



Modified Newton's method for systems of nonlinear equations with singular Jacobian[☆]

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ABSTRACT

It is well known that Newton's method for a nonlinear system has quadratic convergence when the Jacobian is a nonsingular matrix in a neighborhood of the solution. Here we present a modification of this method for nonlinear systems whose Jacobian matrix is singular. We prove, under certain conditions, that this modified Newton's method has quadratic convergence. Moreover, different numerical tests confirm the theoretical results and allow us to compare this variant with the classical Newton's method.

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1. Introduction

Let us consider the problem of finding a real zero of a function $F : D \subseteq \mathbb{R}^n \rightarrow \mathbb{R}^n$, that is, a solution $\alpha \in D$ of the nonlinear system $F(x) = 0$. The most known iterative method is the classical Newton's method. For $n = 1$, this method converges quadratically if, between other conditions, the derivative is nonzero at the solution. Quadratic convergence can be reestablished for multiple roots by modifying the iteration function. If α is a zero of function F , with multiplicity $m > 1$, we can write $F(x) = (x - \alpha)^m h(x)$, with $h(\alpha) \neq 0$. In this case, the modified Newton's iteration

$$x_{k+1} = x_k - m \frac{F(x_k)}{F'(x_k)}, \quad k = 0, 1, \dots, \quad (1)$$

converges quadratically under certain conditions.

In recent papers (see [2,5]) methods for acceleration of iterative processes for solving a nonlinear equation with multiple roots have been presented. We will generalize the idea for nonlinear systems.

For $n > 1$ Newton's iteration is given by

$$x^{(k+1)} = x^{(k)} - J_F(x^{(k)})^{-1} F(x^{(k)}), \quad k = 0, 1, \dots,$$

where $J_F(x)$ is the Jacobian matrix of F . This method requires that the Jacobian matrix is nonsingular in a neighborhood of α , in order to get quadratic convergence. This condition restricts to some extent the application of Newton's method.

For this reason, in [3,8] the authors propose variants of Newton's method which converge quadratically in spite of the Jacobian matrix being singular in some iterations.

In this paper, we present a modified Newton's method for nonlinear systems $F(x) = 0$, allowing that the Jacobian matrix to be singular at the solution α .

Now, we recall some notions about the convergence of an iterative method.

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Definition 1. Let $\{x^{(k)}\}_{k \geq 0}$ be a sequence in \mathbb{R}^n convergent to α . Then, the convergence is said to be

(a) *linear*, if there exists M , $0 < M < 1$, and k_0 such that

$$\|x^{(k+1)} - \alpha\| \leq M \|x^{(k)} - \alpha\|, \quad \forall k \geq k_0.$$

(b) *of order p* , $p \geq 2$, if there exists M , $M > 0$, and k_0 such that

$$\|x^{(k+1)} - \alpha\| \leq M \|x^{(k)} - \alpha\|^p, \quad \forall k \geq k_0.$$

Proposition 1 (See [7]). Let α be a zero of the function F and suppose that $x^{(k-1)}$, $x^{(k)}$ and $x^{(k+1)}$ are three consecutive iterations close to α . Then, the computational order of convergence ρ can be approximated using the formula

$$\rho \approx \frac{\ln(\|x^{(k+1)} - \alpha\| / \|x^{(k)} - \alpha\|)}{\ln(\|x^{(k)} - \alpha\| / \|x^{(k-1)} - \alpha\|)}. \quad (2)$$

Since the iterative methods that we propose can be considered as iterative fixed point methods, we study their convergence by using the following result.

Theorem 1 ([6]). Let $G(x)$ be a fixed point function with continuous partial derivatives of order p with respect to all components of x . The iterative method $x^{(k+1)} = G(x^{(k)})$ is of order p if

$$\begin{aligned} G(\alpha) &= \alpha; \\ \frac{\partial^k g_i(\alpha)}{\partial x_{j_1} \partial x_{j_2} \dots \partial x_{j_k}} &= 0, \quad \text{for all } 1 \leq k \leq p-1, 1 \leq i, j_1, \dots, j_k \leq n; \\ \frac{\partial^p g_i(\alpha)}{\partial x_{j_1} \partial x_{j_2} \dots \partial x_{j_p}} &\neq 0, \quad \text{for at least one value of } i, j_1, \dots, j_p, \end{aligned}$$

where g_i , $i = 1, 2, \dots, n$, are the component functions of G .

The rest of the paper is structured as follows. In Section 2 we prove the quadratic convergence of the modified Newton's method for systems of a particular form. In Section 3 we extend the modified Newton's method for general nonlinear systems whose Jacobian matrix is singular at the solution. We prove that, under certain conditions, this method has quadratic convergence. The last section is devoted to the numerical results obtained by applying the described methods to several nonlinear systems. From this results we compare the different methods, confirming the theoretical results.

We denote by $\text{diag}(d_i)$ the $n \times n$ diagonal matrix whose main diagonal entries are d_1, d_2, \dots, d_n .

2. A modification of Newton's method

The performance of Newton's method for a nonlinear system degrades if the Jacobian matrix is singular at the solution. Following the idea of the modified Newton's method for multiple roots in the scalar case (1), we replace the fixed point function

$$G(x) = x - (J_F(x))^{-1} F(x) \quad (3)$$

by the modified iteration function

$$\widehat{G}(x) = x - (J_F(x))^{-1} M F(x), \quad (4)$$

where M is a diagonal matrix that allows to reestablish quadratic convergence, under some conditions.

In the following result we consider a particular case where the elements of matrix M can be determined analytically. Let us suppose that there exist integers $p_i \geq 1$ and real functions h_i , $i = 1, 2, \dots, n$, such that the component functions of F can be expressed as

$$f_i(x) = (x_i - \alpha_i)^{p_i} h_i(x), \quad i = 1, 2, \dots, n, \quad (5)$$

where $h_i(\alpha) \neq 0$, $i = 1, 2, \dots, n$, and $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_n)^T$ is a solution of $F(x) = 0$.

Theorem 2. Let $F : D \subseteq \mathbb{R}^n \rightarrow \mathbb{R}^n$ and $\alpha = (\alpha_1, \dots, \alpha_n)^T \in D$ a solution of the nonlinear system $F(x) = 0$. Suppose that there exist integers $p_i \geq 1$, $i = 1, 2, \dots, n$, such that the i -th component of $F(x)$ can be expressed as (5), with $h_i(\alpha) \neq 0$, and $h_i(x) \in C^2(D)$. Then there exists a subset $S \subseteq D$ such that, if we choose $x^{(0)} \in S$, the fixed point function $\widehat{G}(x)$ given by (4), with $M = \text{diag}(p_i)$, has quadratic convergence in S .

Proof. The Jacobian matrix $J_F(x)$ can be expressed as the product of two matrices

$$J_F(x) = A(x)B(x),$$

where

$$A(x) = \text{diag}((x_i - \alpha_i)^{p_i-1})$$

and

$$B(x) = \begin{pmatrix} p_1 h_1 + (x_1 - \alpha_1) \frac{\partial h_1}{\partial x_1} & (x_1 - \alpha_1) \frac{\partial h_1}{\partial x_2} & \dots & (x_1 - \alpha_1) \frac{\partial h_1}{\partial x_n} \\ (x_2 - \alpha_2) \frac{\partial h_2}{\partial x_1} & p_2 h_2 + (x_2 - \alpha_2) \frac{\partial h_2}{\partial x_2} & \dots & (x_2 - \alpha_2) \frac{\partial h_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ (x_n - \alpha_n) \frac{\partial h_n}{\partial x_1} & (x_n - \alpha_n) \frac{\partial h_n}{\partial x_2} & \dots & p_n h_n + (x_n - \alpha_n) \frac{\partial h_n}{\partial x_n} \end{pmatrix}.$$

Obviously, matrix $A(x)$ is invertible in the subset S_1 of D such that $x_i \neq \alpha_i, \forall i = 1, \dots, n$, and matrix $B(x)$ is invertible in a neighborhood S_2 of α since,

$$B(\alpha) = \text{diag}(p_i h_i(\alpha))$$

and so we get

$$|B(\alpha)| = \prod_{i=1}^n p_i h_i(\alpha) \neq 0. \quad (6)$$

So, by continuity $B(x)$ is nonsingular in the neighborhood S_2 of α . Then $J_F(x)$ is nonsingular in $S = S_1 \cap S_2$ and

$$(J_F(x))^{-1} = B^{-1}(x)A^{-1}(x).$$

Consider the iteration function $\widehat{G}(x) = x - (J_F(x))^{-1}MF(x)$, where $M = \text{diag}(m_i)$ has to be determined in order to get quadratic convergence. In these terms, we have

$$\begin{aligned} \widehat{G}(x) &= x - B^{-1}(x) \text{diag}((x_i - \alpha_i)^{1-p_i}) M \begin{pmatrix} (x_1 - \alpha_1)^{p_1} h_1(x) \\ (x_2 - \alpha_2)^{p_2} h_2(x) \\ \vdots \\ (x_n - \alpha_n)^{p_n} h_n(x) \end{pmatrix} \\ &= x - B^{-1}(x) \begin{pmatrix} m_1 (x_1 - \alpha_1) h_1(x) \\ m_2 (x_2 - \alpha_2) h_2(x) \\ \vdots \\ m_n (x_n - \alpha_n) h_n(x) \end{pmatrix}. \end{aligned} \quad (7)$$

If $B_{ij}(x)$ represents the adjoint of the element (i, j) of matrix $B(x)$, the inverse matrix has the expression

$$B^{-1}(x) = \frac{1}{|B(x)|} (B_{ji}(x))$$

and substituting in (7) it can be concluded that the associated fixed point function $\widehat{g}_i(x)$ is

$$\widehat{g}_i(x) = x_i - \frac{1}{|B(x)|} \sum_{j=1}^n m_j B_{ji}(x) (x_j - \alpha_j) h_j(x) = x_i - \sum_{j=1}^n (x_j - \alpha_j) H_j(x),$$

where we have taken $H_j(x) = m_j B_{ji}(x) h_j(x) / |B(x)|$ in order to simplify the notation. Observe that $\widehat{g}_i(\alpha) = \alpha_i$ since $|B(\alpha)| \neq 0$ and so $H_j(\alpha)$ is well defined.

By direct differentiation with respect to x_i we get

$$\frac{\partial \widehat{g}_i(x)}{\partial x_i} = 1 - H_i(x) - \sum_{j=1}^n (x_j - \alpha_j) \frac{\partial H_j(x)}{\partial x_j}.$$

Taking into account that $H_j(x)$ is a linear combination of functions with continuous derivatives in S , the last term is zero in $x = \alpha$. Then

$$\frac{\partial \widehat{g}_i(\alpha)}{\partial x_i} = 1 - H_i(\alpha) = 1 - m_i \frac{B_{ii}(\alpha) h_i(\alpha)}{|B(\alpha)|}. \quad (8)$$

From expression of $B(\alpha)$, we deduce the form of the adjoint

$$B_{ii}(\alpha) = \prod_{j \neq i} p_j h_j(\alpha).$$

By substituting in (8) and using (6) we have

$$\frac{\partial \widehat{g}_i(\alpha)}{\partial x_i} = 1 - m_i \frac{\prod_{j \neq i} p_j h_j(\alpha) h_i(\alpha)}{\prod_{j=1}^n p_j h_j(\alpha)} = 1 - m_i \frac{1}{p_i}. \quad (9)$$

By taking $m_i = p_i$ we get

$$\frac{\partial \widehat{g}_i(\alpha)}{\partial x_i} = 0.$$

On the other hand, for all $k = 1, 2, \dots, n, k \neq i$

$$\frac{\partial \widehat{g}_i(x)}{\partial x_k} = -H_k(x) - \sum_{j=1}^n (x_j - \alpha_j) \frac{\partial H_j(x)}{\partial x_k}.$$

The last term is zero in α , as we have commented for getting (8) and

$$H_k(x) = m_k \frac{B_{ki}(x) h_k(x)}{|B(x)|}.$$

Setting $x = \alpha$ obviously the adjoint $B_{ki}(\alpha) = 0$, then $H_k(\alpha) = 0$ since $|B(\alpha)| \neq 0$. So we have

$$\frac{\partial \widehat{g}_i(\alpha)}{\partial x_k} = 0.$$

Therefore, by applying Theorem 1 the iterates $x^{(k+1)} = \widehat{G}(x^{(k)})$ converge at least quadratically in S . \square

Theorem 2 states that for systems of the form (5) taking $m_i = p_i, i = 1, 2, \dots, n$, the iteration (4) converges at least quadratically.

The main diagonal entries of matrix M are called *weights*. If M is the identity matrix, the iteration (4) is Newton's method. In addition, if we apply Newton's iteration function $G(x) = (g_1(x), \dots, g_n(x))^T$ to a system of the form (5), the proof of Theorem 2 shows that

$$\frac{\partial g_i(\alpha)}{\partial x_i} = 1 - \frac{1}{p_i}$$

and, in this case, the weights are

$$m_i = p_i = \frac{1}{1 - \frac{\partial g_i(\alpha)}{\partial x_i}}.$$

The iterative method

$$\widehat{G}(x) = x - (J_F(x))^{-1} M F(x),$$

can be applied to a general system $F(x) = 0$ by defining

$$m_i = \frac{1}{1 - \frac{\partial g_i(\alpha)}{\partial x_i}}, \quad (10)$$

where $G(x) = (g_1(x), \dots, g_n(x))^T = x - (J_F(x))^{-1} F(x)$. We will refer to it as modified Newton's method (MN). Numerical examples from (c)–(f) show that the number of iterations used by modified Newton's method is smaller than that of Newton's method.

Most papers trying to accelerate the convergence when approaching a singular root establish a connection between multiplicity and the rank of the Jacobian matrix (see, for example, [1] and [4]). In our case for systems of the form (5) it is easy to observe that if $p_i > 1, i = 1, 2, \dots, n$, then $\text{rank}(J_F(\alpha)) = 0$, and if the number of integers p_i greater than 1 is m , then $\text{rank}(J_F(\alpha)) = n - m$.

3. A generalization of the method

In [3,8], the authors establish the following iterate method

$$x^{(k+1)} = x^{(k)} - (\text{diag}(v_i f_i(x^{(k)})) + J_F(x^{(k)}))^{-1} F(x^{(k)}), \quad k = 0, 1, \dots$$

in order to find a zero of a nonlinear system $F(x) = 0$, permitting the Jacobian matrix to be singular in some points. In this section we generalize this iteration for finding a root of a system with singular Jacobian at the solution.

Given the nonlinear system

$$F(x) = 0, \quad (11)$$

where

$$F(x) = (f_1(x), \dots, f_n(x))^T$$

for which $F(\alpha) = 0$ and $|J_F(\alpha)| = 0$, let us consider a new system

$$\hat{F}(x) = (e^{v_1 x_1} f_1(x)^{\frac{1}{m_1}}, \dots, e^{v_n x_n} f_n(x)^{\frac{1}{m_n}}) = 0, \quad (12)$$

where $m_i > 0$, $i = 1, 2, \dots, n$ are given by (10) and $v_i \in \mathbb{R}$, $i = 1, 2, \dots, n$ are chosen in order to obtain $|J_{\hat{F}}(\alpha)| \neq 0$. Notice that, for systems of the form (5), by taking $v_i = 0$, $i = 1, 2, \dots, n$, the condition is satisfied.

Obviously, system (11) is equivalent to (12), so applying Newton's method to system (12) we have

$$x^{(k+1)} = x^{(k)} - (J_{\hat{F}}(x^{(k)}))^{-1} \hat{F}(x^{(k)}). \quad (13)$$

The Jacobian matrix of $\hat{F}(x)$ can be written as follows

$$J_{\hat{F}}(x) = \text{diag}\left(e^{v_i x_i} \frac{1}{m_i} f_i(x)^{\frac{1}{m_i}-1}\right) (\text{diag}(v_i m_i f_i(x)) + J_F(x)).$$

Then Newton's iteration yields

$$\begin{aligned} x^{(k+1)} &= x^{(k)} - (\text{diag}(v_i m_i f_i(x^{(k)})) + J_F(x^{(k)}))^{-1} \text{diag}(m_i e^{-v_i x_i} f_i(x^{(k)})^{1-\frac{1}{m_i}}) \hat{F}(x^{(k)}) \\ &= x^{(k)} - (\text{diag}(v_i m_i f_i(x^{(k)})) + J_F(x^{(k)}))^{-1} \text{diag}(m_i) F(x^{(k)}). \end{aligned} \quad (14)$$

We will refer to this iteration formula as *generalized Newton's method (GN)*. The modified Newton's method (4) is a particular case of (14), by taking $v_i = 0$, $i = 1, 2, \dots, n$. The main difference between methods *MN* and *GN* is that *GN* allows a higher degree of freedom in parameters v_i in order to obtain convergent iterates.

In the following theorem we study the convergence of method *GN*. We use in it the same notation for the n -dimensional case as for the one-dimensional case by simply interpreting the symbols appropriately.

Theorem 3. Under the above mentioned conditions, if $f_i(x) \in C^2(D) : D \subseteq \mathbb{R}^n$, $\alpha \in D$ and $x^{(0)}$ is chosen sufficiently close to the solution, then the method defined by (14) has quadratic convergence.

Proof. Taylor's series of $\hat{F}(x)$ about $x^{(k)}$ is

$$\hat{F}(x) = \hat{F}(x^{(k)}) + \hat{F}'(x^{(k)})(x - x^{(k)}) + O(\|x - x^{(k)}\|^2).$$

Setting $x = \alpha$ we obtain

$$0 = \hat{F}(\alpha) = \hat{F}(x^{(k)}) + \hat{F}'(x^{(k)})(\alpha - x^{(k)}) + O(\|\alpha - x^{(k)}\|^2)$$

and replacing $e^{(k)} = x^{(k)} - \alpha$ it results

$$\hat{F}(x^{(k)}) = \hat{F}'(x^{(k)})e^{(k)} - O(\|e^{(k)}\|^2). \quad (15)$$

Adding the term $-\alpha$ in both sides of (13) and using (15) we have

$$e^{(k+1)} = e^{(k)} - \hat{F}'(x^{(k)})^{-1} [\hat{F}'(x^{(k)})e^{(k)} - O(\|e^{(k)}\|^2)].$$

Therefore, by the nonsingularity of the Jacobian matrix in a neighborhood of α , we have the quadratic convergence of the method

$$e^{(k+1)} = O(\|e^{(k)}\|^2). \quad \square$$

Table 1
Numerical results for different methods

System		(a)	(b)	(c)	(d)	(e)	(f)
$x^{(0)}$		(1.5, 2.5)	(2, 1, -2)	(0.7, 0.7)	(-0.5, 0.5)	(0.2, 0.2, -0.2)	(0, 1, 2)
m		(2, 5)	(4, 5, 6)	(2, 1)	(4, 1)	(1, 2, 1)	(1, 1, 3)
Iter	CN	108	143	28	91	37	67
	MN	7	6	5	5	NC	6
	GN ($v_i = 1.1$)	6	8	7	8	9	8
	GN ($v_i = 1$)	6	8	6	8	9	7
	GN ($v_i = 0.01$)	7	6	5	4	NC	6
ρ	CN	1.0	1.0	1.0	1.0	1.0	1.0
	MN	2.0	2.0	2.0	1.2	–	1.8
	GN ($v_i = 1.1$)	2.0	2.0	2.0	2.0	1–2 ^a	1.9
	GN ($v_i = 1$)	2.0	2.0	2.0	2.0	1–2 ^a	1.6
	GN ($v_i = 0.01$)	2.0	2.0	2.0	1.6	–	1.8

^a During the first steps ρ is between the indicated values.

4. Numerical results

In this section we check the effectiveness of the methods *MN* and *GN* compared with classical Newton's method. The considered systems present singular Jacobian at the solution. Examples (a) and (b) verify the hypothesis of [Theorem 2](#), whereas examples from (c) to (f) are of a general form. In this case, the values of the weights m_i are obtained from (10) by symbolic computation in MATLAB.

$$\begin{aligned}
 \text{(a)} \quad & \begin{cases} (x-1)^2(x-y) = 0 \\ (y-2)^5 \cos(2x/y) = 0 \end{cases} & \text{(b)} \quad & \begin{cases} (x-1)^4 e^y = 0 \\ (y-2)^5 (xy-1) = 0 \\ (z+4)^6 = 0 \end{cases} \\
 \text{(c)} \quad & \begin{cases} e^x - y - 1 = 0 \\ x - y = 0 \end{cases} & \text{(d)} \quad & \begin{cases} (6x-y)^4 = 0 \\ \cos(x) - 1 + y = 0 \end{cases} \\
 \text{(e)} \quad & \begin{cases} 3x - \cos(yz) - 0.5 = 0 \\ x^2 - 625y^2 - 0.25 = 0 \\ e^{-xy} + 20z + (10\pi - 3)/3 = 0 \end{cases} & \text{(f)} \quad & \begin{cases} e^{x^2} - 8x \sin(y) = 0 \\ x + y - 1 = 0 \\ (z-1)^3 = 0 \end{cases}
 \end{aligned}$$

whose solutions are, respectively:

- (a) (1, 2)
- (b) (1, 2, -4)
- (c) (0, 0)
- (d) (0, 0)
- (e) (0.5, 0, $-\pi/6$)
- (f) (0.175599, 0.824401, 1).

Numerical computations have been carried out in double precision in MATLAB 7.1.

The stopping criterion used is $\|x^{(k+1)} - x^{(k)}\| + \|F(x^{(k)})\| < 10^{-12}$. Therefore, we check that the iterates converge to a limit and that this limit is a solution of the nonlinear system. For every method, we analyze the number of iterations needed to converge to the solution and the computational order of convergence ρ , approximated by (2). The value of ρ that appears in [Table 1](#) is the last coordinate of vector ρ when the variation between its coordinates is small. In some cases, the computational order of convergence is not stable and we consider it not conclusive. In this cases it does not appear in the table.

In [Table 1](#), several results obtained by using classical Newton's method, *CN*, and methods *MN* and *GN* in order to estimate the zeros of nonlinear systems from (a) to (f) can be observed. For every system we specify the initial estimation $x^{(0)}$ and, for each method, the number of iterations and the estimated computational order of convergence ρ . For method *GN* we take a vector $v = (v_1, v_2, \dots, v_n)$ with $v_1 = v_2 = \dots = v_n$ and different values for these components.

We can observe that, in general, the number of iterations of new methods *MN* and *GN* is smaller than that of Newton's method. In addition, whereas the computational order of convergence of Newton's method is 1.0, the corresponding of the new methods is near to 2. However, the modified Newton's method tends to be numerically unstable, even in the one-dimensional case.

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