

Original Article

Numerical differential continuation approach for systems of nonlinear equations with singular Jacobian

Mohammad Ali Mehrpouya^{*a}

^aDepartment of Mathematics, Tafresh University, 39518-79611, Tafresh, Iran

ABSTRACT: It is well known that, one of the useful and rapid methods for a nonlinear system of algebraic equations is Newton’s method. Newton’s method has at least quadratic convergence when the Jacobian is a nonsingular matrix in a neighborhood of the solution. In this paper, a differential continuation method is presented for solving the nonlinear system of algebraic equations whose Jacobian matrix is singular at the solution. For this purpose, at first, an auxiliary equation named the homotopy equation is constructed. Then, by differentiating from the homotopy equation, a system of differential equations is replaced instead of the target problem and solved. In other words, the solution of the nonlinear system of algebraic equations with singular Jacobian is transformed to the solution of a system of differential equations. Some numerical tests are presented at the end and the computational efficiency of the method is described.

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1. Introduction

Nonlinear systems of algebraic equations arise frequently in science and engineering. For instance, many methods in solving differential and integral equations, eventually solve the problem by converting the problem into a system of algebraic equations. Because, the analytical solution of nonlinear systems of algebraic equations is rarely found, so, the numerical methods should be entered. Undoubtedly one of the most widely used numerical methods in solving nonlinear systems of algebraic equations is the classical Newton’s method.

Let us consider the problem of finding the solution of the nonlinear system

$$\mathbf{F}(\mathbf{x}) = \begin{pmatrix} f_1(x_1, \dots, x_n) \\ \vdots \\ f_n(x_1, \dots, x_n) \end{pmatrix} = \mathbf{0} \tag{1}$$

in which, $\mathbf{F} : D \subseteq \mathbb{R}^n \rightarrow \mathbb{R}^n$. It is assumed that, the Eq. (1) has a solution \mathbf{x}^* , so that, $\mathbf{F}(\mathbf{x}^*) = \mathbf{0}$. It is worthwhile to note that, the Newton’s iteration formula for numerical solution of the Eq. (1) is given by

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \mathbf{J}_{\mathbf{F}}(\mathbf{x}^{(k)})^{-1}\mathbf{F}(\mathbf{x}^{(k)}), \quad k = 0, 1, \dots, \tag{2}$$

^{*}Corresponding author.
E-mail addresses: mehrpouya@tafreshu.ac.ir

where, $\mathbf{J}_{\mathbf{F}}(\mathbf{x}) = \frac{\partial \mathbf{F}(\mathbf{x})}{\partial \mathbf{x}}$ is the Jacobian matrix of \mathbf{F} . Obviously, for the success of this method, the Jacobian matrix should be nonsingular in a neighborhood of \mathbf{x}^* . Of course, the Eq. (2) can be rewritten so that there is no need to evaluate the inverse of the Jacobian matrix. For this purpose, we have

$$\mathbf{J}_{\mathbf{F}}(\mathbf{x}^{(k)})\mathbf{x}^{(k+1)} = \mathbf{J}_{\mathbf{F}}(\mathbf{x}^{(k)})\mathbf{x}^{(k)} - \mathbf{F}(\mathbf{x}^{(k)}), \quad k = 0, 1, \dots \quad (3)$$

The Eq. (3) is actually a system of linear algebraic equations in which for each $k = 0, 1, \dots$ should be solved.

The aim of this paper is to propose a differential continuation method for solving the nonlinear system of algebraic equations whose Jacobian matrix is singular. The plan is to solve a specified target problem starting from the solution of an easy problem, so that, the easy problem is continuously deformed into the original problem. For this purpose, at first, an auxiliary equation named the homotopy equation is constructed which is a set of subproblems that are obtained from changing of the easier problem into the original problem. Then, by differentiating from the homotopy equation, a system of differential equations is replaced instead of the target problem. So, the solution of each subproblem is fed as an initial guess for other problems in this set and this procedure is followed to the solution of the target problem. The continuation methods are well-known subject in numerical computations. They have been frequently utilized to successfully solve nonlinear equations, boundary value problems and different kinds of engineering problems [6, 7, 1, 9, 8].

2. Preliminary considerations

To solve the nonlinear system of algebraic equations (1) in the classical version of continuation methods, at first, the original set of functions $\mathbf{F}(\mathbf{x})$ is transformed into the homotopy function

$$\mathcal{H}(\mathbf{x}, \lambda) = \mathbf{F}(\mathbf{x}) + (\lambda - 1)\mathbf{F}(\mathbf{x}^{(0)}),$$

where, $\lambda \in [0, 1]$ is the homotopy parameter. Now, a family of subproblems is formed as

$$\mathcal{H}(\mathbf{x}, \lambda) = \mathbf{F}(\mathbf{x}) + (\lambda - 1)\mathbf{F}(\mathbf{x}^{(0)}) = \mathbf{0}, \quad (4)$$

for different values of λ , so that, for $\lambda = 0$, this homotopy equation comes in the shape

$$\mathbf{0} = \mathcal{H}(\mathbf{x}, 0) = \mathbf{F}(\mathbf{x}) - \mathbf{F}(\mathbf{x}^{(0)}),$$

and $\mathbf{x}(0) = \mathbf{x}^{(0)}$ is a solution and when $\lambda = 1$, the equation comes in the shape

$$\mathbf{0} = \mathcal{H}(\mathbf{x}, 1) = \mathbf{F}(\mathbf{x}),$$

and $\mathbf{x}(1) = \mathbf{x}^*$, which is the solution of the Eq. (1), is obtained. Indeed, the $\mathbf{x}(\lambda)$ is supposed to be a solution of the homotopy equation (4) for each $\lambda \in [0, 1]$. Consequently, the set

$$\{\mathbf{x}(\lambda) \mid 0 \leq \lambda \leq 1\},$$

can be looked as a curve from $\mathbf{x}(0) = \mathbf{x}^{(0)}$ to $\mathbf{x}(1) = \mathbf{x}^*$ parameterized by λ . This curve is nominated as the zero curve [10]. A continuation method detects a sequence of steps along the zero curve corresponding to $\{\mathbf{x}(\lambda_k)\}_{k=0}^l$, where $0 = \lambda_0 < \lambda_1 < \dots < \lambda_l = 1$. If the functions $\mathbf{x}(\lambda)$ and \mathcal{H} are continuously differentiable, by differentiating from the homotopy equation (4) regarding to the λ gets

$$\mathbf{0} = \frac{\partial \mathcal{H}(\mathbf{x}(\lambda), \lambda)}{\partial \mathbf{x}} \dot{\mathbf{x}}(\lambda) + \frac{\partial \mathcal{H}(\mathbf{x}(\lambda), \lambda)}{\partial \lambda},$$

and subsequently, we have

$$\dot{\mathbf{x}}(\lambda) = - \left(\frac{\partial \mathcal{H}(\mathbf{x}(\lambda), \lambda)}{\partial \mathbf{x}} \right)^{-1} \frac{\partial \mathcal{H}(\mathbf{x}(\lambda), \lambda)}{\partial \lambda}. \quad (5)$$

The Eq. (5) which is a system of differential equations together with the initial condition $\mathbf{x}(0) = \mathbf{x}^{(0)}$, forms an initial value problem as

$$\begin{cases} \dot{\mathbf{x}}(\lambda) = - \left(\frac{\partial \mathbf{F}(\mathbf{x}(\lambda), \lambda)}{\partial \mathbf{x}} \right)^{-1} \mathbf{F}(\mathbf{x}^{(0)}), \\ \mathbf{x}(0) = \mathbf{x}^{(0)}, \quad 0 \leq \lambda \leq 1, \end{cases} \quad (6)$$

where, $\frac{\partial \mathbf{F}(\mathbf{x}(\lambda), \lambda)}{\partial \mathbf{x}}$ is the Jacobian matrix of \mathbf{F} regarding to the \mathbf{x} . So, the problem of finding the root of the original nonlinear system of equations is equivalent to the solution of the system of initial value problems (6) over the interval $[0, 1]$. Unfortunately, although the mentioned differential continuation is uncomplicated and intelligible, it fails at $(\mathbf{x}(\lambda), \lambda)$ where the Jacobian matrix $\frac{\partial \mathbf{F}(\mathbf{x})}{\partial \mathbf{x}}$ is singular. The next section is about overcoming this problem.

3. The proposed method

To treat the failure of the mentioned differential continuation, we reparameterize the problem by introducing the arc length parameter, s , so that both \mathbf{x} and λ depend on s [3]. This method is an arc length differential continuation method. So this time, we will face a new homotopy equation as below

$$\mathbf{0} = \mathcal{H}(\mathbf{x}(s), \lambda(s)) = \mathbf{F}(\mathbf{x}(s)) + (\lambda(s) - 1)\mathbf{F}(\mathbf{x}(0)).$$

Therefore, the problem can be treated as the solution of differential equation

$$\frac{d}{ds} \mathcal{H}(\mathbf{x}(s), \lambda(s)) = \mathbf{0}.$$

Now, from the chain rule, we have

$$\mathbf{0} = \frac{\partial \mathbf{F}(\mathbf{x}(s))}{\partial \mathbf{x}} \dot{\mathbf{x}}(s) + \mathbf{F}(\mathbf{x}(0)) \dot{\lambda}(s). \tag{7}$$

Since, a new parameter s is introduced, an additional equation should be added beside the system of differential equations (7) to make the number of differential equations equal to the number of unknown functions. Because the parameter s is the arc length parameter, so, with the Euclidean norm, the equation

$$\| \dot{\mathbf{x}}(s) \|_2^2 + |\dot{\lambda}(s)|^2 = 1, \tag{8}$$

is considered beside the system of differential equations (7). Therefore, considering the boundary conditions $\lambda(0) = 0$ and $\lambda(1) = 1$, together with Eqs. (7) and (8), we will finally get to the following boundary value problem

$$\begin{cases} \frac{\partial \mathbf{F}(\mathbf{x}(s))}{\partial \mathbf{x}} \dot{\mathbf{x}}(s) + \mathbf{F}(\mathbf{x}(0)) \dot{\lambda}(s) = \mathbf{0}, \\ \| \dot{\mathbf{x}}(s) \|_2^2 + |\dot{\lambda}(s)|^2 = 1, \\ \lambda(0) = 0, \quad \lambda(1) = 1. \end{cases} \tag{9}$$

It is noted that, in this paper, a simple finite difference scheme is utilized for solving the boundary value problem (9). For this purpose, at first, the total domain $[0, 1]$ is discretized as follows

$$0 = s_1 < s_2 < \dots < s_{n-1} < s_N = 1.$$

For simplicity, we will take these nodes to be equally spaced. So, with considering $h = 1/(N - 1)$, we have

$$s_k = s_1 + (k - 1)h, \quad k = 1, 2, \dots, N.$$

Then, we discretize the derivatives in the boundary value problem (9) for each $i = 1, 2, \dots, N - 1$, in the following manner

$$\begin{aligned} \dot{\mathbf{x}}(s) &\simeq \frac{\mathbf{x}(s_{i+1}) - \mathbf{x}(s_i)}{h}, \\ \dot{\lambda}(s) &\simeq \frac{\lambda(s_{i+1}) - \lambda(s_i)}{h}. \end{aligned}$$

Consequently, the boundary value problem (9) is discretized as follows

$$\begin{cases} \frac{\partial \mathbf{F}(\mathbf{x}(s_i))}{\partial \mathbf{x}} \frac{\mathbf{x}(s_{i+1}) - \mathbf{x}(s_i)}{h} + \mathbf{F}(\mathbf{x}(0)) \frac{\lambda(s_{i+1}) - \lambda(s_i)}{h} = \mathbf{0}, \\ \| \frac{\mathbf{x}(s_{i+1}) - \mathbf{x}(s_i)}{h} \|_2^2 + | \frac{\lambda(s_{i+1}) - \lambda(s_i)}{h} |^2 = 1, \\ \lambda(s_1 = 0) = 0, \quad \lambda(s_N = 1) = 1. \end{cases} \tag{10}$$

It is worthwhile to note that, the Eqs.(10) form a system of algebraic equations with $N(n + 1)$ unknown values $\mathbf{x}(s_1), \dots, \mathbf{x}(s_N), \lambda(s_1), \dots, \lambda(s_N)$ and $(N - 1)(n + 1) + 2$ algebraic equations. So, it is an underdetermined system of algebraic equations with nonsingular Jacobian matrix. Consequently, the Newton's iterations (3) can be easily implemented and eventually the problem of dealing with a system of equations with a singular Jacobian will be solved.

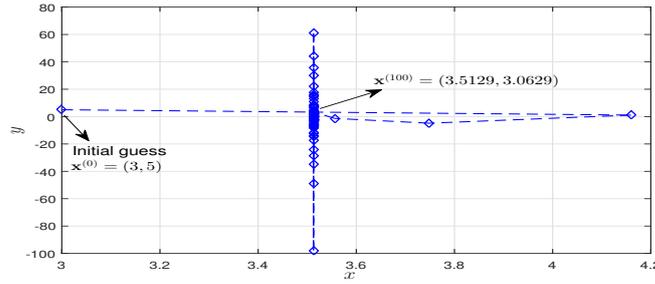


Figure 1: Convergence status of the classical Newton's method.

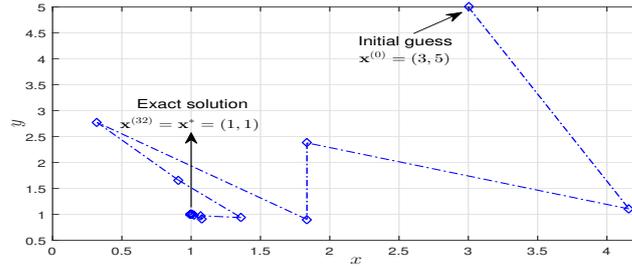


Figure 2: Convergence status of the proposed method.

4. Numerical results

This section is dedicated to the numerical examples. Two examples are considered and the effectiveness of the presented method compared with the classical Newton's method is checked. It is noted that, in the implementation of both classical Newton's and the proposed methods, we calculate the elements of the Jacobian matrix, $\mathbf{J}_F(\mathbf{x})$, via the central finite difference scheme as follows

$$\frac{\partial f_i(\mathbf{x})}{\partial x_j} \simeq \frac{f_i(\mathbf{x} + \mathbf{e}_j h) - f_i(\mathbf{x} - \mathbf{e}_j h)}{2h},$$

where, \mathbf{e}_j is the unit vector whose the j -th element is one and all other elements are zeros. Also, the stopping criterion is considered as $\|\mathbf{F}(\mathbf{x}^{(k)})\|_2 < 10^{-14}$. Furthermore, all computations are carried out on a 2.53 GHz Core i5 PC Laptop with 4 GB of RAM running in MATLAB R2016a.

4.1. Example 1

In the first example, a nonlinear system with two algebraic equations is considered [4, 5]. In this example, the system is described by

$$\begin{cases} x^2 + y^2 - 2 = 0, \\ e^{x-1} + y^2 - 2 = 0, \end{cases}$$

which has an exact solution $(x^*, y^*) = (1, 1)$. This is an exciting example because the iterations of Newton's method stagnate with an initial guess $\mathbf{x}^{(0)} = (3, 5)$ [4]. It means that, the search for the exact solution fails because the Jacobian of the system is singular at $(3.5192, 0)$. Now, the problem is solved using the proposed method starting with an initial guess $\mathbf{x}^{(0)} = (3, 5)$. The convergence status of both classical Newton's and the proposed methods is shown in Fig. 1 and Fig. 2. As we can see, after 100 iterations, the classical Newton's method obtains the approximation $\mathbf{x}^{(100)} = (3.5129, 3.0629)$ which is not close to the solution of the problem. Also, the oscillations around the point $(3.5192, 0)$ are seen when using the classical Newton's method. However, the proposed method converges to the exact solution after 32 iterations. Moreover, to demonstrate the efficiency of the proposed method, we restart this time with an initial guess $\mathbf{x}^{(0)} = (0, 0)$ in which the Jacobian of the system is also singular. It is seen that, while the classical Newton's method diverges immediately, the proposed method, as shown in Fig. 3, captures the exact solution after 25 iterations.

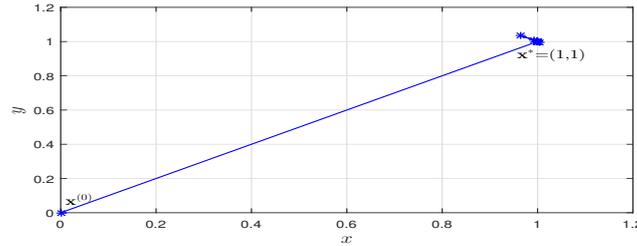


Figure 3: Convergence status of the proposed method, with an initial guess $\mathbf{x}^{(0)} = (0, 0)$.

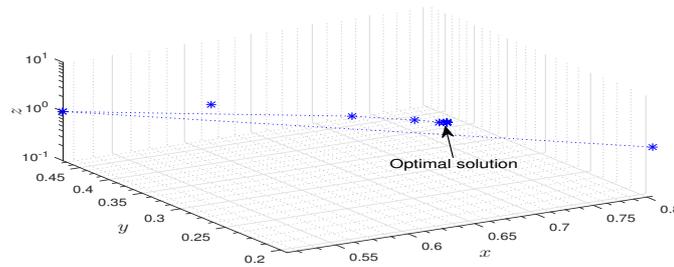


Figure 4: Convergence status of the proposed method, with an initial guess $\mathbf{x}^{(0)} = (0, 0, 1)$.

4.2. Example 2

This example is a nonlinear system with three algebraic equations [2]. In this example, the system is described by

$$\begin{cases} e^{x^2} - 8xy = 0, \\ x + y - 1 = 0, \\ (z - 1)^3 = 0, \end{cases}$$

and has an approximated solution, $(x^*, y^*, z^*) = (0.70854330022, 0.29145669978, 1)$. Now, the problem is solved using the classical Newton's and the proposed methods starting with an initial guess $\mathbf{x}^{(0)} = (0, 0, 1)$ in which the Jacobian of the system is singular. It is seen that, while the classical Newton's method diverges immediately, the proposed method, as shown in Fig. 4, captures the approximated solution after 29 iterations with the residual in the order of 10^{-11} .

5. Conclusion

In this paper, a differential continuation approach for nonlinear systems of algebraic equations with singular Jacobian was applied. It is found that, despite encountering the singular points, the proposed continuation approach succeeds as an effective procedure for tracing the optimal solution. Therefore, the difficulty of the classical Newton's method in dealing with the singular Jacobian systems is solved.

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