Computing 74, 23–39 (2005)
Digital Object Identifier (DOI) 10.1007/s00607-004-0083-1

Computing
Printed in Austria

On the Quadratic Convergence of the Levenberg-Marquardt Method without Nonsingularity Assumption

Jin-yan Fan and **Ya-xiang Yuan,** Beijing

Received October 16, 2001; revised March 9, 2004
Published online: January 10, 2005

Abstract

Recently, Yamashita and Fukushima [11] established an interesting quadratic convergence result for the Levenberg-Marquardt method without the nonsingularity assumption. This paper extends the result of Yamashita and Fukushima by using $\mu_k = \|F(x_k)\|^{\delta}$, where $\delta \in [1, 2]$, instead of $\mu_k = \|F(x_k)\|^2$ as the Levenberg-Marquardt parameter. If $\|F(x)\|$ provides a local error bound for the system of nonlinear equations $F(x) = 0$, it is shown that the sequence $\{x_k\}$ generated by the new method converges to a solution quadratically, which is stronger than $dist(x_k, X^*) \to 0$ given by Yamashita and Fukushima. Numerical results show that the method performs well for singular problems.

AMS Subject Classifications: 34G20, 65K05, 90C30.

Keywords: Nonlinear equations, Levenberg-Marquardt method, quadratic convergence.

1. Introduction

We consider the problem for solving nonlinear equations

$$F(x) = 0, \tag{1.1}$$

where $F(x) : R^n \to R^m$ is continuously differentiable and $F'(x)$ is Lipschitz continuous. Throughout the paper, we assume that the solution set of (1.1) is nonempty and denote it by X^*. And in all cases $\|\cdot\|$ refers to the 2-norm.

The classical Levenberg-Marquardt method (see [2], [3]) for nonlinear Eqs. (1.1) computes the trial step by

$$d_k = -(J(x_k)^T J(x_k) + \mu_k I)^{-1} J(x_k)^T F(x_k), \tag{1.2}$$

where $J(x_k) = F'(x_k)$ is the Jacobian, and $\mu_k \geq 0$ is a parameter being updated from iteration to iteration. Levenberg-Marquardt step (1.2) is a modification of the Gauss-Newton's step

$$d_k^{GN} = -(J(x_k)^T J(x_k))^{-1} J(x_k)^T F(x_k). \tag{1.3}$$

The parameter μ_k is used to prevent d_k from being too large when $J(x_k)^T J(x_k)$ is nearly singular. Furthermore, when $J(x_k)^T J(x_k)$ is singular, the Gauss-Newton's step is undefined. A positive μ_k guarantees that (1.2) is well defined.

It is well known that the Levenberg-Marquardt method has a quadratic rate of convergence when $m = n$, if the Jacobian at the solution x^* is nonsingular and if the parameter is chosen suitably at each step. However, the condition of the nonsingularity of $J(x^*)$ is too strong. Recently, Yamashita and Fukushima [11] have shown that under the weaker condition that $\|F(x)\|$ provides a local error bound near the solution, the Levenberg-Marquardt method still has a quadratic conver gence if the parameter is chosen as $\mu_k = \|F(x_k)\|^2$. This is a very interesting result. However, the quadratic term $\mu_k = \|F(x_k)\|^2$ has some unsatisfactory properties. When the sequence is close to the solution set, $\mu_k = \|F(x_k)\|^2$ may be smaller than the machine precision, so it will lose its role. On the other hand, when the sequence is far away from the solution set, $\mu_k = \|F(x_k)\|^2$ may be very large, and the step d_k will be too small, consequently, it prevents the iterates moving to the solution set quickly. Because of these observations, we consider the choice $\mu_k = \|F(x_k)\|^\delta$ with $\delta \in [1, 2]$. We prove that with this parameter, if $\|F(x)\|$ provides a local error bound near some $x^* \in X$, then the sequence $\{x_k\}$ generated by the new Levenberg-Marquardt method converges quadratically to the solution of (1.1), that is

$$\|x_{k+1} - \bar{x}\| \leq Q\|x_k - \bar{x}\|^2$$

holds for all sufficiently large k, where $\bar{x} \in X^*$ and $Q > 0$ is a positive constant.

Definition 1.1: *Let N be a subset of R^n such that $N \cap X^* \neq \emptyset$. We say that $\|F(x)\|$ provides a local error bound on N for system (1.1), if there exists a positive constant $c > 0$ such that*

$$\|F(x)\| \geq c\,dist(x, X^*), \qquad \forall x \in N.$$

Note that, if $J(x^*)$ is nonsingular at a solution x^* of (1.1), then x^* is an isolated solution, hence $\|F(x)\|$ provides a local error bound on some neighborhood of x^*. However, the converse is not necessarily true, see the example in [11]. So a local error bound condition is weaker than that of the nonsingularity.

In the next section, we show that under the local error bound condition, the sequence generated by the new Levenberg-Marquardt method without line search converges to the solution quadratically. In Sect. 3, the global convergence result is given when the line search is used. Finally in Sect. 4, we present the numerical results for some singular nonlinear equations.

2. Local Convergence of the Levenberg-Marquardt Method

To study the convergence properties of the method, we make the following assumptions.

Assumption 2.1: *(a) $F(x)$ is continuously differentiable, and the Jacobian $J(x)$ is Lipschitz continuous on some neighborhood of $x^* \in X^*$, i.e., there exist positive constants L_1 and $b_1 < 1$ such that*

$$\|J(y) - J(x)\| \leq L_1 \|y - x\|, \qquad \forall x, y \in N(x^*, b_1) = \{x \mid \|x - x^*\| \leq b_1\}. \tag{2.1}$$

(b) $\|F(x)\|$ provides a local error bound on $N(x^*, b_1)$ for the system (1.1), i.e., there exists a constant $c_1 > 0$ such that

$$\|F(x)\| \geq c_1 dist(x, X^*), \qquad \forall x \in N(x^*, b_1). \tag{2.2}$$

Note that, by Assumption 2.1a, we have

$$\|F(y) - F(x) - J(x)(y - x)\| \leq L_1 \|y - x\|^2, \qquad \forall x, y \in N(x^*, b_1), \tag{2.3}$$

and, there exists a constant $L_2 > 0$ such that

$$\|F(y) - F(x)\| \leq L_2 \|y - x\|, \qquad \forall x, y \in N(x^*, b_1). \tag{2.4}$$

We discuss the local convergence of the Levenberg-Marquardt method without line search, i.e., the next iterate x_{k+1} is computed by

$$x_{k+1} = x_k + d_k,$$

where d_k is given by (1.2). For simplification, we use the notations $F_k = F(x_k), J_k = J(x_k)$ in the following. And we assume

Assumption 2.2:

$$\mu_k = \|F_k\|^\delta \textit{ for all } k, \quad \textit{where } \delta \in [1, 2].$$

Yamashita and Fukushima [11] show the quadratic convergence of the Levenberg-Marquardt method when choosing $\mu_k = \|F_k\|^2$, based the analyses on an unconstrained optimization problem. Here, we first prove the superlinear convergence of the new Levenberg-Marquardt method when choosing $\mu_k = \|F_k\|^\delta$, then, based on the singular value decomposition of the Jacobian matrix, we obtain the quadratic convergence. In the following, we denote $\bar{x}_k$ the vector in X^* that satisfies

$$\|x_k - \bar{x}_k\| = \text{dist}(x_k, X^*).$$

Lemma 2.1: *Under the conditions of Assumptions 2.1 and 2.2, if $x_k \in N(x^*, b_1/2)$, then there exists a constant $c_2 > 0$ such that*

$$\|d_k\| \leq c_2 dist(x_k, X^*). \tag{2.5}$$

Proof: Since $x_k \in N(x^*, b_1/2)$, we have

$$\|\bar{x}_k - x^*\| \le \|\bar{x}_k - x_k\| + \|x_k - x^*\| \le \|x_k - x^*\| + \|x_k - x^*\| \le b_1,$$

which means that $\bar{x}_k \in N(x^*, b_1)$. Hence it follows from (2.2) and (2.4) that the Levenberg-Marquardt parameter μ_k satisfies

$$c_1^\delta \|\bar{x}_k - x_k\|^\delta \le \mu_k = \|F_k\|^\delta \le L_2^\delta \|\bar{x}_k - x_k\|^\delta. \tag{2.6}$$

Define

$$\varphi_k(d) = \|F_k + J_k d\|^2 + \mu_k \|d\|^2.$$

It follows from (1.2) that d_k is a stationary point of $\varphi_k(d)$. Hence the convexity of $\varphi_k(d)$ indicates that d_k is also a minimizer of $\varphi_k(d)$. Thus, using $\bar{x}_k \in N(x^*, b_1)$ and $b_1 < 1$, we have

$$\begin{aligned}
\|d_k\|^2 &\le \frac{\varphi_k(d_k)}{\mu_k} \\
&\le \frac{\varphi_k(\bar{x}_k - x_k)}{\mu_k} \\
&= \frac{\|F_k + J_k(\bar{x}_k - x_k)\|^2 + \mu_k \|\bar{x}_k - x_k\|^2}{\mu_k} \\
&\le L_1^2 c_1^{-\delta} \|\bar{x}_k - x_k\|^{4-\delta} + \|\bar{x}_k - x_k\|^2 \\
&\le (L_1^2 c_1^{-\delta} + 1) \|\bar{x}_k - x_k\|^2.
\end{aligned}$$

The above inequality implies that

$$\|d_k\| \le c_2 \ \mathrm{dist}(x_k, X^*),$$

where $c_2 = \sqrt{L_1^2 c_1^{-\delta} + 1}$. □

Lemma 2.2: *Under the conditions of Assumptions 2.1 and 2.2, if* $x_{k+1}, x_k \in N(x^*, b_1/2)$, *then we have*

$$dist(x_k + d_k, X^*) \le c_3 \ \mathrm{dist}(x_k, X^*)^{\frac{2+\delta}{2}}, \tag{2.7}$$

where $c_3 = \left(\sqrt{L_1^2 + L_2^\delta} + L_1 c_2^2\right)/c_1$.

Proof: Since

$$\begin{aligned}
\varphi_k(d_k) &\le \varphi_k(\bar{x}_k - x_k) \\
&= \|F_k + J_k(\bar{x}_k - x_k)\|^2 + \mu_k \|\bar{x}_k - x_k\|^2 \\
&\le L_1^2 \|\bar{x}_k - x_k\|^4 + L_2^\delta \|\bar{x}_k - x_k\|^{2+\delta} \\
&\le (L_1^2 + L_2^\delta) \|\bar{x}_k - x_k\|^{2+\delta},
\end{aligned}$$

we have

$$\begin{aligned}\|F(x_k+d_k)\| &\le \|F_k+J_kd_k\|+L_1\|d_k\|^2\\ &\le \sqrt{\varphi_k(d_k)}+L_1\|d_k\|^2\\ &\le \sqrt{L_1^2+L_2^\delta}\|\bar{x}_k-x_k\|^{\frac{2+\delta}{2}}+L_1c_2^2\|\bar{x}_k-x_k\|^2\\ &\le \left(\sqrt{L_1^2+L_2^\delta}+L_1c_2^2\right)\|\bar{x}_k-x_k\|^{\frac{2+\delta}{2}}.\end{aligned}$$

Hence

$$\operatorname{dist}(x_k+d_k,X^*)\le \frac{1}{c_1}\|F(x_k+d_k)\|\le c_3\ \operatorname{dist}(x_k,X^*)^{\frac{2+\delta}{2}},$$

where $c_3=\left(\sqrt{L_1^2+L_2^\delta}+L_1c_2^2\right)/c_1$. The proof is completed. □

Theorem 2.1: *Under the conditions of Assumptions 2.1 and 2.2, if x_0 is chosen sufficiently close to X^*, then $\{x_{k+1}=x_k+d_k\}$ converges to some solution $\bar{x}$ of (1.1) superlinearly.*

Proof: Let $r=\min\left\{\frac{b_1}{2(1+11c_2)},\frac{1}{2c_3^{\frac{2}{\delta}}}\right\}$. First we show by induction that if $x_0\in N(x^*,r)$, then $x_k\in N(x^*,b_1/2)$ for all k. It follows from Lemma 2.1 that

$$\begin{aligned}\|x_1-x^*\| &= \|x_0+d_0-x^*\|\le\|x_0-x^*\|+\|d_0\|\\ &\le \|x_0-x^*\|+c_2\|x_0-\bar{x}_0\|\le(1+c_2)r\le b_1/2,\end{aligned}$$

which means $x_1\in N(x^*,b_1/2)$. Suppose $x_i\in N(x^*,b_1/2)$ for $i=2,\dots,k$. Then we have from Lemma 2.2 that

$$\|x_i-\bar{x}_i\|\le c_3\|x_{i-1}-\bar{x}_{i-1}\|^{\frac{2+\delta}{2}}\le\dots\le c_3^{\frac{2}{\delta}\left(\left(\frac{2+\delta}{2}\right)^i-1\right)}\|x_0-x^*\|^{\left(\frac{2+\delta}{2}\right)^i}\le r\left(\frac{1}{2}\right)^{\left(\frac{2+\delta}{2}\right)^i-1}\le 2r\left(\frac{1}{2}\right)^{\left(\frac{3}{2}\right)^i}.$$

Hence, it follows from the definition of r that

$$\begin{aligned}\|x_{k+1}-x^*\| &\le \|x_1-x^*\|+\sum_{i=1}^{k}\|d_k\|\\ &\le (1+c_2)r+c_2\sum_{i=1}^{k}\|x_i-\bar{x}_i\|\\ &\le (1+c_2)r+2rc_2\sum_{i=1}^{k}\left(\frac{1}{2}\right)^{\left(\frac{3}{2}\right)^i}\\ &\le (1+c_2)r+2rc_2\left(4+\sum_{i=1}^{k}\left(\frac{1}{2}\right)^{\left(\frac{3i}{2}\right)}\right)\\ &\le (1+9c_2)r+2rc_2\sum_{i=1}^{\infty}\left(\frac{1}{2}\right)^{i}\\ &\le (1+11c_2)r\\ &\le b_1/2,\end{aligned}$$

so $x_{k+1} \in N(x^*, b_1/2)$. Therefore, if x_0 is chosen sufficiently close to X^*, then all x_k are in $N(x^*, b_1/2)$. Now it follows from (2.7) that

$$\sum_{k=0}^{\infty} \operatorname{dist}(x_k, X^*) < +\infty,$$

which implies, due to Lemma 2.1, that

$$\sum_{k=0}^{\infty} \|d_k\| < +\infty.$$

Thus $\{x_k\}$ converges to some point $\bar{x} \in X^*$. It is obvious that

$$\operatorname{dist}(x_k, X^*) \leq \operatorname{dist}(x_k + d_k, X^*) + \|d_k\|.$$

The above inequality and (2.7) imply that

$$\operatorname{dist}(x_k, X^*) \leq 2\|d_k\| \tag{2.8}$$

for all large k. Thus from (2.5), (2.7) and (2.8) we obtain that

$$\|d_{k+1}\| = O(\|d_k\|^{\frac{2+\delta}{2}}).$$

Hence, $\{x_k\}$ converges to some solution $\bar{x} \in X$. Therefore, we have

$$\lim_{k\to\infty} \frac{\|x_{k+1} - \bar{x}\|}{\|x_k - \bar{x}\|^{\frac{2+\delta}{2}}} = \lim_{k\to\infty} \frac{\|\sum_{j=k+1}^{\infty} d_j\|}{\|\sum_{j=k}^{\infty} d_j\|^{\frac{2+\delta}{2}}} = \lim_{k\to\infty} \frac{\|d_{k+1}\|}{\|d_k\|^{\frac{2+\delta}{2}}} \leq \tilde{c},$$

where $\tilde{c} \geq 0$ is a constant. The above inequality implies that $\{x_k\}$ converges to the solution $\bar{x}$ quadratically when $\delta = 2$ and superlinearly when $\delta \in [1, 2)$. $\square$

Without loss of generality, we assume that $\{x_k\}$ converges to $x^* \in X^*$, and the singular value decomposition (SVD) of $J(x^*)$ is

$$\begin{aligned} J(x^*) &= U^* \Sigma^* V^{*T} \\ &= U^* \begin{pmatrix} \sigma_1^* & & & & & \\ & \ddots & & & & \\ & & \sigma_r^* & & & \\ & & & 0 & & \\ & & & & \ddots & \\ & & & & & 0 \end{pmatrix} V^{*T} \\ &= U_1^* \Sigma_1^* V_1^{*T}, \end{aligned}$$

where $\sigma_1^* \geq \sigma_2^* \geq \ldots \geq \sigma_r^* > 0$ and $\operatorname{rank}(\Sigma_1^*) = r$. Suppose the SVD of $J(x_k)$ and its decomposition form is as follows:

$$
\begin{aligned}
J(x_k) &= U_k \Sigma_k V_k^T \\
&= (U_{k,1}, U_{k,2}, U_{k,3}) \begin{pmatrix} \sigma_1^{(k)} & & & & & & & & \\ & \ddots & & & & & & & \\ & & \sigma_r^{(k)} & & & & & & \\ & & & \sigma_{r+1}^{(k)} & & & & & \\ & & & & \ddots & & & & \\ & & & & & \sigma_{r+q}^{(k)} & & & \\ & & & & & & 0 & & \\ & & & & & & & \ddots & \\ & & & & & & & & 0 \end{pmatrix} \begin{pmatrix} V_{k,1}^T \\ V_{k,2}^T \\ V_{k,3}^T \end{pmatrix} \\
&= U_{k,1}\Sigma_{k,1}V_{k,1}^T + U_{k,2}\Sigma_{k,2}V_{k,2}^T,
\end{aligned}
\tag{2.9}
$$

where $\Sigma_{k,1}, \Sigma_{k,2} > 0$, $\operatorname{rank}(\Sigma_{k,1}) = r$ and $\operatorname{rank}(\Sigma_{k,2}) = q \geq 0$. In the following, if the context is clear, we supress the subscription k in $\Sigma_{k,i}$ and $U_{k,i}, V_{k,i} (i = 1, 2, 3)$. Consequently, (2.9) can be written as

$$J_k = U_1\Sigma_1V_1^T + U_2\Sigma_2V_2^T.$$

To prove quadratic convergence when $\delta \in [1, 2)$, we first give the following lemma.

Lemma 2.3: *Under the conditions of Assumption 2.1, if $x_k \in N(x^*, b_1/2)$, then we have*

(a) $\|U_1U_1^TF_k\| \leq L_2\|x_k - \bar{x}_k\|$;

(b) $\|U_2U_2^TF_k\| \leq 2L_1\|x_k - x^*\|^2$;

(c) $\|U_3U_3^TF_k\| \leq L_1\|x_k - \bar{x}_k\|^2$.

Proof: Result (a) follows immediately from (2.4). By the theory of matrix perturbation [10] and Assumption 2.1(a), we have

$$\|\operatorname{diag}(\Sigma_1 - \Sigma_1^*, \Sigma_2, 0)\| \leq \|J_k - J^*\| \leq L_1\|x_k - x^*\|.$$

The above relation gives

$$\|\Sigma_1 - \Sigma_1^*\| \leq L_1\|x_k - x^*\| \qquad \text{and} \qquad \|\Sigma_2\| \leq L_1\|x_k - x^*\|. \tag{2.10}$$

Let $s_k = -J_k^+F_k$, where J_k^+ is the pseudo-inverse of J_k. It is easy to see that s_k is the least squares solution of $\min\|F_k + J_ks\|$, so we obtain from (2.3) that

$$\|U_3U_3^TF_k\| = \|F_k + J_ks_k\| \leq \|F_k + J_k(\bar{x}_k - x_k)\| \leq L_1\|x_k - \bar{x}_k\|^2.$$

Let $\tilde{J}_k = U_1\Sigma_1 V_1^T$ and $\tilde{s}_k = -\tilde{J}_k^+ F_k$. Since $\tilde{s}_k$ is the least squares solution of $\min \|F_k + \tilde{J}_k s\|$, it follows from (2.3) and (2.10) that

$$\begin{aligned}
\|(U_2U_2^T + U_3U_3^T)F_k\| &= \|F_k + \tilde{J}_k\tilde{s}_k\| \\
&\le \|F_k + \tilde{J}_k(\bar{x}_k - x_k)\| \\
&\le \|F_k + J_k(\bar{x}_k - x_k)\| + \|(\tilde{J}_k - J_k)(\bar{x}_k - x_k)\| \\
&\le L_1\|\bar{x}_k - x_k)\|^2 + \|U_2\Sigma_2V_2^T(\bar{x}_k - x_k)\| \\
&\le L_1\|\bar{x}_k - x_k\|^2 + L_1\|x^* - x_k\|\|\bar{x}_k - x_k\| \\
&\le 2L_1\|x_k - x^*\|^2.
\end{aligned}$$

Due to the orthogonality of U_2 and U_3, we get result (b). □

Theorem 2.2: *Under the conditions of Assumptions 2.1 and 2.2, if the sequence $\{x_k\}$ is generated by the new Levenberg-Marquardt method without line search with x_0 sufficiently close to x^*, then $\{x_k\}$ converges to the solution of (1.1) quadratically.*

Proof: By the SVD of J_k, we know the step at the current iterate is

$$d_k = -V_1(\Sigma_1^2 + \mu_k I)^{-1}\Sigma_1 U_1^T F_k - V_2(\Sigma_2^2 + \mu_k I)^{-1}\Sigma_2 U_2^T F_k. \tag{2.11}$$

So we have

$$\begin{aligned}
F_k + J_k d_k &= F_k - U_1\Sigma_1(\Sigma_1^2 + \mu_k I)^{-1}\Sigma_1 U_1^T F_k - U_2\Sigma_2(\Sigma_2^2 + \mu_k I)^{-1}\Sigma_2 U_2^T F_k \\
&= \mu_k U_1(\Sigma_1^2 + \mu_k I)^{-1} U_1^T F_k + \mu_k U_2(\Sigma_2^2 + \mu_k I)^{-1} U_2^T F_k + U_3 U_3^T F_k. \qquad (2.12)
\end{aligned}$$

Since $\{x_k\}$ converges to x^* superlinearly, without loss of generality, we assume that $L_1\|x_k - x^*\| < \sigma_r^*/2$ holds for all sufficient large k. Then we obtain from (2.10) that

$$\|(\Sigma_1^2 + \mu_k I)^{-1}\| \le \|\Sigma_1^{-2}\| \le \frac{1}{(\sigma_r^* - L_1\|x_k - x^*\|)^2} < \frac{4}{\sigma_r^{*2}},$$

and

$$\|(\Sigma_2^2 + \mu_k I)^{-1}\| \le \mu_k^{-1}.$$

The above two inequalities, together with (2.6) and Lemma 2.3 imply that

$$\begin{aligned}
\|F_k + J_k d_k\| &\le \frac{4L_2^{1+\delta}}{\sigma_r^{*2}}\|x_k - x^*\|^{1+\delta} + 3L_1\|x_k - x^*\|^2 \\
&\le \left(\frac{4L_2^{1+\delta}}{\sigma_r^{*2}} + 3L_1\right)\|x_k - x^*\|^2. \qquad (2.13)
\end{aligned}$$

Let $c_4 = 4L_2^{1+\delta}/\sigma_r^{*2} + 3L_1$, then we get

$$\begin{aligned} c_1 \mathrm{dist}(x_{k+1}, X^*) &\leq \|F(x_k + d_k)\| \\ &\leq \|F_k + J_k d_k\| + L_1\|d_k\|^2 \\ &\leq (c_4 + c_2^2 L_1)\|x_k - x^*\|^2. \end{aligned}$$

It now follows from (2.8) and Lemma 2.1 that

$$\|d_{k+1}\| = O(\|d_k\|^2),$$

which implies that $\{x_k\}$ converges quadratically to x^*, namely,

$$\|x_{k+1} - x^*\| = O(\|x_k - x^*\|^2).$$

The proof is completed. □

Remark: *From the proof above, we can see that if the Levenberg-Marquardt parameter is chosen as $\mu_k = \|F_k\|^\delta$ with $\delta \in [1, 2]$, then under the local error bound condition we have*

$$\frac{\mu_{k+1}}{\mu_k^2} = \frac{\|F_{k+1}\|^\delta}{\|F_k\|^{2\delta}} \leq O\left(\frac{\|x_{k+1} - \bar{x}_{k+1}\|^\delta}{\|x_k - \bar{x}_k\|^{2\delta}}\right) = O\left(\frac{\|d_{k+1}\|^\delta}{\|d_k\|^{2\delta}}\right) = O(1),$$

which implies the Levenberg-Marquardt parameter $\{\mu_k\}$ and $\{\|F_k\|\}$ converges quadratically to zero as the sequence $\{x_k\}$ converges quadratically to the solution of the nonlinear equations.

Another natural question one may ask is whether we could extend the results for even larger Levenberg-Marquardt parameters μ_k. For example, whether the quadratic convergence result remains true if $\mu_k = \|F(x_k)\|^\delta$ for $\delta \in (0, 1)$. It seems that the parameter $\mu_k/\|F(x_k)\|$ should be bounded to maintain quadratic convergence. At least this is true for the case when $n = m$ and $J(x^*)$ is nonsingular. In this case, we have that

$$J_k^T J_k(x^* - x_k) + J_k^T F_k = O(\|x_k - x^*\|^2).$$

If d_k is a quadratic convergent step, we would have

$$x_k + d_k - x^* = O(\|x_k - x^*\|^2).$$

It follows from the definition of d_k (1.2) and the above two relations that

$$\mu_k d_k = O(\|x_k - x^*\|^2),$$

which implies that

$$\mu_k = O(\|x_k - x^*\|).$$

The nonsingularity of $J(x^*)$ implies that $\|x_k - x^*\| = O(\|F(x_k)\|)$, thus it follows that

$$\mu_k = O(\|F(x_k)\|).$$

Hence, we have shown that our results cannot be further improved to $\mu_k = \|F(x_k)\|^\delta$ for $\delta < 1$.

3. Global Convergence of the New Levenberg-Marquardt Method

In this section, we consider the globalization of our new Levenberg-Marquardt method. Similar to unconstrained optimization problems, we impose line search conditions on every iteration to guarantee convergence. The line search conditions are based on the reduction of the following merit function

$$\phi(x) = \frac{1}{2}\|F(x)\|^2.$$

At iteration k, we compute the next iterate by

$$x_{k+1} = x_k + \alpha_k d_k,$$

where d_k is computed by (1.2) and α_k satisfies certain line search conditions. One commonly used inexact line search is the Wolfe line search which requires $\alpha_k > 0$ to satisfy

$$\|F(x_k + \alpha_k d_k)\|^2 \leq \|F(x_k)\|^2 + \alpha_k \beta_1 F_k^T J_k d_k \tag{3.1}$$

and

$$F(x_k + \alpha_k d_k)^T J(x_k + \alpha_k d_k) d_k \geq \beta_2 F_k^T J_k d_k, \tag{3.2}$$

where $\beta_1 \leq \beta_2$ are two constants in $(0, 1)$. Another famous inexact line search is the Armijo line search which sets $\alpha_k = \delta^t \bar{\alpha}$, where $\bar{\alpha} > 0$ and $\delta \in (0, 1)$ are two positive constants, and t is the smallest nonnegative integer satisfying

$$\|F(x_k + \delta^t \bar{\alpha} d_k)\|^2 \leq \|F(x_k)\|^2 + \beta_1 \delta^t \bar{\alpha} F_k^T J_k d_k. \tag{3.3}$$

Both inexact line searches imply that

$$\|F(x_{k+1})\|^2 \leq \|F(x_k)\|^2 - \beta_1 \beta_3 \frac{(F_k^T J_k d_k)^2}{\|d_k\|^2}, \tag{3.4}$$

where β_3 is some positive constant. For more details, please see [13].

Algorithm 3.1: *(New Levenberg-Marquardt method with line search):*

Step 1: Given $x_0 \in R^n, \delta \in [1,2], \eta \in (0,1),\ k := 0.$

Step 2: If $\|J_k^T F_k\| = 0$ *then stop; Set* $\mu_k := \|F_k\|^\delta$*; Compute* d_k *by (1.2).*

Step 3: If d_k *satisfies*

$$\|F(x_k + d_k)\| \le \eta \|F(x_k)\|, \tag{3.5}$$

then $x_{k+1} = x_k + d_k$ *otherwise* $x_{k+1} = x_k + \alpha_k d_k$ *where* α_k *is obtained by Wolfe or Armijo line search.*

Step 4 $k := k+1$*; go to Step 2.*

Theorem 3.1: *Suppose Assumption 2.2 holds and* $F(x)$ *is continuously differentiable. Let the sequence* $\{x_k\}$ *be generated by Algorithm 3.1. Then any accumulation point of* $\{x_k\}$ *is a stationary point of* ϕ*. Moreover, if an accumulation point* x^* *is a solution of nonlinear Eq. (1.1) and if Assumption 2.1 holds, then the whole sequence* $\{x_k\}$ *converges to* x^* *quadratically.*

Proof: It is easy to see that $\|F(x_k)\|$ is monotonically decreasing and bounded below. If $\|F(x_k)\|$ converges to zero, any accumulation point of $\{x_k\}$ is a solution of (1.1). Otherwise, $\|F(x_k)\| \to \gamma > 0$, which means that (3.5) holds for only finitely many times. Thus, inequality (3.4) is satisfied for all large k, which gives that

$$\sum_{k=1}^{\infty} \frac{(F_k^T J_k d_k)^2}{\|d_k\|^2} < +\infty. \tag{3.6}$$

The above inequality, the definition of d_k and $\|F(x_k)\| \ge \gamma > 0$ imply that

$$(F_k^T J_k d_k)^2 = (d_k^T (J_k^T J_k + \mu_k I) d_k)^2 \ge \gamma^{2\delta} \|d_k\|^4. \tag{3.7}$$

Relations (3.6) and (3.7) show that

$$\lim_{k\to\infty} \|d_k\| = 0. \tag{3.8}$$

This limit, (1.2) and the continuity of $J(x)$ imply that at any accumulation point x^* of $\{x_k\}$, we have that $J(x^*)^T F(x^*) = 0$, which says that x^* is a stationary point of $\phi(x)$.

We now proceed to prove the second part of the theorem. It suffices to prove that (3.5) holds for all sufficiently large k. Since the stationary point x^* is a solution of (1.1), there exists a large $\tilde{k}$ such that $x_{\tilde{k}} \in N(x^*, r)$ and $\|F_{\tilde{k}}\| \le \left(\frac{\eta c_1^{\frac{2+\delta}{2}}}{L_2 c_3}\right)^{\frac{2}{\delta}}$, where c_1, c_3, r and L_2 are defined in Sect. 2. We now verify that (3.5) holds for all $k \ge \tilde{k}$. Since $x_{\tilde{k}} \in N(x^*, r)$, we have $x_k \in N(x^*, b_1/2)$ for all $k \ge \tilde{k}$. In view of (2.6), we see

$$\frac{\|F(x_{k+1})\|}{\|F(x_k)\|} \le \frac{L_2 \|x_{k+1} - \bar{x}_{k+1}\|}{c_1 \|x_k - \bar{x}_k\|} \le \frac{L_2 c_3}{c_1} \|x_k - \bar{x}_k\|^{\frac{\delta}{2}} \le \frac{L_2 c_3 \|F(x_k)\|^{\frac{\delta}{2}}}{c_1^{\frac{2+\delta}{2}}}.$$

Hence, it follows from $\|F(x_{\tilde{k}})\| \leq (\frac{\eta c_1^{\frac{2+\delta}{2}}}{L_2 c_3})^{\frac{2}{\delta}}$ that $\|F(x_{\tilde{k}+1})\| \leq \eta \|F(x_{\tilde{k}})\|$ and so $\|F(x_{k+1})\| \leq \eta \|F(x_k)\|$ for all $k \geq \tilde{k}+1$, which implies that the step size $\alpha_k = 1$ holds for all sufficiently large k in Algorithm 3.1. Thus, we have $\{x_k\}$ converges to the solution quadratically. $\square$

4. Numerical Results

We tested our new Levenberg-Marquardt algorithm on some singular problems, and compared it with the traditional trust region algorithm for nonlinear Eqs. (1.1).

The traditional trust region algorithm for nonlinear equations computes the trial step d_k at the k-th iterate by solving the following subproblem:

$$\begin{aligned} \min_{d \in R^n} \ & \|F_k + J_k d\|^2 \triangleq \bar{\varphi}_k(d) \\ s.\ t.\ & \|d\| \leq \Delta_k, \end{aligned} \tag{4.1}$$

where $\Delta_k > 0$ is the current trust region bound. The ratio between the actual reduction and the predicted reduction of the function is defined by

$$r_k = \frac{Ared_k}{Pred_k} = \frac{\|F_k\|^2 - \|F(x_k + d_k)\|^2}{\bar{\varphi}_k(0) - \bar{\varphi}_k(d_k)},$$

which is used to decide whether the trial step is acceptable and to adjust the new trust region radius Δ_k. The algorithm can be stated as follows:

Algorithm 4.1: *(Trust region algorithm for nonlinear Eqs. [12]):*

Step 1: Given $x_1 \in R^n, \Delta_1 > 0, \varepsilon \geq 0, 0 \leq p_0 \leq p_1 \leq p_2 < 1, k := 1.$

Step 2: If $\|J_k^T F_k\| \leq \varepsilon$, *then stop;*

Solve (4.1) giving d_k.

Step 3: Compute $r_k = Ared_k / Pred_k$;

set

$$x_{k+1} = \begin{cases} x_k + d_k, & \text{if } r_k > \text{p0}, \\ x_k, & \text{otherwise} . \end{cases} \tag{4.2}$$

Step 4: Choose Δ_{k+1} *as*

$$\Delta_{k+1} = \begin{cases} \min\left\{\frac{\Delta_k}{4}, \frac{\|d_k\|}{2}\right\}, & \text{if } r_k < \text{p1}, \\ \Delta_k, & \text{if } r_k \in [\text{p1, p2}], \\ \max\{4\|d_k\|, 2\Delta_k\}, & \text{if } r_k > \text{p2}; \end{cases} \tag{4.3}$$

$k := k+1$; *go to Step 2.*

Both the trust region algorithm and the Levenberg-Marquardt algorithm have the advantage of preventing the trial step from being too large, which is especially useful for solving the singular nonlinear equations. However, the trust region algorithm achieves it by updating the trust region directly, while the Levenberg-Marquardt algorithm modifies the parameter μ_k. Many papers have considered the relationship between these two algorithms, for more details, please see [4, [5], [12], [14], etc.

First we test the Powell singular function [8], where $n = 4$ and $\mathrm{rank}(J(x^*)) = 2$. The results are given in Table 1.

The other test problems were created by modifying the nonsingular problems given by Moré, Garbow and Hillstrom [6], and have the same form as in [9],

$$\hat{F}(x) = F(x) - J(x^*)A(A^TA)^{-1}A^T(x - x^*), \tag{4.4}$$

where $F(x)$ is the standard nonsingular test function, x^* is its root, and $A \in R^{n\times k}$ has full column rank with $1 \le k \le n$. Obviously, $\hat{F}(x^*) = 0$ and

$$\hat{J}(x^*) = J(x^*)(I - A(A^TA)^{-1}A^T)$$

has rank $n - k$. A disadvantage of these problems is that $\hat{F}(x)$ may have roots that are not roots of $F(x)$. We created two sets of singular problems, with $\hat{J}(x^*)$ having rank $n - 1$ and $n - 2$, by using

$$A \in R^{n\times 1}, \qquad A^T = (1, 1, \ldots, 1)$$

and

$$A \in R^{n\times 2}, \qquad A^T = \begin{pmatrix} 1 & 1 & 1 & 1 & \cdots & 1 \\ 1 & -1 & 1 & -1 & \cdots & \pm 1 \end{pmatrix},$$

respectively. Meanwhile, we made a slight alteration on the variable dimension problem, which has $n + 2$ equations in n unknowns; we eliminated the $(n - 1)$-th and n-th equations. (The first n equations in the standard problem are linear.)

We used $p_0 = 0.0001, p_1 = 0.25$ and $p_2 = 0.75$, which are popular for tests in trust region method. And we applied Algorithm 2.6 in [7] to solve the trust region subproblem (4.1) in Algorithm 4.1. And the initial trust region radius is chosen as

Table 1. Results on Powell singular problem

			$\mu_k = \alpha\|F(x_k)\|$		$\mu_k = \alpha\|F(x_k)\|^2$		TR
			$\alpha = 1$	$\alpha = 10^{-4}$	$\alpha = 1$	$\alpha = 10^{-4}$	
Problem	n	x_0	NF	NF	NF	NF	NF/NG
Powell singular	4	1	13	10	15	10	11
		10	34	13	485	13	13
		100	198	16	–	22	16

$$\Delta_1 = \|(J_1^T J_1 + \mu_1 \|F_1\| I)^{-1} J_1^T F_1\|. \quad (4.5)$$

We test several choices of the Levenberg-Marquardt parameter in the Levenberg-Marquardt method. We choose $\mu_k = \alpha \|F_k\|^\delta$, with $\alpha = 1$ or 10^{-4} and $\delta = 1$ or 2. The algorithm is terminated when the norm of $J_k^T F_k$, e.g., the derivative of $\frac{1}{2}||F(x)||^2$ at the k-th iterate, is less than 10^{-5}, or when the number of the iterations exceeds $100(n+1)$. The results for the first set problems of rank $n-1$ are listed in Table 2, and the second set of rank $n-2$ in Table 3. The third column of the table indicates that the starting point is $x_0, 10x_0$, and $100x_0$, where x_0 is suggested by Moré, Garbow and Hillstrom in [6]; "NF" and "NJ" represent the numbers of function calculations and Jacobian calculations, respectively. We only present the values of "NF" in the Levenberg-Marquardt method as "NF" is equal to "NJ" and in the trust region method if "NF" and "NJ" are the same. If the method

Table 2. Results on first singular test set with $rank(F'(x^*)) = n-1$

			$\mu_k = \alpha\|F(x_k)\|$		$\mu_k = \alpha\|F(x_k)\|^2$		TR
			$\alpha = 1$	$\alpha = 10^{-4}$	$\alpha = 1$	$\alpha = 10^{-4}$	
Problem	n	x_0	NF	NF	NF	NF	NF/NG
1	2	1	43	15	24	15	15
		10	63	18	125	19	17
		100	234	21	–	25	21
3	2	1	64	OF	OF	OF	OF
		10	46	OF	OF	OF	OF
		100	–	OF	–	OF	OF
4	4	1	25	16	28	16	16
		10	31	19	–	18	19
		100	62	22	–	47	22
5	3	1	18	8	16	8	8
		10	22	8	68	8	8
		100	32	8	–	10	8
8	10	1	9	8	10	8	9
		10	23	23	35	23	23
		100	45	OF	OF	45	OF
9	10	1	4	4	3	3	4
		10	311	7	23	8	8
		100	100	9	515	9	10
10	30	1	13	5	6	5	6
		10	87	7	43	6	9
		100	28	10	–	10	10
11	30	1	6	12	7	–	23/13
		10	12	–	–	13	–
		100	–	–	260	–	–
12	10	1	14	14	15	14	14
		10	16	16	112	16	16
		100	36	19	–	20	19
13	30	1	14	–	–	–	9
		10	26	–	–	–	14
		100	30	–	–	–	18
14	30	1	12	11	112	11	13
		10	18	17	519	17	19
		100	24	22	–	28	24

Table 3. Results on second singular test set with $\text{rank}(F'(x^*)) = n - 2$

			$\mu_k = \alpha\|F(x_k)\|$		$\mu_k = \alpha\|F(x_k)\|^2$		TR
			$\alpha = 1$	$\alpha = 10^{-4}$	$\alpha = 1$	$\alpha = 10^{-4}$	
Problem	n	x_0	NF	NF	NF	NF	NF/NG
1	2	1	11	11	12	11	24
		10	14	13	58	13	31
		100	17	17	–	17	38
3	2	1	–	33	35	OF	59/51
		10	3	27	14	OF	4
		100	3	114	3	OF	4
4	4	1	14	14	23	14	4
		10	17	17	–	17	–
		100	21	20	–	26	–
5	3	1	29	13	21	13	13
		10	35	14	74	14	14
		100	83	15	–	17	66/44
6	31	1	16	19	60	20	–
8	10	1	9	8	10	8	328
		10	23	23	35	23	–
		100	44	OF	–	45	–
9	10	1	4	688	–	76	4
		10	311	216	384	70	8
		100	113	10	517	10	10
10	30	1	13	–	20	–	6
		10	87	–	45	–	9
		100	142	–	–	–	10
11	30	1	–	13	9	–	20/13
		10	12	–	13	23	–
		100	–	–	261	–	–
12	10	1	14	14	15	14	–
		10	16	16	109	16	–
		100	36	19	–	20	–
13	30	1	14	–	461	–	9
		10	23	–	–	–	14
		100	30	–	–	–	18
14	30	1	12	11	12	11	13
		10	18	17	519	17	9
		100	24	22	–	28	24

failed to find the solution in $100(n+1)$ iterations, we denoted it by the sign "–", and if the iterations have underflows or overflows, we denoted it by OF.

From the results, we can see that our new Levenberg-Marquardt algorithm performs almost the same as the traditional trust region algorithm for problems with $\text{rank}(J(x^*)) = n - 1$. However it performs much better than the traditional trust region algorithm when $\text{rank}(J(x^*)) = n - 2$. Hence, it seems that our new Levenberg-Marquardt algorithm may be more efficient for nonlinear equations with higher rank deficiency.

When the starting point is far away from the solution set of the nonlinear equations, the choice of $\alpha = 10^{-4}$ is better than that of $\alpha = 1$ and the choice of $\delta = 1$ is better than that of $\delta = 2$, whatever the rank of $J(x^*)$ is. These facts indicate that $\mu_k = \|F_k\|^2$ may be very large at the beginning of the iterations, which may lead to smaller steps, and so prevent the sequence from converging quickly, and sometimes the method can not solve the problem in $100(n+1)$ iterations.

All in all, the Levenberg-Marquardt algorithm with the parameter being $\mu_k = \|F_k\|$ performs most stable among the traditional trust region algorithm and the Levenberg-Marquardt algorithm with other three choices of the parameter. Hence, the choice of $\mu_k = \|F_k\|$ may be preferable to an arbitrary problem with unknown rank.

Finally, it is worth pointing out that on the $100x_0$ case for Problem 11, when the parameter is chosen as $\mu_k = \|F_k\|^2$, the new Levenberg-Marquardt algorithm converges to a stationary point of $\min_{x \in R^n} \|F(x)\|$, instead of that of $F(x) = 0$.

Acknowledgements

Supported by Chinese NSF grants 19731010, 10231060 and the Knowledge Innovation Program of CAS. It was pointed out by Prof. C.T. Keller (private communication) that the choice $\mu_k = \|F(x_k)\|$ was suggested in his book [1]. We would like to thank two anonymous referees for their valuable comments.

References

[1] Kelley, C. T: Iterative methods for optimization (Frontiers in Applied Mathematics 18). Philadelphia: SIAM 1999.
[2] Levenberg, K.: A method for the solution of certain nonlinear problems in least squares. Quart. Appl. Math. *2*, 164–166 (1944).
[3] Marquardt, D. W.: An algorithm for least-squares estimation of nonlinear inequalities. SIAM J. Appl. Math. *11*, 431–441 (1963).
[4] Moré, J. J.: The Levenberg-Marquardt algorithm: implementation and theory. In: Lecture Notes in Mathematics 630: Numerical analysis (Watson, G. A., ed.), pp. 105–116. Berlin: Springer 1978.
[5] Moré, J. J.: Recent developments in algorithms and software for trust region methods. In: Mathematical programming: The state of art. (Bachem, A., Grötschel, M., Korte, B., eds.), pp. 258–287. Berlin: Springer 1983.
[6] Moré, J. J., Garbow, B. S., Hillstrom, K. H.: Testing unconstrained optimization software. ACM Trans. Math. Software *7*, 17–41 (1981).
[7] Nocedal, J., Yuan, Y.X.: Combining trust region and line search techniques. In: Advances in nonlinear programming (Yuan, Y., ed.), pp. 153–175. Kluwer 1998.
[8] Powell, M. J. D.: An iterative method for finding stationary values of a function of several variables. Comput. J. *5*, 147–151 (1962).
[9] Schnabel, R. B., Frank, P.D.: Tensor methods for nonlinear equations. SIAM J. Numer. Anal. *21*, 815–843 (1984).
[10] Stewart, G. W., Sun, J. G.: Matrix perturbation theory. San Diego: Academic Press 1990.
[11] Yamashita, N., Fukushima, M.: On the rate of convergence of the Levenberg-Marquardt method. Computing (Suppl. 15): 237–249 (2001).
[12] Yuan, Y. X.: Trust region algorithms for nonlinear equations. Information *1*, 7–20 (1998).
[13] Yuan, Y. X.: Problems on convergence of unconstrained optimization algorithms. In: Numerical linear algebra and optimization (Yuan, Y. X., ed.), pp. 95–107. Beijing: Science Press 1999.
[14] Yuan, Y. X.: A review of trust region algorithms for optimization. In: ICM99: Proc. 4th Int. Congress on Industrial and Applied Mathematics (Ball, J. M., Hunt, J. C. R., eds.), pp. 271–282. Oxford: Oxford University Press 2000.

Jin-yan Fan
State Key Laboratory of Scientific/
Engineering Computing
Institute of Computational
Mathematics and Scientific/
Engineering Computing
The Academy of Mathematics and
Systems Sciences
Chinese Academy of Sciences
P.O. Box 2719
Beijing, 100080
P.R. China
e-mail: jyfan@sjtu.edu.cn

Ya-xiang Yuan
State Key Laboratory of Scientific/
Engineering Computing
Institute of Computational
Mathematics and Scientific/
Engineering Computing
The Academy of Mathematics and
Systems Sciences
Chinese Academy of Sciences
P.O. Box 2719
Beijing, 100080
P.R. China
e-mail: yyx@lsec.cc.ac.cn