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<td>Kanzawa, Yuichi; Oishi, Shin'ichi</td>
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Kyoto University
Approximate Singular Solutions of Nonlinear Equations and a Numerical Method of Proving their Existence

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Abstract

A new concept of "an approximate singular solution" is defined as an approximate solution which becomes a singular solution by adding a suitable small perturbation to the original equations. A numerical method is presented for proving the existence of approximate singular solutions of nonlinear equations with guaranteed accuracy. A few numerical examples are also presented for illustration.

1 Introduction

In this paper we are concerned with the problem of proving numerically the existence of singular solutions for the following system of nonlinear equations:

\[ f(x) = 0, \quad f: \mathbb{R}^n \rightarrow \mathbb{R}^n \]  \hspace{1cm} (1)

Various methods such as Krawczyk's method have been proposed for calculating the regular solutions of Eq. (1) with guaranteed accuracy [3]. Thus one way of calculating singular solutions is to resolve the singularity. The bordering methods have been proposed in this way. In these methods, extended systems are proposed such that singular solutions of the original systems become regular ones for the extended systems. Thus it is natural to consider that it may be possible to prove the existence of the singular solutions of Eq. (1) by applying Krawczyk's method to the extended systems. However, in the extended systems additional variables are necessary to introduce in order to resolve the singularities. A regular solution of the extended system becomes a singular solution of Eq. (1) when these additional variables are equal to zero. Usually, it is numerically undecidable whether such variables are equal to zero or not.

In this paper, based on this consideration the concept of an approximate singular solution of Eq. (1) is proposed as an exact solution of the extended system of Eq. (1) whose additional variables have norms smaller the prescribed values. Thus, an approximate singular solution is either a true singular solution, a set of regular solutions, or not a solution of the original equation. However, it always becomes a true singular solution if additional variables are added to the original equation Eq. (1) as perturbations. This is the motivation why we have introduced a new concept.

Then a numerical method is proposed for proving the existence of approximate singular solutions to Eq. (1). Previously, the extended systems have been proposed for a specific kind of singularity. Therefore, for instance, the codimension of the Jacobian matrix at the solution and the multiplicity of the solution must be known a priori. Moreover, one must prepare various kinds of extended systems according to the types of singularities. In this paper, a new type of extended system is proposed. The proposed system is based on a map from \( \mathbb{R}^l \) to \( \mathbb{R}^n \), where \( l \) is greater than \( n \). It is manageable for any codimension of Jacobian matrix at the solution and any multiplicity of the solution. A numerical method is also proposed to prove the existence of the approximate singular solution of the new system. It is shown that the new method always succeeds if the given approximate solution is sufficiently close to the approximate singular solution of Eq. (1). Finally, numerical examples are also presented for illustration.

2 Notations and Definitions

In this section, we shall explain briefly notations and definitions which will be used in the paper. We will use the terminologies of the interval analysis according to the paper[3].

Let \( D \) be a set. The set of intervals, interval vectors, or interval matrices included in \( D \) are represented by \( I(D) \) The mid point \( \text{mid}(I) \), the radius \( \text{rad}(I) \) and the absolute value \( |I| \) of interval
$I = [p, q] \in I(R)$ are defined by

\[
\text{mid}(I) = \frac{p + q}{2}, \quad \text{rad}(I) = \frac{q - p}{2}
\]

and \(|I| = \max(|p|, |q|)|

respectively. \(\text{mid}(I), \text{rad}(I), |I|\) of interval vector \(I\) or interval matrices \(I\) are obtained by \(\text{mid}(I), \text{rad}(I), |I|\) of their elements. The norm of the interval vector \(I \in I(R^n)\) is defined as

\[
||I|| = \max\{|I_i|\} \text{ for all } i.
\]

That of the interval matrix \(I \in I(C(R^n; R^n))\) as

\[
||A|| = ||A[u]||, \quad u = (1, 1, \ldots, 1)^T.
\]

The map \(F : I(D) \to I(Y)\) constructed by a map \(f : D \to R^n\) is called interval map, where \(D \subset X = R^n\) and \(Y = R^n\).

In order to calculate the solution of a nonlinear system of equations with guaranteed accuracy, range of the map \(f\) used in the theorem is also needed to calculate with guaranteed accuracy. Interval enclosure is defined as representation of maps in computers. Let \(D\) be a bounded open subset of \(R^d\). Interval map \(F : I(D) \to I(R^n)\) is an interval enclosure of a map \(f : D \to R^n\) if

\[
F(I) \supset f(I) \text{ for all } I \in I(D).
\]

Regularity of functions is defined as follows:

Let \(D\) be a bounded open subset of \(R^d\). Let \(f : D \to R^n\) be \(C^1\). \(f\) is regular at \(x\) if the Jacobian matrix \(f'(x)\) is regular, otherwise \(f\) is singular at \(x\). such a point \(x\) is called singular point. \(y \in R^n\) is singular value of \(f\) if \(f^{-1}(y)\) includes a singular point of \(f\) at least, otherwise \(y\) is regular value of \(f\).

Let \(E = \{e_1, \ldots, e_l\}\) be the basis of \(R^l\), where \(e_1 = (1, 0, \ldots, 0), e_2 = (0, 1, 0, \ldots, 0), \ldots \). Let \(N \subset 2^E\) be whole subsets of \(n\) elements of \(E\). Let \(X_a\) be the subspace spanned by the elements of \(a \in N\). Let \(Y_a\) be the orthogonal complement of \(X_a\). Let \(P_{ax} : D \to R^n\) be \(l \times n\) dimensional matrix by row vectors of elements of \(a\). Let \(P_{ay} : D \to R^{l-n}\) be \(l \times (l-n)\) dimensional matrix by row vectors of elements of \(E \backslash a\). Let \(P_{az} : R^n \times R^{l-n} \to R^l\) be defined as

\[
P_{az}(x, y) = P_{ax}^t \mathbf{x} + P_{ay}^t \mathbf{y}
\]

For example, let \(E\) be \(\{e_1, \ldots, e_3\}\), let \(N\) be whole subsets of \(3\) elements of \(E\), and let \(a \in N\) be \(\{e_1, e_3, e_5\}\). Then,

\[
P_{az} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix},
\]

\[
P_{ay} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix},
\]

that is, \(P_{az}, P_{ay}\) map \(z = (z_1, z_2, z_3, z_4, z_5)^T \in R^5\) as

\[
P_{az} z = (z_1, z_3, z_5)^T
\]

\[
P_{ay} z = (z_2, z_4)^T.
\]

\(P_{az}\) constructed by the above \(P_{ax}, P_{ay}\) maps \((x, y) = (x_1, x_2, x_3, y_1, y_2)^T\) as

\[
P_{az}(x, y) = (x_1, y_1, x_2, y_2, x_3)^T.
\]

The function \(f_a : R_n \times R^{l-n} \to R^n\) is defined as

\[
f_a(x, y) = f(P_{ax}(x, y)), \quad x \in R_n, y \in R^{l-n}.
\]

Let \(f'_{ax}, f'_{ay}\) be \(f'_{ax} = \frac{\partial f_a}{\partial x}, f'_{ay} = \frac{\partial f_a}{\partial y}\) for the function \(f_a(x, y)\) defined by \(a \in N\). Interval enclosures of \(f'_{ax}, f'_{ay}\) can be constructed from \(P_{ax} F', P_{ay} F'\) and is denoted as \(F'_{ax}, F'_{ay}\).

The following theorem guarantees the existence of the solution of Eq. (1).
Theorem 2.1 Let $f : \mathbb{R}^n \to \mathbb{R}^n$ be $C^1$. For a given interval $I \in I(D)$, define interval matrix $M$ and interval map $K$ as

$$M := E - L^{-1}f'(I),$$
$$K(I) := c - L^{-1}f(c) + M(I - c),$$

where $E$ is $n \times n$-unit vector, $c$ is mid$(I)$ and $L$ is a regular non-interval matrix approximating the Jacobian matrix $f'(c)$. If the following conditions

$$\begin{align*}
K(I) &\subseteq I, \\
\|M\| &< 1.
\end{align*}$$

(3)

are valid, there exists a unique solution of the equation $g(x) = 0$ in $I$.

The following theorem guarantees the existence of the solution of parameter dependent systems of equations defined by

$$g(z) = 0, \quad g : \mathbb{R}^l \to \mathbb{R}^n.$$

Theorem 2.2 Let $g : \mathbb{R}^l \to \mathbb{R}^n$ be $C^1$. Let $F, F'$ be the interval enclosures of $f, f'$, respectively. Let $0 < r < 1$. For a given interval $I \in I(\mathbb{R}^l)$, let $c = \text{mid}(I)$, $C$ be the small interval satisfying mid$(C) = \text{mid}(I)$ and rad$(C) = r \text{rad}(I)$. Let $T_x, T_y, c_x, C_x, C_y$ be $P_{ax}T, P_{ay}T, P_{ax}c, P_{ax}C, P_{ay}C$, respectively. For the interval $I$ and an element $a \in N$, define interval matrix $M$ and interval map $K$ as

$$M = E - L^{-1}_a F'_a(T_x, T_y),$$
$$K(T) = c_x - L^{-1}_a F_a(C_x, T_y) + M(T_x - c_x),$$

where $E$ is $n \times n$-unit vector, and $L_a$ is a regular non-interval matrix, which describes an approximate Jacobian in $I$:

$$L_a \in P_{ax} F'_a(C_x, C_y).$$

If the following conditions

$$\begin{align*}
K(I) &\subseteq I, \\
\|M\| &< 1,
\end{align*}$$

(4)

are valid, there exists a unique solution of the equation $g(z) = 0$ in $I$.

Definition 2.1 The solution $x^*$ of Eq. (1) is called the singular solution of codimension $m$ if

$$\text{codim}(\text{Range}D_x f(x^*)) = m$$

holds. The solution $x^*$ of Eq. (1) is isolated simple singular solution if

$$\begin{align*}
\text{codim}(\text{Range}D_x f(x^*)) &\neq 1, \\
\psi(D_x^2 f(x^*) \phi^*) &\neq 0
\end{align*}$$

hold, where $\phi^*$ is a elements of ker($D_x f(x^*)$) and $\psi$ is a functional satisfying

$$\psi(D_x f(x^*) \phi^*) = 0.$$

3 approximate isolated simple singular solutions

The following extended system

$$\begin{align*}
\bar{f} := \begin{cases}
\bar{f}(x) + \lambda \phi, \\
\phi_k^{-1}
\end{cases}
\end{align*}$$

(5)

$$F : \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^{2n+1}$$
has been proposed to calculate isolated simple singular solutions of Eq. (1). where $\lambda \in R, \phi \in R^n, \phi_k$ is the $k$-th element of $\phi$, and $z = (x, \lambda, \phi)$. The second equation of (5) expresses that the rank of the Jacobian matrix $D_2 f(x^*)$ on the solution $x^*$ is less than $n$. It is known that a regular solution of Eq. 5 becomes a true isolated simple singular solution $x^*$ of the original equation provided that $\lambda$ is zero. While using Krawczyk's method one can find a regular solution of Eq. 5 with guaranteed accuracy, it cannot be numerically decidable whether $\lambda$ is zero or not.

Thus we define an approximate isolated simple singular solution as the point which becomes an isolated simple singular solution by adding a suitable small perturbation to the original equation:

**Definition 3.1** The element $\bar{x}$ of the solution $\bar{z} = (\bar{x}, \bar{\lambda}, \bar{\phi})$ of Eq. (5) is called the $\varepsilon$-approximate isolated simple singular solution of Eq. (1) if $\bar{\lambda}$ is not greater than $\varepsilon > 0$.

For any $\varepsilon > 0$, the existence of $\varepsilon$-approximate isolated simple singular solution can be proved by applying Krawczyk's method to Eq. (5).

4 More complex singular solution

We can define an approximate singular solution for other type of singular solution using the same technique as the definition 3.1. Moreover, we can also present a method of proving its existence applying Krawczyk's method to the expanded system. However, there are many cases that one cannot know a priori the type of singularity of the solution to find.

Thus, we propose a new type of extended system for singular solutions for any codimension $m$.

**Definition 4.1** Let $\lambda_1, \lambda_2 \in R^n, \phi \in R^n$ and $z = (x, \lambda_1, \lambda_2, \phi)$. A new extended system is defined by

$$g(z) = 0,$$

where

$$g(z) = \left\{ \begin{array}{c} f(x) + \lambda_1 \vspace{1em} \\
D_x f(x)\phi + \lambda_2 \
\phi \vspace{1em} \\
\phi_\varepsilon - 1 \end{array} \right\},$$

$$g : R^n \times R^n \times R^n \times R^n \rightarrow R^{2n+1}.$$

The first equation of Eq. (7) is constructed by adding the vector $\lambda_1$ to the original equation. The second one is constructed by adding the vector $\lambda_2$ to the second one of Eq. (5). The third one is the same as the third one of Eq. (5). The first and second ones avoid the short of rank of Jacobian matrices $D_2 f(x^*)$ and $D_2 f(x^*)\phi^*$ on the singular solution $x^*$ of the original equation and on the element $\phi^*$ of the null space of $D_x f(x^*)$. The solutions of proposed expand system Eq. (7) includes the singular solution of Eq. (1) of codimension $m_1$ and of the multiplicity $m_2$ for all $1 \leq m_1 \leq n, 1 \leq m_2$. The element $x$ of the obtained solution of Eq. (7) becomes a true singular solution of Eq. (1) provided that both elements $\lambda_1$ and $\lambda_2$ of the obtained solution are equal to zero.

We now define a concept of an approximate singular solution as the point which becomes the singular solution by adding a suitable small perturbation to the original equation. More precisely, by

**Definition 4.2** The element $\bar{x}$ of the solution $\bar{z} = (\bar{x}, \bar{\lambda_1}, \bar{\lambda_2}, \bar{\phi})$ of Eq. (7) is the $\varepsilon_1, \varepsilon_2$-approximate singular solution of Eq. (1) if the element $\|\bar{\lambda_1}\|, \|\bar{\lambda_2}\|$ is not greater than $\varepsilon_1 > 0, \varepsilon_2 > 0$, respectively.

The existence of a solution of extended system $g(z) = 0$ can be proved by applying the method of [2], which is the method of finding solutions of the equation $g(x) = 0$, $g$ being a map from $R^n \times R^n \times R^n \times R^n$ to $R^{2n+1}$. Now, we propose the algorithm to prove the existence of the solution of $g(z) = 0$ for a given approximate solution $x = c_x, \phi = c_{\phi}, \lambda_1 = c_{\lambda_1}, \lambda_2 = c_{\lambda_2}$ as follows:

**Algorithm 4.1** Let $X$ an open subset of $R^{4n}$ and let $g : X \rightarrow R^{2n+1}$ be $C^1$. Set $\rho > 1$ and $r > 0$. Let $G, G'$ be the interval enclosures of $g, g'$, respectively. Let $g'_{ax} = \frac{\partial^2 a}{\partial x \partial y}$ and $g'_{ay} = \frac{\partial^2 a}{\partial y \partial y}$, respectively for $a \in N$. Let $c = (c_x, c_{\lambda_1}, c_{\lambda_2}, c_{\phi})$ be a approximate solution of Eq. (7).

1. Check the existence of $g'_{ax}(c)^{-1}$ for all $a \in N$. If for any $a \in N$, $g'_{ax}(c)$ becomes singular, end with failure.
2. Let $s$ be a $a \in N$ for which $g'_{ax}(c)$ exits and $\|g'_{ax}(c)\|$ becomes the smallest for all $a \in N$. Let $L$ be $g'_{ax}(c)$.
(3) Let \( c_x, c_y \) be \( P_{sx}c, P_{sy}C \). Calculate
\[
I_y = c_y + rB,
\]
where \( B \) is the \( 2n - 1 \) dimensional unit ball. Calculate
\[
I_x = c_x + \rho\|L^{-1}G(P_{sx}(c_x, I_y))\|B
\] (8)

(4) Calculate
\[
M = E - L^{-1}G'(P_{sx}(I_x, I_y)),
K(I) = c_x - L^{-1}G(P_{sx}(c_x, I_y)) + M(I_x - c_x).
\]

(5) If
\[
\|M\| < 1, \quad (9)
\]
\[
K(I) \subset I \quad (10)
\]
hold, there exists the unique solution of Eq. (7) in the interval \( I_x \) for the fixed \( y \in I_y \). Otherwise, let \( r \) be \( r/2 \) and go to the step 2.

We now show that Algorithm 4.1 ends with succeed provided that if one starts with an approximate solution sufficiently close to a true solution of Eq. (7).

**Theorem 4.1** Assume that the series of approximate solution converges to the true solution of Eq. (7), that is, \( c_k \rightarrow c^* \), holds, where \( c^* \) is the true solution of Eq. (7). Then, Algorithm 4.1 succeeds for the sufficient large \( k \).

**Proof**

Let \( c_x^{(k)}, c_y^{(k)}, L_k, I_x^{(k)} \), \( f_y^{(k)}, j_y^{(k)} \), \( M_k \) be \( c_x, c_y, L, I_x, I_y, M \) for \( c_k \), respectively. Let \( \{r_j\} \) be the series of \( r \) obtained in the case that Algorithm 4.1 fails. The proof is completed by indicating that the tests (9),(10) succeed for the sufficiently large \( k, j \).

We have the sufficient condition of (10) as
\[
\|L^{-1}\{G_{xy}(P_{sx}(c_x, I_y))\}\| + \|M\|\|I_x - c_x\| < \|I_x - c_x\|.
\]
From (8) and (9), we have
\[
\|M\| < 1 - \frac{1}{\rho} \quad (11).
\]
Thus the proof is completed by indicating that (11) holds for the sufficiently large \( k, j \).

\( g'(c) \) is described concretely as
\[
g'(c) = \begin{pmatrix}
f'(c_x) & E & 0 & 0 \\
0 & f_y'(c_x) & c_h & E & 0 \\
0 & 0 & 0 & 0 & e_k^t\end{pmatrix}.
\]

If we select
\[
a = \{e_{n+1}, \cdots, e_{3n}, e_{3n+k}\}
\]
for all \( k \), there exists \( L_k^{-1} \) and we have
\[
\|L_k^{-1}\| = \|E^{-1}\| = 1
\]
for all \( k \). Thus,
\[
\|L_k^{-1}\| \leq 1
\] (12)
holds for the determined $L^{-1}_k$ in Algorithm 4.1.

From (12), we have

$$
\|I_x^{(k)} - c_x^{(k)}\| \\
= \rho \|L^{-1}_k \{g(c_k) + G'_{x}c_x^{(k)}(I_y^{(k)} - c_y^{(k)})\}\| \\
\leq \rho \|L^{-1}_k\| \|g(c_k) + G'_{x}c_x^{(k)}(I_y^{(k)} - c_y^{(k)})\| \\
\leq \rho \|g(c_k)\| + \|G'_{x}c_x^{(k)}\| \|I_y^{(k)} - c_y^{(k)}\| \\
\leq \rho \|g(c_k)\| + \|G'_{x}c_x^{(k)}\| \|I_y^{(k)} - c_y^{(k)}\|.
$$

We have

$$r_j \rightarrow 0, \quad (j \rightarrow \infty)$$

as Algorithm 4.1 proceeds. We have

$$
\|g(c_k)\| \rightarrow 0, \quad (k \rightarrow \infty)
$$

From (13), (14), we have

$$
\|I_x^{(k)} - c_x^{(k)}\| \rightarrow 0, \quad (k \rightarrow \infty).
$$

Thus, we have

$$
\|M_k\| = \|E - L^{-1}_k G'_{x}c_x^{(k)}(I_y^{(k)} + I_y^{(k)})\| \\
\leq \|L^{-1}_k\| \|G'_{x}c_x^{(k)}(I_y^{(k)} + I_y^{(k)})\| \\
\leq \|g'(c_k) - G'(I_x^{(k)} + I_y^{(k)})\| \\
\rightarrow 0, \quad (k \rightarrow \infty)
$$

by the continuity of $G'$.

\[\square\]

5 Numerical Examples

In order to realize an arithmetical system for the algorithms mentioned in this paper, we use a programming language which Kashiwagi made by improving a programming language called CALC. In this language, instead of the floating-point arithmetic, the rational arithmetic is used.

Our program was implemented by the technique of automatic differentiation. Our system can automatically validate the approximate (isolated simple) solution of Eq. 1 only by providing two inputs: a program expressing the system of equations and an approximate solution.

Example 5.1 Consider a system of equations described as

$$
\begin{cases}
    x_1(x_1 - 1)^2(x_1 - 3) + (x_2 - 1)(x_2 - 2) &= 0, \\
    (x_2 - 1)(x_1 - 1)(x_2 - 2) + x_1(x_1 - 3)(x_2 - 1) &= 0
\end{cases}
$$

We construct the extended system (5). For a given approximate solution

$$(x_1, x_2, \lambda, \phi_1, \phi_2) = (1, 1, 0, 1, 0),$$

we can obtain the solution of the expanded system (See Table 6).

Since $\lambda$ is in $[-0.0000000000000001, 0.0000000000000001]$, we obtained $0.0000000000000001$-approximate isolated simple singular solution for Eq. (15).

\[\square\]

Example 5.2 Consider a system of equation described as

$$
\begin{cases}
    x_1^3(x_1 - 1)^2(x_1 - y) + x_2^3(x_2 - 2)^2(x_2 - 3) &= 0, \\
    x_1^3(x_1 - 1)^2(x_1 - 3) + x_2(x_2 - 2)(x_2 - 3) &= 0
\end{cases}
$$

We construct the extended system (7). For a given approximate solutions as shown in Table 6, we can obtain the solution of the extended system by Algorithm 4.1 (See Table 6).

\[\square\]
6 Consideration on Automation of Calculating Approximate Singular Solutions

We consider now how to calculate an approximate singular solution for a given approximate solution of Eq. (1). Let \( D_x f^{(j)} \) be the matrix by exchanging the \( j \)-th row vector \( D_x f^{(j)} \) of \( Df(x) \) and \( e^*_l \). There exists at least one number \( j \) such that \( D_x f^{(j)}(x) \) is regular for an approximate solution of Eq. (1). We can calculate

\[
\bar{\phi} = D_x f^{(j)}(x)e_l
\]

Thus, we have the following new extended system \( \bar{g}(z) = 0 \) which is equivalent to Eq. (5) for the approximate isolated simple singular solution, where \( z = (x, \lambda) \) and

\[
\bar{g}(z) = \begin{cases} 
  f(x) + \lambda e_l, \\
  D_x f^{(j)}(x)\bar{\phi}.
\end{cases}
\]

(17)

The number of equations and variables are less than Eq. (1). This system can be constructed automatically using the technique of automatic differentiation. The equivalent system for Eq. (7) can be constructed as Eq. (17).

References


| \( x_1 \) | \( \cdot9999999999999999, 1.0000000000000000 \) |
| \( x_2 \) | \( \cdot9999999999999999, 1.0000000000000000 \) |
| \( \lambda \) | \(-\cdot0000000000000000, \cdot0000000000000000 \) |
| \( \phi_1 \) | \( \cdot9999999999999999, 1.0000000000000000 \) |
| \( \phi_2 \) | \(-\cdot0000000000000000, \cdot0000000000000000 \) |

Table.1 Interval including the approximate isolated simple singular solution of Eq. (15)
Table 2: Approximate solutions of Eq. (16)

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Table 3: Intervals including the approximate singular solutions of Eq. (16), Respectively

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