the rank-4 Newton’s iteration in (25) in the follow computing demo of NACLAB in which \texttt{pplus}, \texttt{pminus}, \texttt{ptimes} are polynomial utilities for +, − and \( \times \).

\[
\begin{align*}
\text{Step 0: residual} & = 5.35e-02 \\
\text{Step 1: residual} & = 2.26e-04 & \text{shift} & = 3.70e-03 \\
\text{Step 2: residual} & = 7.87e-06 & \text{shift} & = 3.63e-05 \\
\text{Step 3: residual} & = 7.86e-06 & \text{shift} & = 1.22e-09 \\
\text{Step 4: residual} & = 7.86e-06 & \text{shift} & = 6.58e-16 \\
\end{align*}
\]

The process terminates at the approximate factorization

\[
0.999035(0.667678y^3 + 0.858444x^2z^4)^3(-0.998210 + 0.453732yz + 1.728948x^5)^2
\]

toward a point in the 2-dimensional solution (21) with coefficients accuracy \( 6.8 \times 10^{-6} \) that is in the same order as the data accuracy. Again, residual does not approach zero since the mapping \( f \) in (22) does not have a zero at the data \( f = \tilde{p} \). However, the shifts approaching zero implies the iteration solves the stationary equation

\[
\frac{\partial f_{u_0u_1u_2}(u_0, u_1, u_2, \tilde{p})}{\partial \tilde{p}}\bigg|_{\text{rank-4}} = 0
\]

that regularizes the singular equation (20) with a near optimal condition number 4.92. The NACLAB equation solving interface [27] makes the entire process intuitive.
10 Application: Defective eigenvalues

Computing defective eigenvalues of matrices is a well-known singular problem and a formidable challenge to achieve accurate results from empirical data. We shall demonstrate that defective eigenvalues are semiregular and can be regularized through the low-rank Newton’s iteration, advancing from sensitivity theory and the computational method in [26].

Let $\hat{\lambda}$ be a defective eigenvalue of a matrix $A \in \mathbb{C}^{n \times n}$. We say the multiplicity support of $\hat{\lambda}$ is $m \times k$ if $\hat{\lambda}$ is of geometric multiplicity $m$ with the smallest Jordan block size $k$. Finding such an eigenvalue can naturally modeled as solving the eigenequation

$$AX - \lambda X - XS = O \quad (27)$$

for $(\lambda, X) \in \mathbb{C} \times \mathbb{C}^{n \times k}$ where $S \in \mathbb{C}^{k \times k}$ satisfies

$$S = [s_{ij}], \quad s_{ij} = 0 \text{ for } i \leq j \text{ and } s_{12}s_{23} \cdots s_{k-1,k} \neq 0. \quad (28)$$

Any solution of (27) is a zero of the mapping $(\lambda, X) \mapsto f(\lambda, X, A)$ where

$$f : \mathbb{C} \times \mathbb{C}^{n \times k} \times \mathbb{C}^{n \times n} \rightarrow \mathbb{C}^{n \times k}$$

$$(\lambda, X, G) \mapsto GX - \lambda X - XS \quad (29)$$

Lemma 5 (Semiregularity of Defective Eigenvalues) Let $\hat{\lambda}$ be an eigenvalue of $A \in \mathbb{C}^{n \times n}$ with a multiplicity support $m \times k$. For any fixed parameter $S$ satisfying (28), the solution of (27) is semiregular with dimension $mk$ in the form of

$$\{(\hat{\lambda}, \hat{X}) \mid \hat{X} = X_0 + Y_0 Z, \ Z \in \mathbb{C}^{m \times k}\} \quad (30)$$

where $X_0, Y_0 \in \mathbb{C}^{n \times k}$ with $\text{Range}(Y_0) = \text{Kernel}(A - \hat{\lambda}I)$. Furthermore, the partial Jacobian $f_{\lambda X}(\hat{\lambda}, \hat{X}, A)$ at any solution is of rank

$$r = \text{rank}(f_{\lambda X}(\hat{\lambda}, \hat{X}, A)) = 1 + (n - m)k. \quad (31)$$

Proof. Write $X = [x_1, \ldots, x_k]$ columnwise. Then the equation (27) with $\lambda = \hat{\lambda}$ can be expanded as $(A - \hat{\lambda}I)x_1 = 0$ along with

$$Ax_j - \hat{\lambda}x_j = s_{ij}x_1 + \cdots + s_{j-1,j}x_{j-1}, \ \text{for } j = 2, \ldots, k.$$ 

by picking any specific solution $X = X_0$ satisfying the above system and any $Y_0 \in \mathbb{C}^{n \times m}$ whose columns form a basis for $\text{Kernel}(A - \hat{\lambda}I)$, we have the solution (30) since $\text{nullity}(A - \hat{\lambda}I) = m$. The mapping $\phi : Z \mapsto (\lambda, X_0 + Y_0 Z)$ is injective and the Jacobian $\phi'_Z : Z \mapsto Y_0 Z$ is of rank $mk$ since $Y_0$ is of full column rank. Define the mapping

$$g : \mathbb{C} \times \mathbb{C}^{n \times k} \rightarrow \mathbb{C}^{n \times k}$$

$$(\lambda, X) \mapsto (A - \lambda I)X - XS$$
Thus the Jacobian $g_{\lambda X}$ at any solution in (30) is of nullity at least $mk$. By [26, Lemma 2], appending a linear mapping $X \mapsto C^m X \in \mathbb{C}^{m \times k}$ with a constant matrix $C \in \mathbb{C}^{m \times m}$ to $g_{\lambda X}(\lambda, X)$ reduces the nullity to zero, implying $\text{nullity}(g_{\lambda X}(\lambda, X))$ is no more than $mk$. Hence every solution in (30) is semiregular. The rank (31) follows accordingly.

Upon establishing semiregularity and setting the projection rank $r$ in (31), we can now compute a defective eigenvalue from empirical data $\hat{A}$ by applying the rank-$r$ Newton’s iteration

$$(\lambda_{j+1}, X_{j+1}) = (\lambda_j, X_j) - f_{\lambda X}(\lambda_j, X_j, \hat{A})_{\text{rank-}r} \cdot f(\lambda_j, X_j, \hat{A}) \quad (32)$$

**Theorem 4 (Regularization of Defective Eigenvalues)** Let $\lambda$ be an eigenvalue of $A \in \mathbb{C}^{m \times n}$ with a multiplicity support $m \times k$. Then, for any $\hat{A} \in \mathbb{C}^{m \times n}$ sufficiently close to $A$ as empirical data and $r$ as in (31), the rank-$r$ Newton’s iteration (32) from any initial iterate $(\lambda_0, X_0)$ close to a solution in (30) converges to a point $(\lambda, \hat{X}) \in \mathbb{C} \times \mathbb{C}^{m \times k}$ with an error bound

$$\| (\hat{\lambda}, \hat{X}) - (\lambda, \hat{X}) \| \leq \alpha \| f_{\lambda X}(\hat{\lambda}, \hat{X}, \hat{A})_{\text{rank-}r} \| \| \hat{X} \|_2 \| A - \hat{A} \|_F + O(\| A - \hat{A} \|_F^2) \quad (33)$$

where $\alpha = O(1)$ is a constant and $(\hat{\lambda}, \hat{X})$ is an exact solution in (30). The convergence is quadratic if $\hat{A} = A$. The condition number of $\lambda$ can be defined as $\| f_{\lambda X}(\lambda, X, A)_{\text{rank-}r} \|$

**Proof.** The assertions directly follow Lemma 2 and Lemma 3 with $\| f_{\hat{C}}(\hat{\lambda}, \hat{X}, A) \| \leq \| \hat{X} \|_2$ since $f_{\hat{C}}(\hat{\lambda}, \hat{X}, A) : G \mapsto G \hat{X}$. The $\| \hat{X} \|_2$ component in the condition number of $\lambda$ can be eliminated since the $\hat{X}$ can be chosen with orthonormal columns. \qed

The error estimate (33) can be improved by eliminating the factor $\| \hat{X} \|_2$ by a thin-QR decomposition $\hat{X} = QR$, resetting the component $S$ as $RSR^{-1}$ and one additional step of the iteration (32) from the initial iterate $(\lambda_0, X_0) = (\hat{\lambda}, Q)$. The resulting $X$ component will have nearly orthonormal columns and 2-norm approximately one. This normalization process is much simpler than that in [26].

**Example 3 (Defective eigenvalue from empirical data)** Let $\hat{\lambda} = 2$ be a 7-fold eigenvalue of $A$ with multiplicity support $2 \times 2$ but $A$ is known through data $\hat{A}$ below with entry error bound $0.5 \times 10^{-4}$.

$$A = \begin{bmatrix} -0.1047 & 2.6711 & -7.7657 & -7.6782 & -0.1741 & -2.8614 & -1.5102 & 10.1186 \\ 1.1993 & 1.3389 & 2.5196 & -2.4136 & -0.5598 & 1.1995 & 1.5892 & -3.1106 \\ 1.5919 & -4.4314 & 10.3181 & -7.9651 & 0.8970 & 1.3103 & 0.2183 & -11.4464 \\ 3.0877 & -4.2142 & 9.8737 & -7.5953 & 0.4991 & 3.1022 & 1.4778 & -13.1894 \\ 1.3996 & 0.6824 & 0.3731 & -0.3272 & 1.2337 & 0.4494 & 0.6920 & -0.0206 \\ 0.2930 & -0.4477 & 1.8217 & -2.4647 & -0.3103 & 3.4128 & 0.7911 & -2.8883 \\ 0.8370 & -0.3341 & 1.7179 & -0.9933 & 0.4461 & 0.2581 & 1.8852 & -1.4502 \\ -1.7541 & 0.4549 & -2.9046 & 2.8613 & 0.4216 & -1.9328 & -1.5465 & 5.5124 \end{bmatrix}$$

Matlab built-in function `eig` produces scattered eigenvalues

$$1.7733 \pm 0.1345i, 2.0341 \pm 0.2668i, 2.1931 \pm 0.0454i, 1.9976, 2.0025$$
of errors at least 0.0024. From an initial estimate \( \lambda_0 = 1.98 \), we first calculate the component \( X_0 \) of the initial iterate by solving
\[
AX - \lambda_0 X - XS = 0
\]
for \( X \in \mathbb{C}^{8 \times 2} \) within error tolerance \( 3 \times 10^{-2} \) in the following NACLAb calling sequence:

```
>> A = [-0.1047 2.6711 -7.6782 ...]; % enter data matrix
>> S = [0 1; 0 0]; % matrix parameter S
>> L = @(X,e0,G,S) G*X-e0*X-X*S; % function handle for \( L : X \to G*X-e0*X-X*S \)
>> [~,K]=LinearSolve([L,{ones(8,2)},{1.98,A,S}],zeros(8,2),3e-2) % solve \( L(X)=0 \)
```

obtaining the initial iterate \( (\lambda_0, X_0) \) where \( X_0 \) is a random linear combination of the four solutions in output \( K \) of \texttt{LinearSolve}. The rank-13 Newton’s iteration is carried out as follows.

```
>> f = @(e,X,G,S) G*X-e*X-X*S; % function handle for mapping \( f(e,X)\to G*X-e*X-X*S \)
>> fjac = @(e,X,e0,X0,G,S) G*X-e*X0-e0*X-X*S; % Jacobian \( (e,X)\to G*X-e*X0-e0*X-X*S \)
>> domain = {1,ones(8,2)}; % domain of \( f \) as \( C \times C^{(8x2)} \)
>> param = {A,S}; % parameters \( A \) and \( S \) for mapping \( f \)
>> [Z,res,fcnd]=Newton({f,domain,param},{fjac,13},{e0,X0},1); % rank-13 Newton
```

obtaining an accurate defective eigenvalue \( \tilde{\lambda} = 2.000072 \) with an accuracy \( .7 \times 10^{-4} \) in the same level of the data error.

### 11 On ultrasingular equations

We say an equation is ultrasingular if its Jacobian at a desired solution has a (column) rank-deficiency larger than the dimension of the solution. Ultrasingularity occurs in cases such as at a zero whose dimension is undefined (e.g. intersection points of solution branches), isolated multiple zeros, isolated ultrasingular zeros embedded in a semiregular zero set and entire branch of nonisolated ultrasingular zeros. Difficulties in computing ultrasingular zeros including slow convergence rate of iterative methods (c.f. [6]) and, more importantly, barriers of low attainable accuracy [19, 24].

Singular equations with isolated multiple zeros can be accurately solved by the depth-deflation method [4, 5]. A singular isolated zero \( x^* \) of a mapping \( f : \Omega \subset \mathbb{C}^m \to \mathbb{C}^n \) derives an isolated zero \((x^*,y^*)\) of an expanded mapping

\[
g : \Sigma \subset \mathbb{C}^m \times \mathbb{C}^m \longrightarrow \mathbb{C}^n \times \mathbb{C}^m \times \mathbb{C}^{m-r} \\
(x,y) \longmapsto (f(x), J(x)y, Ry - e)
\] (34)
where $J(x)$ is the Jacobian of $f(x)$, $R$ is a random $(m - r) \times m$ matrix and $e \neq 0$ with $r = \text{rank}(J(x_*))$. The deflation process terminates if $(x_*, y_*)$ is a regular zero of $g$ or, otherwise, continues recursively by expanding $g$. It is proved in [4, 5] that the number of deflation steps is bounded by the \textit{depth} of $x_*$. When depth-deflation terminates, the ultrasingular zero $x_*$ of $f$ is a component of the regular zero of the final expanded mapping. As a result, the Gauss-Newton iteration locally converges to an accurate zero at quadratic rate. An earlier deflation strategy in [15] is also proven to terminate with the number of steps bounded by the multiplicity.

By definition, a branch of $k$-dimensional semiregular zero of a mapping $f$ can be parameterized as $x = \phi(z)$ for $z$ in an open set. As the parameter $z$ varies, there is a significant likelihood that $\text{nullity}(f_x(\phi(z)))$ degenerates below the dimension $k$ and reaches ultrasingularity. Such ultrasingular zeros can be of particular interest. The following example shows that we can proactively seek such ultrasingularity by applying the depth-deflation method.

\textbf{Example 4 (Ultrasingularity embedded in a semiregular solution set)} The cyclic-4 system arises in applications such as biunimodular vectors that comes from a notion traces back to Gauss [9]. It is in the form of $f(x) = 0$ where $x = (x_1, x_2, x_3, x_4)$ and

$$f(x) = \begin{pmatrix} x_1 + x_2 + x_3 + x_4 \\ x_1 x_2 + x_2 x_3 + x_3 x_4 + x_4 x_1 \\ x_1 x_2 x_3 + x_2 x_3 x_4 + x_3 x_4 x_1 + x_4 x_1 x_2 \\ x_1 x_2 x_3 x_4 - 1 \end{pmatrix}$$

(35)

The solution consists of two 1-dimensional branches

$$\{x_1 = -x_3, x_2 = -x_4, x_3 x_4 = \pm 1\}. \quad (36)$$

All zeros in the branches are semiregular except eight ultrasingular zeros in the form of $(\pm 1, \pm 1, \pm 1, \pm 1)$ and $(\pm i, \pm i, \pm i, \pm i)$ with proper choices of signs. The cyclic-4 system becomes an ultrasingular equation at, say $x_* = (1, -1, -1, 1)$, for being 1-dimensional in (36) but the nullity of the Jacobian $f_x(x_*)$ is 2. However, it is a straightforward verification that, for almost all matrices $R \in \mathbb{C}^{2 \times 4}$, there is a unique $y_*$ such that the point $(x_*, y_*)$ is a regular zero of the deflation mapping $g$ in (34). As a result, the rank-8 Newton’s iteration on $g$ becomes the Gauss-Newton iteration that locally quadratically converges to $(x_*, y_*)$, solving the ultrasingular equation $f(x) = 0$. The same assertion can be verified in the same way for all eight ultrasingular solutions. The results show that, at least for cyclic-4 system the depth-deflation methods deflates the ultrasingularity into regularity.

The rank-8 Newton’s iteration on $g$ converges specifically to those eight ultrasingular zeros of $f$ and does not converge to other semiregular zeros in the same solution branch since they are not zeros of the deflation mapping $g$ in (34). Consequently, the depth-deflation method can be proactively deployed to compute ultrasingular zeros if so desired. At this point, however, the theories of the depth-deflation are lacking at ultrasingularity embedded in semiregular branches of zeros and require
further studies. Similar gaps exist in cases such as computing ultrasingular zeros at intersections of semiregular branches, and in cases where the entire branch of zeros are ultrasingular as shown in the following example proposed by Barry Dayton.

**Example 5 (High dimension ultrasingularity)** Consider the mapping below with \( \mathbf{x} = (x_1, \ldots, x_5) \)

\[
\mathbf{f}(\mathbf{x}) = \begin{bmatrix}
    x_2^3 x_4^2 + x_2^2 x_5^2 + x_1^5 - 2 x_2 x_4 \\
    x_2^3 x_4^2 - 2 x_2 x_3^2 + x_2^2 x_5^2 + x_5^7 + 3 x_2 x_4 - 2 \\
    x_1^2 x_5^2 + x_2^2 x_4 + x_5^7 - 2 x_2 x_4
\end{bmatrix}
\]

The solution set \( S = \{(0, s, t, 1/s, 1/t) \mid s, t \neq 0\} \) is 2-dimensional but the nullity of the Jacobian is \( 4 > 2 \), making the entire branch ultrasingular. We apply the depth-deflation method by setting up the deflation mapping \( \mathbf{g} \) in (34) with a random matrix \( R \in \mathbb{C}^{4 \times 5} \). For every \( \mathbf{x}_* \in S \), there is a unique \( \mathbf{y}_* \) such that \( \mathbf{g}(\mathbf{x}_*, \mathbf{y}_*) = 0 \). Namely \( \mathbf{g} \) also has a corresponding 2-dimensional zero set. Anticipating this zero set to be semiregular, we set \( r = 10 - 2 = 8 \) and test the rank-8 Newton’s iteration on \( \mathbf{g} \) from an initial iterate near \( S \), say \( \mathbf{x}_0 = (0.001, .698, 1.201, 1.428, 0.833) \). The rank-8 Newton’s iteration converges to a point \( (\tilde{x}, \tilde{y}) \) with the component \( \tilde{x} \) as

\[
(0.0, .699835056282962, 1.201681873936643, 1.428908127739848, 0.832167000009791)
\]

approximating a zero of \( \mathbf{f} \) with an accuracy at hardware precision. The condition number 28.7 indicates the Jacobian is indeed rank 8 and the solution is a semiregular zero of deflation mapping \( \mathbf{g} \).

The result of this experiment shows that, at least for this polynomial system, the depth-deflation method deflates the ultrasingularity into semiregularity.

Open questions remain such as: Does the depth-deflation deflates ultrasingularity in general? If so, under what conditions does the deflation terminate? If not, are there proper modifications to overcome its limitations? In fact, a numeric-symbolic deflation proposed by Hauenstein and Wampler is proved to terminate in finitely many steps [11]. Our preliminary experimental results also suggest the potential effectiveness of the depth-deflation method combined with the novel low-rank Newton’s iteration.

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