Finding zeros of Hölder metrically subregular mappings via globally convergent Levenberg–Marquardt methods

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Abstract

We introduce LMLS and LMQR, two globally convergent Levenberg–Marquardt methods for finding zeros of Hölder metrically subregular mappings that may have non-isolated zeros. The first method unifies the Levenberg–Marquardt direction and an Armijo-type line search, while the second incorporates this direction with a non-monotone quadratic regularization technique. For both methods, we prove the global convergence to a first-order stationary point of the associated merit function. Furthermore, the worst-case global complexity of these methods are provided, indicating that an approximate stationary point can be computed in at most $O\left(\varepsilon^{-2}\right)$ function and gradient evaluations, for an accuracy parameter $\varepsilon > 0$. We also study the conditions for the proposed methods to converge to a zero of the associated mappings. Computing a moiety conserved steady state for biochemical reaction networks can be cast as the problem of finding a zero of a Hölder metrically subregular mapping. We report encouraging numerical results for finding a zero of such mappings derived from real-world biological data, which supports our theoretical foundations.

1. Introduction

We consider the problem of finding zeros of the nonlinear mapping $h : \mathbb{R}^m \to \mathbb{R}^n$, i.e.

$$h(x) = 0, \quad x \in \mathbb{R}^m,$$

where $m \geq n$ and $h$ is continuously differentiable and satisfies the Hölder metric subregularity (see below). The set of zeros of such mappings is denoted by $\Omega$, which is assumed to be non-empty.
A classical approach for finding a solution of (1) is to search for a minimizer of the nonlinear least-squares problem

$$\min_{x \in \mathbb{R}^m} \psi(x), \quad \text{with } \psi : \mathbb{R}^m \to \mathbb{R} \text{ given by } \psi(x) := \frac{1}{2} \| h(x) \|^2,$$

(2)

where \( \| \cdot \| \) denotes the Euclidean norm. In order to guarantee the quadratic or superlinear convergence of many Newton-type schemes for solving (2), the existence of some constant \( \beta > 0 \) satisfying

$$\beta \dist(x, \Omega) \leq \| h(x) \|, \quad \forall x \in B(x^*, \varepsilon)$$

(3)
is assumed, where \( B(x^*, \varepsilon) \) stands for the closed ball centred at \( x^* \in \Omega \) with radius \( \varepsilon > 0 \), cf. [27,48]. Such an inequality is referred as an error bound (Lipschitzian error bound or metric regularity) condition. The notion of error bound has been very popular during the last few decades to study the local convergence of optimization methodologies; however, there are many important mappings where (3) is not satisfied, see, e.g. [4,34]. This motivated the authors of [4] to propose a weaker condition so-called the Hölder metric subregularity (Hölderian error bound), where a mapping \( h : \mathbb{R}^m \to \mathbb{R}^n \) is said to be Hölder metrically subregular of order \( \delta > 0 \) around \((x, y)\) with \( y = h(x) \) if there exist some constants \( r > 0 \) and \( \beta > 0 \) such that

$$\beta \dist(x, h^{-1}(y)) \leq \| y - h(x) \|^\delta, \quad \forall x \in B(x^*, r).$$

(4)

For any solution \( x^* \in \Omega \) of the system of nonlinear equations (1), the Hölder metric subregularity of \( h \) around \((x^*, 0)\) reduces to

$$\beta \dist(x, \Omega) \leq \| h(x) \|^\delta, \quad \forall x \in B(x^*, \varepsilon),$$

(4)

for \( \delta \in ]0, 1[ \) and \( \varepsilon \in ]0, 1[ \). There are many mappings satisfying this condition, see, e.g. [4,34] and references therein. See also Section 5 for a real-world nonlinear system satisfying (4), but not (3).

The Levenberg–Marquardt method is a standard technique used to solve (1), where, in the current point \( x_k \) and for a positive parameter \( \mu_k \), the convex subproblem

$$\min_{d \in \mathbb{R}^m} \phi_k(d), \quad \text{with } \phi_k : \mathbb{R}^m \to \mathbb{R} \text{ given by } \phi_k(d) := \| \nabla h(x_k)^T d + h(x_k) \|^2 + \mu_k \| d \|^2,$$

(5)

is solved to compute a direction \( d_k \) in which \( \nabla h(x_k) \in \mathbb{R}^{m \times n} \) is the gradient of \( h \) at \( x_k \). This requires finding the unique solution of the linear system

$$\left( \nabla h(x_k)^T \nabla h(x_k) + \mu_k I \right) d_k = -\nabla h(x_k) h(x_k),$$

(6)

where \( I \in \mathbb{R}^{m \times m} \) denotes the identity matrix. Then, the next iteration is generated by \( x_{k+1} = x_k + d_k \) and this scheme is continued until a stationary point of (2) is found, which may correspond to a zero \( h \), when certain conditions are satisfied.

The choice of the parameter \( \mu_k \) has substantial impacts on the global convergence, the local convergence rate, and the computational efficiency of Levenberg–Marquardt methods, cf. [4,31,38,47,48]. Hence, several ways to specify and to adapt this parameter have
been proposed; see, e.g. [18,19,48]. A recently proposed Levenberg–Marquardt method by the authors [4] suggests an adaptive parameter $\mu_k$ based on the order $\delta \in ]0, 1]$ of the Hölder metric subregularity (4), i.e.

$$\mu_k = \xi_k \|h(x_k)\|^\eta + \omega_k \|\nabla h(x_k) h(x_k)\|^\eta,$$

where $\eta \in ]0, 4\delta[$, $\xi_k \in [\xi_{\min}, \xi_{\max}]$ and $\omega_k \in [\omega_{\min}, \omega_{\max}]$ with $\xi_{\min} + \omega_{\min} > 0$. In [4], this Levenberg–Marquardt method, with adaptive regularization (LM-AR), was presented and its local convergence was studied for Hölder metrically subregular mappings.

If one assumes that the starting point $x_0$ is close enough to a solution $x^*$ of (2), then when $m = n$ the Levenberg–Marquardt method is known to be quadratically convergent if $\nabla h(x^*)$ has full rank, in which case it is clearly convergent to a solution to (1). In this case, the full rank assumption implies that the solution of the minimization problem (2) must be locally unique; see [10,28,48]. However, assuming local uniqueness of the solution might be restrictive for many applications since the underlying mappings might have non-isolated zeros. Therefore, much attention has been devoted to the study of local convergence of the Levenberg–Marquardt method under local error bounds, which enables the solution of mappings with non-isolated zeros; see, e.g. [10,18,19,48]. In particular, the local convergence of the Levenberg–Marquardt method was studied in [4] under the Hölder metric subregularity condition (4).

As it is the case in many applications, one cannot provide a sufficiently close starting point $x_0$ to a solution $x^*$, and therefore the convergence of the Levenberg–Marquardt method is not guaranteed, which decreases the chance of practical applicability. To overcome this shortcoming, two globalization techniques have been proposed to be combined with the Levenberg–Marquardt direction, namely, line search and quadratic regularization; see, e.g. [3,30,31,44]. Generally, a line search method finds a descent direction $d_k$, specifies a step-size $\alpha_k$, generates the new iteration $x_{k+1} = x_k + \alpha_k d_k$, and repeats this scheme until a stopping criterion holds. The step-size is usually determined by an inexact line search such as Armijo, Wolfe, or Goldstein backtracking schemes; see [14,43]. In particular, the Armijo line search usually finds $\alpha_k$ using a backtracking procedure, which ends up with a step-size satisfying

$$\psi(x_k + \alpha_k d_k) \leq \psi(x_k) + \sigma \alpha_k \nabla \psi(x_k)^T d_k,$$

where $\sigma \in ]0, 1[$. In order to provide an outline for quadratic regularization methods, let us define, firstly, the quadratic function $q_k : \mathbb{R}^m \to \mathbb{R}$ with

$$q_k(d) := \frac{1}{2} \|\nabla h(x_k)^T d + h(x_k)\|^2.$$

Then, a Levenberg–Marquardt quadratic regularization method solves the quadratic subproblem (5) to find a direction $d_k$, computes the ratio of the actual reduction to the predicted reduction

$$r_k := \frac{\psi(x_k) - \psi(x_k + d_k)}{q_k(0) - q_k(d_k)},$$

and updates the parameter $\mu_k$ using $r_k$. For line search and quadratic regularization methods, the global convergence to a first-order stationary point of $\psi$ can be guaranteed, which results in a monotone sequence of function values, i.e. $\psi(x_{k+1}) \leq \psi(x_k)$. 
Regardless of the fact that the monotonicity seems natural for the minimization goal, it has some drawbacks. We address two of them here: (i) the monotone method may lose its efficiency if iterations are trapped at the bottom of a curved narrow valley, where the monotonicity forces the iterations to trace the valley floor (causing very short steps or even an undesired zigzagging); (ii) the Armijo-type line search can break down for very small step-sizes because of rounding errors, when \( \psi(x_k + \alpha_k d_k) \approx \psi(x_k) \). In this case, the point \( x_k \) may still be far from a stationary point of \( \psi \); however, the Armijo rule cannot be satisfied due to indistinguishability of \( \psi(x_k + \alpha_k d_k) \) from \( \psi(x_k) \) in floating-point arithmetic. To overcome such limitations, the seminal article by Grippo et al. [22] addressed a variant of the Armijo rule (8) by substituting \( \psi(x_k) \) with \( \psi_l(k) = \max_{0 \leq j \leq m(k)} \psi(x_{k-j}) \), where \( m(0) = 0 \) and \( 0 \leq m(k) \leq \min\{m(k-1) + 1, M\} \), for some non-negative integer constant \( M \) for all \( k \geq 1 \). This does not guarantee the monotonicity condition \( \psi(x_{k+1}) \leq \psi(x_k) \) and therefore called nonmonotone. Non-monotonicity has also been studied for trust-region methods by replacing \( \psi(x_k) \) with a non-monotone term; cf. [1]. On the basis of many studies in this area, non-monotone methods have been recognized to be globally convergent and computationally efficient, even for highly nonlinear problems; see [1,5] and references therein.

1.1. Motivation and contribution

Our analysis was motivated by the problem of finding moiety conserved steady states of deterministic equations representing the dynamical evolution of molecular species abundance in biochemical reaction networks. This problem can be considered as an application of finding zeros of a mapping \( h : \mathbb{R}^m \rightarrow \mathbb{R}^n \), that may not satisfy the local error bound (3). It was previously established [4] that this mapping is Hölder metrically subregular and that the merit function is real analytic using standard biochemical assumptions; cf. [7]. Applying a novel Levenberg–Marquardt algorithm with adaptive regularization (LM-AR), to this problem, we proved local convergence to a zero of \( h \) for all such networks if the sufficiently closeness of a starting point to \( x^* \) can be assumed [4]. However, providing a starting point close enough to \( x^* \) remains as a limitation in practice, as is the case for all local optimization methods; see, e.g. [14,16].

The global convergence and complexity of iterative methods has been the subject of intense debate within the nonlinear optimization community over the last few decades. While the global convergence guarantees the convergence of the iteration sequence generated by a method for any given starting point \( x_0 \), the worst-case complexity provides an upper bound on the number iterations or function evaluations needed to reach a stationary point of the underlying objective function. These two factors are more important if the convexity or structured non-convexity of the objective function is assumed; see, e.g. [8,11,39–41,49]. In the particular case of solving nonlinear least-squares problems by Levenberg–Marquardt methods, there are fewer results about their global convergence and complexity, compared with the volume of literature concerning Newton-type methods; cf. [45,46]. This motivates our aim to study the global convergence properties and complexity of two Levenberg–Marquardt methods using line search and quadratic regularization techniques.
Our contribution is summarized as follows:

- **(Algorithm development)** We introduce LMLS (Algorithm 1) and LMQR (Algorithm 2), two Levenberg–Marquardt methods using globalization techniques. For LMLS, we use $\mu_k$ defined in (7), solve the linear system (6) to specify $d_k$, and combine this direction with a non-monotone Armijo-type line search. Moreover, we propose a modified version of the Levenberg–Marquardt parameter (7), which is lower bounded, and combines the associated direction $d_k$ with a quadratic regularization technique to adapt the Levenberg–Marquardt parameter that is called LMQR.

- **(Global, local, and complexity analysis)** We analyse the global convergence, and investigate the complexity of both LMLS and LMQR under Hölder metric subregularity. In both cases, it is shown that a first-order stationary point is attained after at most $O(\epsilon^{-2})$ iterations or function evaluations (see Theorems 2.3 and 3.3). We note that if the merit function $\frac{1}{2}\|h(\cdot)\|^2$ satisfies the Łojasiewicz inequality, then the mapping $h$ satisfies Hölder metric subregularity (see [4, Section 2]), which motivates us to study the local convergence of LMQR under the Łojasiewicz inequality (see Section 3).

- **(Finding zeros of nonlinear mappings)** We show that if $\nabla h(x^*)$ is full column rank at accumulation point $x^*$ of $\{x_k\}$ generated by LMLS or LMQR, then it is a solution of (1) (see Theorem 4.1). Further, if $h$ is either monotone or duplomonotone (which is the case for some classes of the mapping (83) appearing in biochemical reaction networks; cf. [6]), then the sequences generated by LMLS and LMQR converge to a solution of (1) (see Theorem 4.2).

- **(Application in biochemical reaction network kinetics)** We demonstrate that the application of LMLS and LMQR to mappings derived from real-world biochemical reaction networks (see Section 5), from a diverse set of biological species, shows encouraging numerical results in practice. To the best of our knowledge, these two algorithms are the first methods that are globally convergent to a stationary point of the mapping $h$ arising in the study of biological networks. These algorithms are available in the COBRA Toolbox v.03 [25], an open source software package for modelling biochemical reaction networks.

This paper has five sections, besides this introductory section. Section 2 describes a globally convergent Levenberg–Marquardt line search method. Section 3 addresses a globally convergent Levenberg–Marquardt quadratic regularization method, where in both sections the global convergence and complexity of these methods are analysed. In Section 4, finding a zero of some specific mappings with the proposed methods is discussed. Section 5 reports encouraging numerical results for a mapping appearing in biochemical reaction networks. Finally, conclusions and area for further research are identified in Section 6.

### 2. Levenberg–Marquardt line search method

For the sake of simplicity, we define $H_k = H(x_k) := \nabla h(x_k) \nabla h(x_k)^T + \mu_k I$. If $x_k$ is not a stationary point of $\psi$, from positive definiteness of $H(x_k)$, we obtain

$$\nabla \psi(x_k)^T d_k = -d_k^T H(x_k) d_k < 0,$$

(11)
which guarantees the descent property of \( d_k \) at \( x_k \). This motivates us to develop a globally convergent Levenberg–Marquardt method using (7). More precisely, we shall combine the Levenberg–Marquardt direction with a non-monotone Armijo-type line search using the non-monotone term

\[
D_k = \begin{cases} 
\psi(x_0) & \text{if } k = 0, \\
(1 - \theta_{k-1})\psi(x_k) + \theta_{k-1}D_{k-1} & \text{if } k \geq 1,
\end{cases}
\]

where \( \theta_{k-1} \in [\theta_{\min}, \theta_{\max}] \) and \( 0 \leq \theta_{\min} \leq \theta_{\max} < 1 \), cf. [2,23].

A combination of the direction \( d_k \) (given by solving (6) using the parameter (7)) with a non-monotone Armijo-type line search using (12) leads to Algorithm 1.

**Algorithm 1: LMLS (Levenberg–Marquardt Line Search algorithm)**

**Input:** \( x_0 \in \mathbb{R}^m, \eta > 0, \alpha > 0, \epsilon > 0, \rho, \sigma \in ]0,1[, \xi_0 \in [\xi_{\min}, \xi_{\max}], \omega_0 \in [0, \omega_{\max}], \theta_0 \in [\theta_{\min}, \theta_{\max}] \);

1. \( k := 0; \mu_0 := \xi_0 \| h(x_0) \|^\eta + \omega_0 \| \nabla h(x_0)h(x_0) \|^\eta; \)
2. \( \text{while a stopping criterion is not satisfied do} \)
3. \( \quad \text{solve the linear system (6) to specify the direction } d_k; \quad \ell = 0; \alpha_k = \alpha; \)
4. \( \quad \text{while } \psi(x_k + \alpha_k d_k) > D_k + \sigma \alpha_k \nabla \psi(x_k)^T d_k \text{ do} \)
5. \( \quad \quad \ell = \ell + 1; \quad \alpha_k = \rho^\ell \alpha; \)
6. \( \quad \text{end} \)
7. \( \quad \ell_k = \ell; \quad x_{k+1} = x_k + \alpha_k d_k; \quad \text{update } \xi_k, \omega_k, \text{ and } \theta_k; \)
8. \( \quad \text{update } \mu_k \text{ and } D_k \text{ by (7) and (12), respectively; } k = k + 1; \)
9. \( \text{end} \)
10. \( \text{end} \)

One may use \( \| h(x_k) \| > \epsilon \) or \( \| \nabla \psi(x_k) \| > \epsilon \) as a stopping criterion in LMLS. In order to prove the global convergence of the sequence \( \{x_k\} \) generated by LMLS to a stationary point of \( \psi \), we assume that the next assumptions hold:

(A1) The mapping \( h \) is continuously differentiable and \( \nabla h \) is Lipschitz continuous, i.e.

\[
\| \nabla h(x) - \nabla h(y) \| \leq L \| x - y \|, \quad \forall \, x, y \in \mathbb{R}^m;
\]

(A2) The lower level set \( L(x_0) := \{ x \in \mathbb{R}^m \mid \psi(x) \leq \psi(x_0) \} \) is bounded;

In the subsequent proposition, we first derive a lower bound for the step-size \( \alpha_k \) and give a bound on the total number of function evaluations needed until the line search (Line 5 of LMLS) is satisfied.

**Proposition 2.1 (well-definedness of LMLS):** Let \( \{x_k\} \) be an infinite sequence generated by LMLS. Then, for all \( k \), the following statements are true:

(i) \( x_k \in L(x_0); \)
(ii) if \( \|h(x_k)\| > \varepsilon \) and \( \|\nabla h(x_k)h(x_k)\| > \varepsilon \) for all \( k = 0, \ldots, k \), then
\[
\alpha_k \geq \frac{\rho(1 - \sigma)\mu^2}{\vartheta (L_0^2 + \mu)} := \hat{\alpha},
\]
with
\[
\vartheta := \frac{1}{2}L_0^2 + \frac{1}{2}\bar{\alpha}^2\rho^{-2}L^2\mu^{-2}L_0^2\|h(x_0)\|^2 + (1 + \bar{\alpha}\rho^{-1}L_0\mu^{-1})L\|h(x_0)\|,
\]
where \( \mu \in [0, \varepsilon] \) and \( L_0 > 0 \) satisfies \( \|\nabla h(x)\| \leq L_0 \) for all \( x \in L(x_0) \). Moreover, the inner loop of LMLS is terminated in a finite number of steps, denoted by \( \ell_k \), which satisfies
\[
0 \leq \ell_k \leq \frac{\log(\hat{\alpha}) - \log(\alpha)}{\log(\rho)}.
\]

**Proof:** We prove Assertions (i) and (ii) by induction at the same time. Let us assume \( i = 1 \). Since \( D_0 = \psi(x_0) \), by the traditional results about the monotone Armijo line search, we have \( \psi(x_1) \leq D_0 = \psi(x_0) \). This implies that \( x_1 \in L(x_0) \). The proof of Assertion (ii) is similar to \( i = k \), i.e. we therefore omit it.

We now assume Assertions (i) and (ii) hold for \( i = 1, \ldots, k - 1 \) and prove them for \( i = k \). Since \( x_{k-1} \) satisfies the line search and \( \nabla \psi(x_{k-1})^T d_{k-1} < 0 \), similar to Lemma 2.3 in [2], we can show \( \psi(x_k) \leq D_{k-1} \). This and
\[
D_k - \psi(x_k) = \theta_{k-1}(D_{k-1} - \psi(x_k)) \geq 0, \quad D_k - D_{k-1} = (1 - \theta_{k-1})(\psi(x_k) - D_{k-1}) \leq 0,
\]

imply \( D_k \leq D_{k-1} \) and
\[
\psi(x_k) \leq D_k.
\]

Therefore,
\[
\psi(x_k) \leq D_{k-1} \leq D_{k-2} \leq \cdots \leq D_0 = \psi(x_0),
\]
leading to \( x_k \in L(x_0) \), i.e. Assertion (i) holds for \( i = k \).

From (A1) and \( x_k \in L(x_0) \), there exists some constant \( L_0 > 0 \) such that
\[
\|\nabla h(x_k)\| \leq L_0,
\]
which implies
\[
\|H(x_k)\| = \|\nabla h(x_k)\nabla h(x_k)^T + \mu_k I\| \leq \|\nabla h(x_k)\|^2 + \mu_k \leq L_0^2 + \mu_k,
\]
leading to
\[
\lambda_{\min}\left(H(x_k)^{-1}\right) = \frac{1}{\lambda_{\max}(H(x_k))} = \frac{1}{\|H(x_k)\|} \geq \frac{1}{L_0^2 + \mu_k}.
\]
From the definition of $d_k$, we obtain
\[
\|d_k\| = \| H(x_k)^{-1} \nabla \psi(x_k) \| \leq \| H(x_k)^{-1} \| \| \nabla \psi(x_k) \| \\
= \frac{1}{\lambda_{\text{min}}(H(x_k))} \| \nabla \psi(x_k) \| \leq \frac{1}{\mu_k} \| \nabla \psi(x_k) \|. \quad \text{(20)}
\]

Since $\|h(x_k)\| > \varepsilon$ and $\| \nabla h(x_k) h(x_k) \| > \varepsilon$, it holds that
\[
\mu_k = \xi_k \|h(x_k)\|^n + \omega_k \| \nabla h(x_k) h(x_k) \|^n > \xi_{\text{min}} \varepsilon^n, \quad \forall \ k \geq 0.
\]

Let us consider a constant $\mu \in ]0, \xi_{\text{min}} \varepsilon^n[$, i.e.
\[
\mu_i > \mu, \quad \forall \ i = 0, \ldots, k. \quad \text{(21)}
\]

We first derive a lower bound on the step-size $\alpha_k$. By (20), (18) and (21), we get
\[
\|d_k\| \leq \mu_k^{-1} \| \nabla \psi(x_k) \| \leq \mu_k^{-1} \| \nabla h(x_k) \| \| h(x_k) \| \leq \mu_k^{-1} L_0 \| h(x_0) \| \leq \mu^{-1} L_0 \| h(x_0) \|. \quad \text{(22)}
\]

Therefore, for all $\alpha > 0$, we have
\[
\| h(x_k) + \alpha \nabla h(x_k) d_k \| \leq \| h(x_k) \| + \alpha \| \nabla h(x_k) \| \| d_k \| \leq (1 + \alpha L_0^2 \mu^{-1}) \| h(x_0) \|. \quad \text{(23)}
\]

Further, for all $t \in [0, 1]$ and $\alpha > 0$, (A3) and (22) yield
\[
\| \nabla h(x_k + t \alpha d_k) - \nabla h(x_k) \| \leq L \alpha \| d_k \| \leq \alpha LL_0 \mu^{-1} \| h(x_0) \|. \quad \text{(24)}
\]

It follows from (18) that
\[
\frac{1}{2} \| h(x_k) + \alpha \nabla h(x_k) d_k \|^2 = \frac{1}{2} \| h(x_k) \|^2 + \alpha h(x_k)^T \nabla h(x_k) d_k + \frac{1}{2} \alpha^2 \| \nabla h(x_k) d_k \|^2 \\
\leq \frac{1}{2} \| h(x_k) \|^2 + \alpha h(x_k)^T \nabla h(x_k) d_k + \frac{1}{2} \alpha^2 \| \nabla h(x_k) \|^2 \| d_k \|^2 \\
\leq \frac{1}{2} \| h(x_k) \|^2 + \alpha h(x_k)^T \nabla h(x_k) d_k + \frac{1}{2} \alpha^2 L_0^2 \| d_k \|^2 \\
= \psi(x_k) + \alpha \nabla \psi(x_k)^T d_k + \frac{1}{2} \alpha^2 L_0^2 \| d_k \|^2. \quad \text{(25)}
\]

By this inequality, the Taylor expansion of $h(x_k + \alpha d_k)$ around $x_k$, and the Cauchy–Schwarz inequality, for any $\alpha > 0$, we come to
\[
\psi(x_k + \alpha d_k) = \frac{1}{2} \bigg\| h(x_k) + \alpha \nabla h(x_k) d_k + \int_0^1 \alpha (\nabla h(x_k + t \alpha d_k) - \nabla h(x_k)) d_k \ dt \bigg\|^2 \\
= \frac{1}{2} \| h(x_k) + \alpha \nabla h(x_k) d_k \|^2 + \frac{1}{2} \bigg\| \int_0^1 \alpha (\nabla h(x_k + t \alpha d_k) - \nabla h(x_k)) d_k \ dt \bigg\|^2 \\
+ (h(x_k) + \alpha \nabla h(x_k) d_k)^T \int_0^1 \alpha (\nabla h(x_k + t \alpha d_k) - \nabla h(x_k)) d_k \ dt \\
\leq \psi(x_k) + \alpha \nabla \psi(x_k)^T d_k + \frac{1}{2} \alpha^2 L_0^2 \| d_k \|^2
\]
\[
\begin{align*}
&\frac{1}{2} \left( \int_0^1 \alpha (\| \nabla h(x_k + t \alpha d_k) - \nabla h(x_k) \| \| d_k \| \, dt \right)^2 \\
&+ \| h(x_k) + \alpha \nabla h(x_k)^T d_k \| \int_0^1 \alpha \| \nabla h(x_k + t \alpha d_k) - \nabla h(x_k) \| \| d_k \| \, dt.
\end{align*}
\]

(26)

This inequality, (18), (23), (24), and (A3) suggest

\[
\psi(x_k + \alpha d_k) \leq \psi(x_k) + \alpha \nabla \psi(x_k)^T d_k \\
+ \left( \frac{1}{2} L_0^2 + \frac{1}{2} \sigma^2 \mu^{-2} L_0^2 \| h(x_0) \|^2 + (1 + \alpha L_0^2 \mu^{-1}) L \| h(x_0) \| \right) \alpha \| d_k \|^2.
\]

From (16), we come to

\[
\psi(x_k + \alpha d_k) \leq D_k + \alpha \nabla \psi(x_k)^T d_k \\
+ \left( \frac{1}{2} L_0^2 + \frac{1}{2} \sigma^2 \mu^{-2} L_0^2 \| h(x_0) \|^2 + (1 + \alpha L_0^2 \mu^{-1}) L \| h(x_0) \| \right) \alpha \| d_k \|^2.
\]

For \( \alpha = \alpha_k / \rho \leq \overline{\alpha} / \rho \), we have

\[
\frac{1}{2} L_0^2 + \frac{1}{2} \sigma^2 \mu^{-2} L_0^2 \| h(x_0) \|^2 + (1 + \alpha L_0^2 \mu^{-1}) L \| h(x_0) \| \\
\leq \frac{1}{2} L_0^2 + \frac{1}{2} \overline{\alpha}^2 \rho^{-2} \mu^{-2} L_0^2 \| h(x_0) \|^2 \\
+ (1 + \overline{\alpha} \rho^{-1} L_0^2 \mu^{-1}) L \| h(x_0) \| =: \vartheta,
\]

which yields

\[
\psi(x_k + \alpha d_k) \leq D_k + \alpha \nabla \psi(x_k)^T d_k + \vartheta \alpha \| d_k \|^2.
\]

(27)

For \( \alpha = \alpha_k / \rho \), the Armijo-type line search (Line 5 of LMLS) does not hold, i.e.

\[
\psi(x_k + \alpha d_k) > D_k + \sigma \alpha \nabla \psi(x_k)^T d_k.
\]

This and inequality (27) lead to

\[
\vartheta \alpha \| d_k \|^2 \geq (\sigma - 1) \nabla \psi(x_k)^T d_k.
\]

Substituting \( \alpha = \alpha_k / \rho \), we have thanks to (20) and (19) that

\[
\vartheta \alpha_k \rho^{-1} \mu_k^{-2} \| \nabla \psi(x_k) \|^2 \geq \vartheta \alpha_k \rho^{-1} \| d_k \|^2 > (\sigma - 1) \nabla \psi(x_k)^T d_k \\
= (1 - \sigma) \nabla \psi(x_k)^T H(x_k)^{-1} \nabla \psi(x_k) \\
\geq (1 - \sigma) \lambda_{\min}(H(x_k)^{-1}) \| \nabla \psi(x_k) \|^2 \\
\geq (1 - \sigma)(L_0^2 + \mu_k)^{-1} \| \nabla \psi(x_k) \|^2 \\
\geq (1 - \sigma)(L_0^2 + \mu)^{-1} \| \nabla \psi(x_k) \|^2.
\]

(28)
It follows from (28) and (21) that (13) is valid. Using $\alpha_k = \rho^k \alpha$ and (13), we end up to

$$\hat{\alpha} \leq \rho^k \alpha \leq \alpha,$$

which proves (14). ■

The first main result of this section demonstrates some properties of the sequence $D_k$ and shows that any accumulation point of the sequence $\{x_k\}$ generated by LMLS is either a solution of (1) or a stationary point of $\psi$.

**Theorem 2.2 (global convergence):** Let $\{x_k\}$ be an infinite sequence generated by LMLS. Then, for all $k \geq 0$, the following assertions hold:

(i) the sequences $\{\psi(x_k)\}$ and $\{D_k\}$ are convergent and

$$\lim_{k \to \infty} D_k = \lim_{k \to \infty} \psi(x_k); \quad (29)$$

(ii) for some $c_1 > 0$, it holds that $\nabla \psi(x_k)^T d_k \leq -c_1 \|\nabla \psi(x_k)\|^2$;

(iii) LMLS either stops at finite number of iterations, satisfying $\|h(x_k)\| \leq \varepsilon$ or $\|\nabla \psi(x_k)\| \leq \varepsilon$, or generates an infinite sequence $\{x_k\}$ such that any accumulation point of this sequence is a stationary point of the merit function $\psi$, i.e.

$$\lim_{k \to \infty} \|\nabla \psi(x_k)\| = 0. \quad (30)$$

**Proof:** From (15), we have $D_k \leq D_{k-1}$. Together with $x_k \in \mathcal{L}(x_0)$ and (A2), this implies that the sequence $\{D_k\}$ is convergent. From $\theta_k \in [\theta_{\min}, \theta_{\max}]$, with $\theta_{\max} \in [\theta_{\min}, 1]$, we obtain $1 - \theta_k \geq 1 - \theta_{\max} > 0$. Taking limits when $k$ goes to infinity from $D_k \leq \psi(x_k) \leq D_{k-1}$ gives (29).

It follows from (19) and the definition of $d_k$ that

$$\nabla \psi(x_k)^T d_k = -\nabla \psi(x_k)^T H(x_k)^{-1} \nabla \psi(x_k) \leq -\lambda_{\min} (H(x_k)^{-1}) \|\nabla \psi(x_k)\|^2$$

$$\leq -\frac{1}{L_0^2 + \mu_k} \|\nabla \psi(x_k)\|^2. \quad (31)$$

By the definition of $\mu_k$, (17), and (18), we get

$$\mu_k = \xi_k \|h(x_k)\|^\eta + \omega_k \|\nabla h(x_k)h(x_k)\|^\eta$$

$$\leq \xi_{\max} \|h(x_k)\|^\eta + \omega_{\max} \|\nabla h(x_k)\|^\eta \|h(x_k)\|^\eta$$

$$\leq (\xi_{\max} + \omega_{\max} L_0^\eta) \|h(x_0)\|^\eta := \overline{\mu}, \quad (32)$$

for all $k \geq 0$. This and (31) yield

$$\nabla \psi(x_k)^T d_k \leq -\left(L_0^2 + \overline{\mu}\right)^{-1} \|\nabla \psi(x_k)\|^2;$$

that is, Assertion (i) holds with $c_1 := \left(L_0^2 + \overline{\mu}\right)^{-1} > 0$.

Let us now prove the assertion (iii). If the algorithm stops in a finite number of iterations by either $\|h(x_k)\| \leq \varepsilon$ or $\nabla \psi(x_k) \leq \varepsilon$, the result is valid. Let us assume that the algorithm
generates an infinite sequence \(\{x_k\}\). For a fixed iteration \(x_k\), the stopping criteria of LMLS do not hold, i.e. \(\|h(x_k)\| > \varepsilon\) and \(\|\nabla h(x_k)h(x_k)\| > \varepsilon\). Therefore, from (21), we have 
\[ \mu_k \geq \mu > 0. \]
It can be deduced from Line 5 of LMLS and Assertion (ii) that
\[ D_k - \psi(x_{k+1}) \geq -\sigma \alpha_k \nabla \psi(x_k)^T d_k \geq c_1 \sigma \alpha_k \|\nabla \psi(x_k)\|^2 \geq c_1 \sigma \hat{\alpha} \|\nabla \psi(x_k)\|^2. \] (33)
Together with the assertion (i), this yields
\[ \lim_{k \to \infty} \|\nabla \psi(x_k)\| = \lim_{k \to \infty} \|\nabla h(x_k)h(x_k)\| = 0, \]
i.e. any accumulation point of \(\{x_k\}\) is a stationary point of \(\psi\).

We continue the analysis of LMLS by providing the worst-case global and evaluation complexities of LMLS, which are upper bounds on the number of iterations and merit function evaluations required to get an approximate stationary point of \(\psi\) satisfying \(\|\nabla \psi(x)\| \leq \varepsilon\), for the accuracy parameter \(\varepsilon\), respectively. Let us denote by \(N_i(\varepsilon)\) and \(N_f(\varepsilon)\) the total number of iterations and merit function evaluations of LMLS required to find an \(\varepsilon\)-stationary point of (2).

**Theorem 2.3 (complexity analysis):** Let \(\{x_k\}\) be the sequence generated by LMLS and (A1) and (A2) hold. Then, the following statements are true:

(i) the total number of iterations to guarantee \(\|\nabla \psi(x_k)\| \leq \varepsilon\) is bounded above and
\[ N_i(\varepsilon) \leq [c_2^{-1}\psi(x_0)\varepsilon^{-2} + 1], \] (34)
with \(c_2 := c_1 \sigma \hat{\alpha}(1 - \theta_{\text{max}})\);

(ii) the total number of function evaluations to guarantee \(\|\nabla \psi(x_k)\| \leq \varepsilon\) is bounded above and
\[ N_f(\varepsilon) \leq \frac{[c_2^{-1}\psi(x_0)\varepsilon^{-2} + 1](\log(\hat{\alpha}) - \log(\alpha))}{\log(\rho)}. \] (35)

**Proof:** To prove Assertion (i), we define
\[ \hat{k} := [c_2^{-1}\psi(x_0)\varepsilon^{-2} + 1], \]
which suggests
\[ c_2 \varepsilon^{2\hat{k}} = c_2 \varepsilon^2 [c_2^{-1}\psi(x_0)\varepsilon^{-2} + 1] > \psi(x_0). \] (36)
Let us assume by contradiction that \(N_i(\varepsilon) > \hat{k}\), which means that the algorithm does not stop in \(\hat{k}\) iterations. From Line 5 of LMLS, (15), and Theorem 2.2 (ii), we obtain, for all \(k = \hat{k} - 1\),
\[ D_k - D_{k+1} = (1 - \theta_k)(D_k - \psi(x_{k+1})) \geq -\sigma \hat{\alpha}(1 - \theta_k)\nabla \psi(x_k)^T d_k. \]
\[
\geq -\sigma \hat{\alpha}(1 - \theta_{\text{max}}) \nabla \psi(x_k)^T d_k \geq c_1 \sigma \hat{\alpha}(1 - \theta_{\text{max}}) \|\nabla \psi(x_k)\|^2
\]
\[
= c_2 \|\nabla \psi(x_k)\|^2,
\]
leading to
\[
\psi(x_0) = D_0 \geq D_0 - D_k = \sum_{i=0}^{k-1} (D_i - D_{i+1}) \geq c_2 \sum_{i=0}^{k-1} \|\nabla \psi(x_i)\|^2 \geq c_2 \varepsilon^2 k,
\]
which contradicts (36). Therefore, (34) is valid.

Considering the bound on the number of merit function evaluations in step \(k\) (\(\ell_k\), given in Proposition 2.1), the following upper bound on the total number of merit function evaluations can be provided by
\[
N_f(\varepsilon) \leq \sum_{k=0}^{N(\varepsilon)} \ell_k \leq \sum_{k=0}^{N(\varepsilon)-1} \frac{\log(\hat{\alpha}) - \log(\alpha)}{\log(\rho)}
\]
\[
\leq \left[ c_2^{-1} \psi(x_0)\varepsilon^{-2} + 1 \right] \frac{\log(\hat{\alpha}) - \log(\alpha)}{\log(\rho)},
\]
giving the results.

Theorem 2.3 implies that the worst-case global and evaluation complexities of LMLS to attain the approximate stationary point of \(\psi\) are of the order \(O(\varepsilon^{-2})\), which is the same as the gradient method; see, e.g. [39]. However, in practice Levenberg–Marquardt methods usually perform much better than the gradient method.

Let us compute here the second derivative of \(\psi\) at \(x\), i.e.
\[
\nabla^2 \psi(x) = \nabla h(x) \nabla h(x)^T + \sum_{i=1}^{m} h_i(x) \nabla^2 h_i(x) = \nabla h(x) \nabla h(x)^T + S(x),
\]  
(37)
where \(S(x) := \sum_{i=1}^{m} h_i(x) \nabla^2 h_i(x)\). Three types of the problem (1) are recognized with respect to the magnitude of \(\|h(x^*)\|\): (i) if \(h(x^*) = 0\), the problem is called zero residual; (ii) if \(\|h(x^*)\|\) is small, the problem is called small residual; and if \(\|h(x^*)\|\) is large, the problem is called large residual; see, e.g. [16]. Under the full (column) rank assumption of \(\nabla h(x)\) at the limit point \(x^*\) of \(\{x_k\}\) (i.e. rank \(\nabla h(x^*) = n\)) and using (37), we investigate the superlinear convergence of \(\{x_k\}\) generated by LMLS for zero residual problems, which is the same as the convergence rate given for quasi-Newton methods; see [15].

**Theorem 2.4 (local convergence under full rank assumption):** Let \(\psi : \mathbb{R}^m \rightarrow \mathbb{R}\) be twice continuously differentiable on \(L(x_0)\), and \(\{x_k\}\) be the sequence generated by LMLS and (A1)–(A2) hold. If the sequence \(\{x_k\}\) converges to \(x^*\) and \(\nabla h(x^*)\) has full rank, then
\[
\lim_{k \to \infty} \frac{\|\nabla \psi(x_k) + \nabla^2 \psi(x_k)d_k\|}{\|d_k\|} = 0,
\]  
(38)
there exists \(\bar{k} \geq 0\) such that \(\alpha_k = 1\) for all \(k \geq \bar{k}\), and \(\{x_k\}\) converges to \(x^*\) superlinearly.
**Proof:** Since $\nabla h(x^*)$ has full rank, (30) implies $h(x^*) = 0$. This and (37) yield that $\nabla^2 \psi(x^*)$ is positive definite. Hence, $h(x^*) = 0$ leads to

$$\lim_{k \to \infty} \mu_k \leq \xi_{\max} \lim_{k \to \infty} \|h(x_k)\|^n + \omega_{\max} \lim_{k \to \infty} \|\nabla \psi(x_k)\|^n = 0. \tag{39}$$

From (37), we obtain

$$\nabla \psi(x_k) + \nabla^2 \psi(x_k) d_k = (S(x_k) - \mu_k I) d_k,$$

which implies

$$\frac{\|\nabla \psi(x_k) + \nabla^2 \psi(x_k) d_k\|}{\|d_k\|} \leq \frac{\|S(x_k) - \mu_k I\| \|d_k\|}{\|d_k\|} \leq \|S(x_k)\| + \mu_k = \| \sum_{i=1}^m h_i(x) \nabla^2 h_i(x) \| + \mu_k \leq \sum_{i=1}^m \|h_i(x_k)\| \|\nabla^2 h_i(x)\| + \mu_k.$$

Since $\psi$ is twice continuously differentiable in the compact set $\mathcal{L}(x_0)$, $\|\nabla^2 h_i(x)\|$ ($i = 1, \ldots, m$) is bounded. This, the last inequality, and (39) give

$$\lim_{k \to \infty} \frac{\|\nabla \psi(x_k) + \nabla^2 \psi(x_k) d_k\|}{\|d_k\|} \leq \lim_{k \to \infty} \sum_{i=1}^m \|h_i(x_k)\| \|\nabla^2 h_i(x)\| + \lim_{k \to \infty} \mu_k = 0,$$

giving (38).

From Theorem 6.4 in [15] and (38), we have that (8) is valid with $\alpha_k = 1$, for all $k$ sufficiently large. Therefore, the superlinear convergence of $\{x_k\}$ follows from Theorem 3.1 in [15]. \[\square\]

**Remark 2.5:** Instead of full rank assumption in Theorem 2.4, using the technique developed in [4, Theorem 1], we can also deduce the local convergence of LMLS provided that $h$ satisfies Hölder metric subregularity, which is strictly weaker than full rank assumption. Moreover, if the merit function $\psi$ satisfies the Łojasiewicz gradient inequality (see Definition 3.4), then the convergent rate of LMLS can be obtained similarly to that of [4, Theorem 2], see also Theorem 3.5 in Section 3.

3. **Levenberg–Marquardt quadratic regularization method**

This section concerns with the development of a globally convergent Levenberg–Marquardt method using a quadratic regularization technique and the investigation on its convergence analysis and complexity.

Let us start with some details of a quadratic regularization globalization technique that will be coupled with the Levenberg–Marquardt direction. We first draw your attention to some literature, e.g. [1,3] and references therein, about the efficiency of non-monotone quadratic regularization methods compared to monotone ones for either optimization or
nonlinear systems. This motivates us to develop a non-monotone Levenberg–Marquardt quadratic regularization method for solving systems of nonlinear equations. To do so, we take advantage of the quadratic function $q_k$ and define the ratio

$$
\hat{r}_k := \frac{D_k - \psi(x_k + d_k)}{q_k(0) - q_k(d_k)},
$$

where the non-monotone term $D_k$ defined by (12). In this ratio, the nominator is called non-monotone reduction and the denominator is called the predicted reduction. Further, let us introduce a new Levenberg–Marquardt parameter that is a modified version of (7), i.e.

$$
\hat{\mu}_k := \max \{\mu_{\min}, \lambda_k \mu_k\},
$$

where $\mu_k$ is given by (7) with $\eta \in ]0, 4[\), $\xi_k \in [\xi_{\min}, \xi_{\max}]$, $\omega_k \in [\omega_{\min}, \omega_{\max}]$ with $\xi_{\min} + \omega_{\min} > 0$, and $\lambda_k$ is updated by

$$
\lambda_{k+1} := \begin{cases} 
\rho_1 \lambda_k & \text{if } \hat{r}_k < \nu_1, \\
\lambda_k & \text{if } \nu_1 \leq \hat{r}_k < \nu_2, \\
\rho_2 \lambda_k & \text{if } \hat{r}_k \geq \nu_2,
\end{cases}
$$

in which $0 < \rho_2 < 1 < \rho_1$ and $0 < \nu_1 < \nu_2 < 1$ are some constants. A simple comparison between (7) and (41) indicates that $\hat{\mu}_k$ is lower bounded and $\lambda_k$ helps to have a better control on the Levenberg–Marquardt parameter, which shows its effect on numerical performance of the method (see Section 5 for more details).

In our Levenberg–Marquardt quadratic regularization method, we first determine $\hat{\mu}_k$ (41), specify the direction $d_k$ by solving the linear system (6), and compute the ratio $\hat{r}_k$ (40). If $\hat{r}_k \geq \nu_1$, the trial point $d_k$ is accepted, i.e. $x_{k+1} = x_k + d_k$; otherwise, the parameter $\lambda_k$ should be increased by setting $\lambda_k = \rho_1 \lambda_k$. In the case that $\hat{r}_k \geq \nu_2$, the parameter $\lambda_k$ is decreased by setting $\lambda_{k+1} = \rho_2 \lambda_k$. The final step will be the evaluation of stopping criteria, which here is either $\|h(x_{k+1})\| \leq \varepsilon$ or $\|\nabla \psi(x_{k+1})\| \leq \varepsilon$. We summarize this scheme in Algorithm 2.

In LMQR, the loop starts from Line 5 to Line 7 is called the inner loop and the loop starts from Line 3 to Line 14 is called the outer loop. Moreover, one may use $\|h(x_k)\| > \varepsilon$ or $\|\nabla \psi(x_k)\| > \varepsilon$ as a stopping criterion in LMQR.

The subsequent proposition points out that the inner loop of LMQR is terminated after a finite number of steps and provides upper bounds for $\hat{\mu}_k$ and $p_k$.

**Proposition 3.1 (well-definedness of LMQR):** Let $\{x_k\}$ be an infinite sequence generated by LMQR and (A1)–(A2) holds. Then, for all $k \geq 0$, the following statements are true:

1. $q_k(0) - q_k(d_k) \geq 1/(2(L_0^2 + \mu_{\min})) \|\nabla \psi(x_k)\|^2$;
2. $q_k(0) - q_k(d_k) \leq (1/2)L_0^2 + \hat{\mu}_k \|d_k\|^2$;
3. the inner loop is terminated in a finite number of steps. Further, if $\|h(x_k)\| > \varepsilon$ and $\|\nabla h(x_k)h(x_k)\| > \varepsilon$ for all $k = 0, \ldots, k$, then

$$
\hat{\mu}_k \leq \tau,
$$

(42)
Algorithm 2: LMQR (Levenberg–Marquardt Quadratic Regularization algorithm)

**Input:** \( x_0 \in \mathbb{R}^m, \eta > 0, \varepsilon > 0, 0 < \rho_2 < 1 < \rho_1, 0 < \nu_1 < \nu_2 < 1, \mu_{\text{min}} > 0, \)
\( \xi_0 \in [\xi_{\text{min}}, \xi_{\text{max}}], \omega_0 \in [0, \omega_{\text{max}}], \theta_0 \in [\theta_{\text{min}}, \theta_{\text{max}}]; \)

1. begin
   2. \( k := 0; \lambda_0 = 1; \mu_0 := \max \{\mu_{\text{min}}, \lambda_0 (\xi_0 \|h(x_0)\|^\eta + \omega_0 \|\nabla h(x_0)h(x_0)\|^{\eta})\}; \)
   3. while a stopping criterion does not satisfy do
      4. solve the linear system (6) to specify \( d_k; \) compute \( \hat{r}_k \) by (40); \( p = 0; \)
      5. while \( \hat{r}_k < \nu_1 \) do
         6. \( p = p + 1, \lambda_k = \rho_1^p \lambda_k; \) solve (6) to specify \( d_k; \) compute \( \hat{r}_k \) by (40);
      6. end
      7. if \( \hat{r}_k \geq \nu_2 \) then
         8. \( \lambda_{k+1} = \rho_2 \lambda_k; \)
      9. else
         10. \( \lambda_{k+1} = \lambda_k; \)
      11. end
      12. \( p_k = p; x_{k+1} = x_k + d_k; \) update \( \xi_k, \omega_k, \) and \( \theta_k; \) update \( \mu_k \) and \( D_k \) by (7) and (12); \( k = k + 1; \)
   7. end

with
\[
\tau := \frac{\rho_1}{(1 - \nu_1)} \left( \frac{1}{2} (1 + \nu_1)L_0^2 + \frac{1}{2} L_0^2 \mu_{\text{min}}^{-2} \|h(x_0)\|^2 + (1 + L_0^2 \mu_{\text{min}}^{-1}) L \|h(x_0)\| \right),
\]
and
\[
p_k \leq \frac{\log(\tau) - \log(\mu_{\text{min}}))}{\log(\rho_1)}. \tag{43}
\]

**Proof:** By the definition of \( q_k \) in (9) and (19), we get
\[
q_k(0) - q_k(d_k) \geq \frac{1}{2} \|h(x_k)\|^2 - \frac{1}{2} \|\nabla h(x_k)^T d_k + h(x_k)\|^2 - \frac{1}{2} \hat{\mu}_k \|d_k\|^2
\]
\[
= -\frac{1}{2} d_k^T H_k d_k - \nabla \psi(x_k)^T d_k = \frac{1}{2} \nabla \psi(x_k)^T H_k^{-1} \nabla \psi(x_k)
\]
\[
\geq \frac{1}{2(L_0^2 + \mu_{\text{min}})} \|\nabla \psi(x_k)\|^2, \tag{44}
\]
giving Assertion (i).

It follows from (9) that
\[
q_k(0) - q_k(d_k) = \frac{1}{2} \|h(x_k)\|^2 - \frac{1}{2} \|\nabla h(x_k)^T d_k + h(x_k)\|^2
\]
\[
= -\frac{1}{2} d_k^T \nabla h(x_k) \nabla h(x_k)^T d_k - h(x_k)^T \nabla h(x_k)^T d_k
\]
proving Assertion (ii).

For the first part of the assertion (iii), we show that the inner loop is terminated after a finite number of steps. From Assertion (i) and (20), we obtain

\[
q_k(0) - q_k(d_k) \geq \frac{1}{2(L_0^2 + \mu_{\min})} \| \nabla \psi(x_k) \|^2 \geq \frac{\mu_k^2}{2(L_0^2 + \mu_{\min})} \| d_k \|^2.
\]

(46)

By (A1) and (20), for \( t \in [0, 1] \), we get

\[
\| \nabla (h(x_k + td_k) - h(x_k)) \| \leq tL \| d_k \| \leq tL\mu_k^{-1} \| \nabla \psi(x_k) \| \leq LL_0\mu_k^{-1} \| h(x_k) \|.
\]

(47)

By the Taylor expansion of \( \psi(x_k + d_k) \) around \( x_k \), we come to

\[
\psi(x_k + d_k) = \frac{1}{2} \| h(x_k + d_k) \|^2 = \frac{1}{2} \| h(x_k) + \nabla h(x_k)^T d_k \\
+ \int_0^1 (\nabla h(x_k + td_k) - \nabla h(x_k))^T d_k \, dt \|^2
\]

\[
= \frac{1}{2} \| h(x_k) + \nabla h(x_k)^T d_k \|^2 + \frac{1}{2} \| \int_0^1 (\nabla h(x_k + td_k) - \nabla h(x_k))^T d_k \, dt \|^2
\]

\[
+ (h(x_k) + \nabla h(x_k)^T d_k)^T \int_0^1 (\nabla h(x_k + td_k) - \nabla h(x_k))^T d_k \, dt.
\]

(48)

From this, (23), and (47), it consequently holds

\[
|q_k(d_k) - \psi(x_k + d_k)| = \frac{1}{2} \| \nabla h(x_k)^T d_k + h(x_k) \|^2 - \psi(x_k + d_k)
\]

\[
= \frac{1}{2} \left\| \int_0^1 (\nabla h(x_k + td_k) - \nabla h(x_k))^T d_k \, dt \right\|^2
\]

\[
+ (h(x_k) + \nabla h(x_k)^T d_k)^T \int_0^1 (\nabla h(x_k + td_k) - \nabla h(x_k))^T d_k \, dt
\]

\[
\leq \frac{1}{2} \left( \int_0^1 \| \nabla h(x_k + td_k) - \nabla h(x_k) \| \, dt \right)^2
\]

\[
+ \| h(x_k) + \nabla h(x_k)^T d_k \| \int_0^1 \| \nabla h(x_k + td_k) - \nabla h(x_k) \| \, dt
\]

\[
\leq \left( \frac{1}{2} L_0^2 L_0^2 \| h(x_k) \|^2\mu_k^{-2} + (1 + L_0^2 \mu_k^{-1}) \| h(x_k) \| \right) \| d_k \|^2.
\]

(49)

Since \( \hat{r}_{k-1} \geq \nu_1 \), we have \( \psi(x_k) \leq D_{k-1} \). This and

\[
D_k - D_{k-1} = (1 - \theta_{k-1})(\psi(x_k) - D_{k-1}) \leq 0, \quad D_k - \psi(x_k) = \theta_{k-1}(D_{k-1} - \psi(x_k)) \geq 0
\]

(50)
imply \( D_k \leq D_{k-1} \) and \( \psi(x_k) \leq D_k \), leading to \( \psi(x_k) \leq D_k \leq D_{k-1} \leq \ldots \leq D_0 = \psi(x_0) \), i.e.

\[
x_k \in L(x_0).
\]

(51)

It can be deduced from this and (49) that

\[
|q_k(d_k) - \psi(x_k + d_k)| \leq \left( \frac{1}{2}L^2_0 \|h(x_0)\|^2 \tilde{\mu}^{-2} + (1 + L^2_0 \tilde{\mu}^{-1})\|h(x_0)\| \right) \|d_k\|^2
\]

where \( \tilde{\mu} := \frac{1}{2}L^2_0 \|h(x_0)\|^2, \tilde{\mu}_1 := L^2_0\|h(x_0)\|, \) and \( \tilde{\mu}_2 := \|h(x_0)\|. \) For sufficiently large \( p_k \), we have \( \tilde{\mu}_k = \rho_1^p \lambda_k \mu_k \). This, (10), and (46) yield

\[
|r_k - 1| = \frac{|q_k(d_k) - \psi(x_k + d_k)|}{q_k(0) - q_k(d_k)} \leq \frac{2(L^2_0 + \mu_{\min}) (\tilde{\mu}_0 + \tilde{\mu}_1 \rho_1^p \lambda_k \mu_k + \tilde{\mu}_2 \rho_1^2 \lambda_k^2 \mu_k^2)}{\rho_1^{4p} \lambda_k^4 \mu_k^4} \to 0, \text{ as } p_k \to +\infty.
\]

(52)

It can be deduced from this and \( \psi(x_k) \leq D_k \) that \( \tilde{\mu}_k \geq r_k \geq \nu_1 \), for sufficiently large \( p_k \), proving the first part of Assertion (iii).

In the second part of Assertion (iii), we provide upper bounds for \( \tilde{\mu}_k \) and \( p_k \). Let us denote by \( \tilde{\mu}_k \) the solution of the system (6) corresponding to the parameter \( \tilde{\mu}_k := \rho_1^{p_k} \lambda_k \mu_k \) and set \( \tilde{x}_{k+1} = x_k + \tilde{d}_k \). By (20) and (18), we get

\[
\|\tilde{d}_k\| \leq \tilde{\mu}_k^{-1} \|\nabla \psi(x_k)\| \leq \tilde{\mu}_k^{-1} \|\nabla h(x_k)\| \|h(x_k)\| \leq \tilde{\mu}_k^{-1} L_0 \|h(x_0)\| \leq \mu_{\min}^{-1} L_0 \|h(x_0)\|.
\]

(53)

It follows from this and the triangle inequality that

\[
\|h(x_k) + \nabla h(x_k)^T \tilde{d}_k\| \leq \|h(x_k)\| + \|\nabla h(x_k)\| \|\tilde{d}_k\| \leq (1 + L_0^2 \mu_{\min}^{-1}) \|h(x_0)\|.
\]

(54)

For all \( t \in [0, 1] \), (A1) and (53) imply

\[
\|\nabla h(x_k + t\tilde{d}_k) - \nabla h(x_k)\| \leq L \|\tilde{d}_k\| \leq L L_0 \mu_{\min}^{-1} \|h(x_0)\|.
\]

(55)

From (18), (25), (48), and (11), we obtain

\[
\psi(x_k + \tilde{d}_k) \leq \psi(x_k) + \nabla \psi(x_k)^T \tilde{d}_k + \left( \frac{1}{2}L^2_0 + \frac{1}{2}L^2_0 \mu_{\min}^{-2} \|h(x_0)\|^2 + (1 + L^2_0 \mu_{\min}^{-1}) L \|h(x_0)\| \right) \|\tilde{d}_k\|^2.
\]

Following \( \psi(x_k) \leq D_k \) and \( \nabla \psi(x_k)^T \tilde{d}_k = -\tilde{d}_k^T H_k \tilde{d}_k \leq -\tilde{\mu}_k \|\tilde{d}_k\|^2 \), it can be deduced

\[
\psi(x_k + \tilde{d}_k) \leq D_k - \tilde{\mu}_k \|\tilde{d}_k\|^2
\]

\[
+ \left( \frac{1}{2}L^2_0 + \frac{1}{2}L^2_0 \mu_{\min}^{-2} \|h(x_0)\|^2 + (1 + L^2_0 \mu_{\min}^{-1}) L \|h(x_0)\| \right) \|\tilde{d}_k\|^2.
\]

(56)
It follows from (45) and the definition $\overline{\mu}_k$ that $\hat{\mu}_k < \nu_1$ and
\[
D_k - \psi(x_k + \overline{d}_k) < \nu_1(q_k(0) - q_k(\overline{d}_k)) \leq \nu_1 \left( \frac{1}{2} L_0^2 + \overline{\mu}_k \right) \|\overline{d}_k\|^2.
\]
Combining this inequality with that in (56) suggest
\[
\left( \overline{\mu}_k - \frac{1}{2} L_0^2 - \frac{1}{2} L_0^2 L_0^{-2} \mu_{\min} \|h(x_0)\|^2 \right)
- (1 + L_0^{-1} L \|h(x_0)\|) \|\overline{d}_k\|^2 \leq \nu_1 \left( \frac{1}{2} L_0^2 + \overline{\mu}_k \right) \|\overline{d}_k\|^2,
\]
leading to
\[
\hat{\mu}_k = \rho_1 \overline{\mu}_k \leq \frac{\rho_1}{1 - \nu_1} \left( \frac{1}{2} (1 + \nu_1) L_0^2 + \frac{1}{2} L_0^2 L_0^{-2} \mu_{\min} \|h(x_0)\|^2 + (1 + L_0^{-1} L \|h(x_0)\|) \right),
\]
giving (42). Since $\hat{\mu}_k = \rho_1^{pk} \lambda_k \mu_k$, taking the logarithm from both sides of
\[
\tau \geq \rho_1^{pk} \lambda_k \mu_k \geq \rho_1^{pk} \mu_{\min},
\]
implies (43), completing the proof.

We now draw your attention to the global convergence of the sequence $\{x_k\}$ generated by LMQR to a first-order stationary point $x^*$ of $\psi$ satisfying $\nabla \psi(x^*) = 0$.

**Theorem 3.2 (global convergence):** Let $\{x_k\}$ be the sequence generated by LMQR and (A1)–(A2) hold. Then, the sequences $\{\psi(x_k)\}$ and $\{D_k\}$ are convergent and
\[
\lim_{k \to \infty} D_k = \lim_{k \to \infty} \psi(x_k).
\] (57)

Further, the algorithm either stops at finite number of iterations, satisfying $\|h(x_k)\| \leq \varepsilon$ or $\nabla \psi(x_k) \leq \varepsilon$, or generates an infinite sequence $\{x_k\}$ such that any accumulation point of this sequence is a stationary point of the merit function $\psi$, i.e.
\[
\lim_{k \to \infty} \|\nabla \psi(x_k)\| = 0.
\] (58)

**Proof:** From (50) and (51), we have $D_k \leq D_{k-1}$ and $x_k \in \mathcal{L}(x_0)$. Hence, the sequence $\{D_k\}$ is decreasing and bounded below, i.e. it is convergent. From $\theta_k \in [\theta_{\min}, \theta_{\max}]$, with $\theta_{\max} \in [0, 1]$, we obtain $1 - \theta_k \geq 1 - \theta_{\max} > 0$. Taking limits when $k$ goes to infinity from $D_k \leq \psi(x_k) \leq D_{k-1}$ gives (57).

If the algorithm stops in a finite number of iterations by either $\|h(x_k)\| \leq \varepsilon$ or $\nabla \psi(x_k) \leq \varepsilon$, the result is valid. If the algorithm generates the infinite sequence $\{x_k\}$, Proposition 3.1 (i) yields
\[
D_k - \psi(x_{k+1}) \geq \nu_1(q(0) - q(d_k)) \geq \frac{\nu_1}{2(L_0^2 + \mu_{\min})} \|\nabla \psi(x_k)\|^2 \geq 0.
\]
From this and (57), we obtain
\[
\lim_{k \to \infty} \|\nabla \psi(x_k)\| = \lim_{k \to \infty} \|\nabla h(x_k)h(x_k)\| = 0,
\]
i.e. any accumulation point of $\{x_k\}$ is a stationary point of $\psi$. ■
Let us continue this section by providing global and evaluation complexities of the sequence \( \{ x_k \} \) generated by LMQR using the results presented in Proposition 3.1.

**Theorem 3.3 (complexity analysis):** Let \( \{ x_k \} \) be the sequence generated by LMQR and (A1)–(A2) hold. Then, the following statements are true:

(i) the total number of iterations to guarantee \( \| \nabla \psi(x_k) \| \leq \varepsilon \) is bounded above by

\[
N_i(\varepsilon) \leq \lceil \bar{c}_3^{-1}\psi(x_0)\varepsilon^{-2} + 1 \rceil, \tag{59}
\]

where \( \bar{c}_3 := v_1(1 - \eta_{\max})/(2(L_0^2 + \mu_{\min})) \);

(ii) the total number of function evaluations to guarantee \( \| \nabla \psi(x_k) \| \leq \varepsilon \) is bounded above by

\[
N_f(\varepsilon) \leq \lceil \bar{c}_3^{-1}\psi(x_0)\varepsilon^{-2} + 1 \rceil \left( \frac{\log(\tau) - \log(\mu_{\min})}{\log(\rho_1)} \right), \tag{60}
\]

**Proof:** To prove Assertion (i), we first define

\[
\tilde{k} := \lceil \bar{c}_3^{-1}\psi(x_0)\varepsilon^{-2} + 1 \rceil,
\]

which is equivalent to

\[
\bar{c}_3\varepsilon^2\tilde{k} = \bar{c}_3\varepsilon^2\lceil \bar{c}_3^{-1}\psi(x_0)\varepsilon^{-2} + 1 \rceil > \psi(x_0). \tag{61}
\]

Let us assume by contradiction that \( N_i(\varepsilon) > \tilde{k} \), which means that LMQR does not stop in \( \tilde{k} \) iterations. For a successful iteration \( k \) of LMQR, it follows from (15) and Proposition 3.1 (i) that

\[
D_k - D_{k+1} = (1 - \theta_k)(D_k - \psi(x_{k+1})) \geq v_1(1 - \theta_k)(q(0) - q(d_k)) \geq \frac{v_1(1 - \eta_{\max})}{2(L_0^2 + \mu_{\min})}\| \nabla \psi(x_k) \|^2 = \bar{c}_3\| \nabla \psi(x_k) \|^2,
\]

leading to

\[
\psi(x_0) = D_0 \geq D_0 - D_{\tilde{k}} = \sum_{i=0}^{\tilde{k}-1}(D_i - D_{i+1}) \geq \bar{c}_3 \sum_{i=0}^{\tilde{k}-1}\| \nabla \psi(x_i) \|^2 > \bar{c}_3\varepsilon^2\tilde{k},
\]

which contradicts to (61), proving Assertion (i).

From (43) and (59), we obtain

\[
N_f(\varepsilon) \leq \sum_{k=0}^{N_i(\varepsilon)-1} p_k \leq \sum_{k=0}^{N_i(\varepsilon)-1} \frac{\log(\tau) - \log(\mu_{\min})}{\log(\rho_1)} \leq \lceil \bar{c}_3^{-1}\psi(x_0)\varepsilon^{-2} + 1 \rceil \left( \frac{\log(\tau) - \log(\mu_{\min})}{\log(\rho_1)} \right),
\]

giving (60). \( \blacksquare \)
We conclude this section by providing the local convergence rate of LMQR if the corresponding sequence \(\{x_k\}\) is convergent to a solution of (1) under the Łojasiewicz gradient inequality (see [35,36]). To this end, the presence of the subsequent two facts are necessary in our local analysis of LMQR.

**Fact 3.1 ([7, Lemma 1]):** Let \(\{s_k\}\) be a sequence in \(\mathbb{R}_+\) and let \(\zeta, \nu\) be some non-negative constants. Suppose that \(s_k \to 0\) and that the sequence satisfies

\[
s_k^\zeta \leq \nu(s_k - s_{k+1}),
\]

for all \(k\) sufficiently large. Then

(i) if \(\zeta = 0\), the sequence \(\{s_k\}\) converges to 0 in a finite number of steps;

(ii) if \(\zeta \in [0,1]\), the sequence \(\{s_k\}\) converges linearly to 0 with rate \(1 - (1/\nu)\);

(iii) if \(\zeta > 1\), there exists \(\varsigma > 0\) such that, for all \(k\) sufficiently large,

\[
s_k \leq \varsigma k^{(-1/(\zeta-1))}.
\]

**Fact 3.2 ([29, Theorem 2.5 and Lemma 2.3]):** The sequence \(\{x_k\}\) generated by LMQR with \(p = 0\) satisfies

\[
\|d_k\| \leq \frac{1}{2\sqrt{\hat{\mu}_k}}\|h(x_k)\|,
\]

and

\[
\|h(x_{k+1})\|^2 \leq \|h(x_k)\|^2 + d_k^T \nabla h(x_k) h(x_k) + \|d_k\|^2 \left[ \frac{L^2}{4} \|d_k\|^2 + L \|h(x_k)\| - \hat{\mu}_k \right].
\]

Let us describe now the Łojasiewicz gradient inequality in the following definition.

**Definition 3.4 (Łojasiewicz gradient inequality):** Let \(\psi : U \to \mathbb{R}\) be a function defined on an open set \(U \subseteq \mathbb{R}^m\), and assume that the set of zeros \(\Omega := \{x \in \mathbb{R}^m, \psi(x) = 0\}\) is non-empty. The function \(\psi\) is said to satisfy the Łojasiewicz gradient inequality if for any critical point \(\bar{x}\), there exist constants \(\kappa > 0, \varepsilon > 0\) and \(\theta \in [0,1]\) such that

\[
|\psi(x) - \psi(\bar{x})|^\theta \leq \kappa \|\nabla \psi(x)\|, \quad \forall x \in B(\bar{x}, \varepsilon).
\]

This inequality is valid for a large class of functions such as analytic, subanalytic, and semialgebraic functions, cf. [33,35,36]. See Section 5 for a mapping with a real analytic merit function, where finding zeros of this mapping is the main motivation of this study. Here, we further assume that

(A3) the merit function \(\psi\) satisfies the Łojasiewicz gradient inequality (64).

The next theorem is the third main result of this section, which provides the convergence of the sequences \(\{\text{dist}(x_k, \Omega)\}\) and \(\{\psi(x_k)\}\) to 0 if an accumulation point \(x^*\) of \(\{x_k\}\) is a solution of the nonlinear system (1).
Theorem 3.5 (local convergence under Łojasiewicz gradient inequality): Suppose that (A3) holds and assume that the sequence \( \{x_k\} \) generated by LMQR is convergent to a solution \( x^* \) of the nonlinear system (1). Then,

(i) for sufficiently large \( k \), it holds that \( p_k = 0 \);
(ii) there exist constants \( s > 0, \tilde{s} > 0 \), and \( k' \in \mathbb{N} \) such that, for \( x_{k'} \in \mathbb{B}(x^*, s) \),

\[
\{x_k\}_{k \geq k'} \subset \mathbb{B}(x^*, \tilde{s}), \quad \{\psi(x_k)\} \to 0, \quad \{\text{dist}(x_k, \Omega)\} \to 0, \quad \text{as } k \to \infty;
\]

(iii) if \( \theta = 0 \), the sequences \( \{\psi(x_k)\} \) and \( \{\text{dist}(x_k, \Omega)\} \) converge to 0 in a finite number of steps;
(iv) if \( \theta \in [0, \frac{1}{2}] \), the sequences \( \{\psi(x_k)\} \) and \( \{\text{dist}(x_k, \Omega)\} \) converge linearly to 0;
(v) if \( \theta \in ]\frac{1}{2}, 1[ \), there exist some positive constants \( \varsigma_1 \) and \( \varsigma_2 \) such that, for all large \( k \),

\[
\psi(x_k) \leq \varsigma_1 k^{-(1/(2\theta - 1))} \quad \text{and} \quad \text{dist}(x_k, \Omega) \leq \varsigma_2 k^{-(\delta/(2(2\theta - 1)))}.
\]

Proof: Since \( x^* \) is an accumulation point of \( \{x_k\} \) and a solution of the nonlinear system (1), it can be deduced

\[
\lim_{k \to \infty} \|h(x_k)\| = 0.
\]

Together with Proposition 3.1(i), (49), \( \|d_k\| \leq \mu_k^{-1} \|\nabla \psi(x_k)\| \), and \( \overline{\mu}_k \geq \mu_{\min} \), this yields

\[
|r_k - 1| = \left| \frac{q_k(d_k) - \psi(x_k + d_k)}{q_k(0) - q_k(d_k)} \right| \leq \frac{2(L_0^2 + \mu_{\min}) \left( \frac{1}{2} L_0^2 L_0^2 \|h(x_k)\|^2 \overline{\mu}_k^{-2} + (1 + L_0^2 \overline{\mu}_k^{-1}) \|h(x_k)\| \|d_k\|^2 \right.}{\|\nabla \psi(x_k)\|^2}
\]

\[
\leq \frac{2(L_0^2 + \mu_{\min}) \left( \frac{1}{2} L_0^2 L_0^2 \|h(x_k)\|^2 + (\overline{\mu}_k^2 + L_0^2 \overline{\mu}_k) \|h(x_k)\| \right)}{\frac{2 \overline{\mu}_k^2 + \mu_{\min} \|h(x_k)\|^2}{\mu_{\min}^4}} \to 0, \quad \text{as } k \to +\infty,
\]

which implies that there exists a \( \overline{k}_0 \in \mathbb{N} \) such that \( r_k \geq \nu_1 \). Hence, for all \( k \geq \overline{k}_0 \), it follows from \( D_k \geq \psi(x_k) \) that

\[
\overline{\tau}_k = \frac{D_k - \psi(x_k + d_k)}{q_k(0) - q_k(d_k)} \geq \frac{\psi(x_k) - \psi(x_k + d_k)}{q_k(0) - q_k(d_k)} = r_k \geq \nu_1,
\]

which means that \( x_{k+1} = x_k + d_k \) with \( p_k = 0 \) that justifies Assertion (i).

We divide the proof of Assertion (ii) into three parts. First, we will provide the values of \( s \) and \( \tilde{s} \). Let us set \( \varepsilon > 0 \) and \( \kappa > 0 \) such that (64) holds and let \( \tilde{s} := \min \{s, \varepsilon\} > 0 \). By the definition of \( \overline{\mu}_k \), (A2), and (42), we get

\[
\overline{\mu}_k \geq \mu_{\min} \quad \text{and} \quad \|\nabla h(x_k)\| + \overline{\mu}_k \leq L_0^2 + \tau, \quad \text{for } x_k \in \mathbb{B}(x^*, \tilde{s}).
\]
By making \( \tilde{s} \) smaller if needed, we can guarantee
\[
\mu_{\min} \geq \frac{2 + \sqrt{5}}{4} L \|h(x)\|, \quad \forall \ x \in \mathbb{B}(x^*, \tilde{s}). \tag{67}
\]

Lipschitz continuity of \( h \) and \( \tilde{s} \leq r < 1 \), for all \( x \in \mathbb{B}(x^*, \tilde{s}) \), lead to
\[
\psi(x) = \frac{1}{2} \|h(x) - h(x^*)\|^2 \leq \frac{L^2}{2} \|x - x^*\|^2 \leq \frac{L^2}{2} \|x - x^*\|. \tag{68}
\]

We now define
\[
\Delta := \frac{2^\theta \kappa L^2(1-\theta)(L_0^2 + \tau)}{(1-\theta)\mu_{\min}}, \quad s := \left( \frac{\tilde{s}}{1 + \Delta} \right)^{\frac{1}{1-\theta}}.
\]

From \( \tilde{s} < 1 \) and \( \theta \in [0,1[ \), we obtain \( s \leq \tilde{s} \).

For \( k' \geq \tilde{k}_0 \), let us choose any \( x_{k'} \in \mathbb{B}(x^*, s) \). Fact 3.2 and \( d_k = -H_k^{-1}\nabla h(x_k)h(x_k) \) imply, for all \( k \in \mathbb{N} \),
\[
\psi(x_{k+1}) \leq \psi(x_k) - \frac{1}{2} d_k^T H_k d_k + \frac{\|d_k\|^2}{2\mu_k} \left( \frac{L^2}{16} \|h(x_k)\|^2 + L\tilde{\mu}_k \|h(x_k)\| - \tilde{\mu}_k^2 \right). \tag{69}
\]

Next, let us show by induction that, for \( i \in \mathbb{N} \),
\[
x_{k'+i} \in \mathbb{B}(x^*, \tilde{s}), \quad \|d_{k'+i-1}\| \leq \frac{2k(\tilde{L}_0^2 + \tau)}{1-\theta} \mu_{\min} \left( \psi(x_{k'+i-1})^{1-\theta} - \psi(x_{k'+i})^{1-\theta} \right) \tag{70}\]

It follows from \( x_{k'} \in \mathbb{B}(x^*, \tilde{s}) \) and (67) that
\[
\tilde{\mu}_k' \geq \mu_{\min} \geq \frac{2 + \sqrt{5}}{4} L \|h(x_{k'})\|, \]
leading to
\[
\frac{L^2}{16} \|h(x_{k'})\|^2 + L\tilde{\mu}_k' \|h(x_{k'})\| - \tilde{\mu}_k'^2 \leq 0.
\]

Then, from (69), one can deduce
\[
\psi(x_{k'+1}) \leq \psi(x_k) - \frac{1}{2} d_k^T H_k d_k \leq \psi(x_k) - \frac{\mu_{\min}}{2}\|d_k\|^2. \tag{71}
\]

From the convexity of the function \( \psi(t) := -t^{1-\theta} \) with \( t > 0 \), we come to
\[
\psi(x)^{1-\theta} - \psi(y)^{1-\theta} \geq (1-\theta)\psi(x)^{-\theta} \left( \psi(x) - \psi(y) \right), \quad \forall x, y \in \mathbb{R}^m \setminus \Omega. \tag{72}
\]

This and (71) suggest
\[
\psi(x_{k'})^{1-\theta} - \psi(x_{k'+1})^{1-\theta} \geq \frac{(1-\theta)\mu_{\min}}{2} \psi(x_{k'})^{-\theta} \|d_k\|^2. \tag{73}
\]
It follows from $x_0 \in \mathbb{B}(x^*, s) \subseteq \mathbb{B}(x^*, \tilde{s})$ and (66) that $\|H_0\| \leq (L_0^2 + \tau)$. Hence, by the Łojasiewicz gradient inequality (64), we get

$$\psi(x_k')^\theta \leq \kappa \| \nabla \psi(x_k') \| \leq \kappa \| H_k' \| \| d_k' \| \leq \kappa (L_0^2 + \tau) \| d_k' \|.$$ 

This, (73), and (68) yield

$$\| d_k' \| \leq \frac{2\kappa (L_0^2 + \tau)}{(1 - \theta)\mu_{\min}} \left( \psi(x_k')^{1 - \theta} - \psi(x_k)^{1 - \theta} \right) \leq \frac{2\kappa (L_0^2 + \tau)}{(1 - \theta)\mu_{\min}} \psi(x_k')^{1 - \theta} \leq \Delta \| x_k' - x^* \|^{1 - \theta},$$

which, proves the second assertion in (70) for $i = 1$. Then, we have

$$\| x_{k'+1} - x^* \| \leq \| x_k' - x^* \| + \| d_k' \| \leq \| x_k' - x^* \| + \Delta \| x_k' - x^* \|^{1 - \theta} \leq (1 + \Delta) \| x_k' - x^* \|^{1 - \theta} \leq (1 + \Delta) s^{1 - \theta} = \tilde{s},$$

implying $x_{k'+1} \in \mathbb{B}(x^*, \tilde{s})$. Now, let us assume that (70) holds for all $i = 1, \ldots, k$. From $x_k \in \mathbb{B}(x^*, \tilde{s})$ and (67), it can be deduced

$$\hat{\mu}_{k' + k} \geq \mu_{\min} \geq \frac{2 + \sqrt{5}}{4} L \| h(x_{k' + k}) \|,$$

leading to

$$\frac{L^2}{16} \| h(x_{k' + k}) \|^2 + L \hat{\mu}_{k' + k} \| h(x_{k' + k}) \| - \hat{\mu}_{k' + k}^2 \leq 0.$$ 

It follows from this and (69) that

$$\psi(x_{k' + k} + 1) \leq \psi(x_{k' + k}) - \frac{1}{2} d_{k' + k}^T H_{k' + k} d_{k' + k} \leq \psi(x_{k' + k}) - \frac{\mu_{\min}}{2} \| d_{k' + k} \|^2.$$ 

(74)

A combination of this inequality and (72) leads to

$$\psi(x_{k' + k})^{1 - \theta} - \psi(x_{k' + k + 1})^{1 - \theta} \geq \frac{(1 - \theta)\mu_{\min}}{2} \psi(x_{k' + k})^{-\theta} \| d_{k' + k} \|^2$$ 

(75)

Further, from $x_{k' + k} \in \mathbb{B}(x^*, \tilde{s})$, (64), and (66), we obtain

$$\psi(x_{k' + k})^\theta \leq \kappa \| \nabla \psi(x_{k' + k}) \| \leq \kappa \| H_{k' + k} \| \| d_{k' + k} \| \leq \kappa (L_0^2 + \tau) \| d_{k' + k} \|.$$ 

By the latter inequality and (75), we come to

$$\| d_{k' + k} \| \leq \frac{2\kappa (L_0^2 + \tau)}{(1 - \theta)\mu_{\min}} \left( \psi(x_{k' + k})^{1 - \theta} - \psi(x_{k' + k + 1})^{1 - \theta} \right),$$

proving the second assertion in (70) for $i = k + 1$. Then, it follows from (68) that

$$\| x_{k' + k + 1} - x^* \| \leq \| x_{k'} - x^* \| + \sum_{i=k'}^{k'+k} \| d_i \|$$
\[
\|x_{k'} - x^*\| + \frac{2\kappa (L_0^2 + \tau)}{(1 - \theta)\mu_{\min}} \sum_{i=k'}^{k'} (\psi(x_i)^{1-\theta} - \psi(x_{i+1})^{1-\theta}) \\
= \|x_{k'} - x^*\| + \frac{2\kappa (L_0^2 + \tau)}{(1 - \theta)\mu_{\min}} (\psi(x_{k'})^{1-\theta} - \psi(x_{k'+1})^{1-\theta}) \\
\leq \|x_{k'} - x^*\| + \frac{2\kappa (L_0^2 + \tau)}{(1 - \theta)\mu_{\min}} \psi(x_{k'})^{1-\theta} \\
\leq (1 + \Delta)\|x_{k'} - x^*\|^{1-\theta} \leq (1 + \Delta)s^{1-\theta} = \delta.
\]

Hence, the first assertion in (70) is valid for \( i = k + 1 \).

Finally, we are in a position to show that Assertions (ii) is true. As shown in (70), \( x_k \in B(x^*,\delta) \) for all \( k \geq k' \). This and (66), implies that \( \|H_k\| \leq (L_0^2 + \tau) \) for all \( k \geq k' \). Hence, for \( k \geq k' \), we have

\[
d_k^T H_k d_k = \nabla \psi(x_k)^T H_k^{-1} \nabla \psi(x_k) \geq \frac{1}{\|H_k\|} \|\nabla \psi(x_k)\|^2 \geq \frac{1}{(L_0^2 + \tau)} \|\nabla \psi(x_k)\|^2.
\]

Then, by (74), we get

\[
\psi(x_{k+1}) \leq \psi(x_k) - \frac{1}{2(L_0^2 + \tau)} \|\nabla \psi(x_k)\|^2.
\]

From this and (64), it can be deduced

\[
\psi(x_{k+1}) \leq \psi(x_k) - \frac{1}{2\kappa^2(L_0^2 + \tau)} \psi(x_k)^{2\theta}, \quad \forall k \geq k',
\]

which implies that \( \{\psi(x_k)\} \) converges to 0. This and the Hölder metric subregularity validate the statement of the assertion (ii).

Applying Fact 3.1 with \( s_k := \psi(x_k) \), \( v := 2\kappa^2(L_0^2 + \tau) \) and \( \zeta := 2\theta \), we have that the convergence rate are dependent to \( \theta \) as claimed in Assertions (iii)–(v). Therefore, the Hölder metric subregularity of \( h \) implies that \( \{\text{dist}(x_k, \Omega)\} \) converges to 0 with the rate given in (iii)–(v).

\[\blacksquare\]

4. Convergence to a solution of nonlinear systems

Let us emphasis that the algorithms LMLS and LMQR only guarantee the sequence \( \{\|\nabla \psi(x_k)\|\} \) goes to zero, which can be a local non-global minimizer of (2), i.e.

\[
\nabla h(x^*)h(x^*) = 0, \quad h(x^*) \neq 0.
\]

Therefore, the remainder of this section concerns with considering more restrictions on the mapping \( h \) such that the global convergence of \( \{x_k\} \) to a solution of (1) is guaranteed.

The next theorem extracts some classical results for cases that \( \nabla h(x^*) \) has full rank, which implies that \( x^* \) is a solution of (1). Moreover, the worst-case global and evaluation complexities to attain solution of (1) are provided under the non-singularity of \( \nabla h(x) \nabla h(x)^T \) for all \( x \in \mathcal{L}(x_0) \). Under the assumption that all accumulation points of \( \{x_k\} \)
are solutions of (1) and $\nabla h(x^*)$ has full rank at the accumulation point $x^*$, it is proved that the whole sequence $\{x_k\}$ converges to the isolated solution $x^*$ of (1).

**Theorem 4.1:** Let $\{x_k\}$ be the sequence generated by LMLS or LMQR and (A1)–(A2) hold. Then, the following statements are true:

(i) if $\nabla h(x^*)$ has full rank at any accumulation point $x^*$ of $\{x_k\}$, then $x^*$ is a solution of the nonlinear system (1).

(ii) if the matrix $\nabla h(x)\nabla h(x)^T$ is non-singular for all $x \in L(x_0)$, i.e. there exists $\lambda > 0$ such that $\lambda_{\min}(\nabla h(x)\nabla h(x)^T) > \lambda$. Then, for LMLS, the total number of iterations and function values to guarantee $\|h(x_k)\| \leq \varepsilon$ are respectively bounded above by

$$
\bar{N}_i(\varepsilon) \leq \left[ \lambda^{-1}c_2^{-1}\psi(x_0)\varepsilon^{-2} + 1 \right]
$$

and

$$
\bar{N}_f(\varepsilon) \leq \frac{[\lambda^{-1}c_2^{-1}\psi(x_0)\varepsilon^{-2} + 1](\log(\overline{\alpha}) - \log(\overline{\alpha}))}{\log(\rho)},
$$

and, for LMQR, the total number of iterations and function values to guarantee $\|h(x_k)\| \leq \varepsilon$ are, respectively, bounded above by

$$
\bar{N}_i(\varepsilon) \leq \left[ \lambda^{-1}c_3^{-1}\psi(x_0)\varepsilon^{-2} + 1 \right]
$$

and

$$
\bar{N}_f(\varepsilon) \leq \left[ \lambda^{-1}c_3^{-1}\psi(x_0)\varepsilon^{-2} + 1 \right]\left(\frac{\log(\tau) - \log(\mu_{\min})}{\log(\rho_1)}\right).
$$

(iii) if all accumulation points of $\{x_k\}$ are solutions of the nonlinear system (1), $x^*$ is an accumulation point of $\{x_k\}$ such that $\nabla h(x^*)$ has full rank and

$$
\lim_{k \to \infty} \|x_{k+1} - x_k\| = 0,
$$

then $\{x_k\}$ converges to $x^*$.

**Proof:** For any accumulation point $x^*$ of $\{x_k\}$, it follows from Theorem 3.2 that $\nabla h(x^*)h(x^*) = 0$. Together with the full rank assumption of $\nabla h(x^*)$, this implies Assertion (i).

To prove Assertion (ii), we note that

$$
\|\nabla \psi(x_k)\|^2 = h(x_k)\nabla h(x_k)\nabla h(x_k)^T h(x_k) \geq \lambda \|h(x_k)\|^2,
$$

i.e. $\|h(x_k)\| \leq \lambda^{-1/2}\|\nabla \psi(x_k)\|$. This and Proposition 2.3 (i)–(ii) give (76) and (77), respectively. Similarly, (78) and (79) follow from this inequality and Proposition 3.3 (i)–(ii).

In order to prove Assertion (iii), let us assume that all accumulation points of $\{x_k\}$ are solutions of (1), $x^*$ is an accumulation point such that $\nabla h(x^*)$ has full rank, and (80) holds. From the inverse function theorem and the full rank assumption, of $\nabla h(x^*)$, there exists a
neighbourhood around 0 such that $h$ is invertible. Therefore, there exists a neighbourhood $B(x^*, r_1)$ for $r_1 > 0$ such that

$$h(x) \neq 0, \quad \forall x \in B(x^*, r_1) \text{ and } x \neq x^*,$$

implying

$$\|h(x)\| > 0, \quad \forall x \in B(x^*, r_1) \text{ and } x \neq x^*.$$

Since $x^*$ is an accumulation point of $\{x_k\}$, $B(x^*, r_1)$ contains an infinite number of iteration points of $\{x_k\}$. It remains to show that there exists $k_2 \in \mathbb{N}$ such that $x_k \in B(x^*, r_1)$, for all $k \geq k_2$. Hence, for an arbitrary $\varepsilon \in (0, r_1)$, the set $B(x^*, r_1) - B(x^*, \varepsilon)$ involves only a finite number of iterations of $\{x_k\}$, i.e. there exists $k_3 \in \mathbb{N}$ such that $x_k \in B(x^*, \varepsilon), \quad \forall k \geq k_3.$

It follows from (80) that there exists $k_4 \in \mathbb{N}$ such that

$$\|x_{k+1} - x_k\| \leq \delta - \varepsilon, \quad \forall k \geq k_3.$$

Let us set $k_2 := \max\{k_3, k_4\}$ leading to

$$\|x_{k+1} - x^*\| \leq \|x_{k+1} - x_k\| + \|x_k - x^*\| \leq \delta, \quad \forall k \geq k_2,$$

giving the result. ■

The mapping $h : \mathbb{R}^m \rightarrow \mathbb{R}^m$ is called strictly monotone if

$$(h(x) - h(y))^T(x - y) > 0, \quad \forall x, y \in \mathbb{R}^m, \quad x \neq y.$$

In addition, the mapping $h$ is called strictly duplomonotone with constant $\tau > 0$ if

$$(h(x) - h(x - \tau h(x)))^T h(x) > 0, \quad \forall x \in \mathbb{R}^m, \quad \tau \in (0, \tau],$$

whenever $h(x) \neq 0$; see [6,44]. In the next result, we will show that if the mapping $h$ or $-h$ is strictly monotone (duplomonotone), then the sequence $\{x_k\}$ generated by LMLS converges to the unique solution of the nonlinear system (1).

**Theorem 4.2:** Let $\{x_k\}$ be the sequence generated by LMLS or LMQR and (A1)–(A2) hold. Then, the following statements are true:

(i) If the mapping $h$ or $-h$ is strictly monotone, then $\{x_k\}$ converges to the unique solution of the nonlinear system (1).

(ii) If the mapping $h$ or $-h$ is strictly duplomonotone, then $\{x_k\}$ converges to a solution of the nonlinear system (1).

**Proof:** In order to prove Assertion (i), let $h$ or $-h$ be strictly monotone and $x^*$ be an accumulation point of $\{x_k\}$. If $h$ is strictly monotone, for the points $x$ and $x + th$ with $t > 0$ and $h \in \mathbb{R}^m$, we can deduce

$$z^T \nabla h(x) z = z^T \left( \lim_{t \to 0} \frac{h(x + tz) - h(x)}{t} \right)$$
\[
\lim_{t \to 0} \left( z^T \frac{h(x + tz) - h(x)}{t} \right) > 0, \quad \forall x, z \in \mathbb{R}^m.
\]

If \(-h\) is strictly monotone, then
\[
z^T \nabla h(x) z = -z^T \left( \lim_{t \to 0} \frac{h(x + tz) - h(x)}{t} \right) = -\lim_{t \to 0} \left( z^T \frac{h(x + tz) - h(x)}{t} \right) < 0, \quad \forall x, z \in \mathbb{R}^m.
\]

By setting \(z = h(x^*)\) and \(x = x^*\) in the last two inequalities, we get

\[h(x^*)^T \nabla h(x^*) h(x^*) \neq 0, \quad \forall h(x^*) \in \mathbb{R}^m, : h(x^*) \neq 0.
\]

This, (30), and (58) imply \(h(x^*) = 0\).

To prove Assertion (ii), let \(h\) be strictly duplomonotone, which leads to

\[
h(x)^T \nabla h(x) h(x) = \left( \lim_{\tau \to 0} \frac{h(x - \tau h(x)) - h(x)}{-\tau} \right)^T h(x)
\]

\[
= \lim_{\tau \to 0} \left( \frac{h(x) - h(x - \tau h(x))}{\tau} \right)^T h(x) > 0, \quad \forall x \in \mathbb{R}^m, \quad \tau \in (0, \bar{\tau}].
\]

If \(-h\) is strictly duplomonotone, then

\[
-h(x)^T \nabla h(x) h(x) = -\left( \lim_{\tau \to 0} \frac{h(x + \tau h(x)) - h(x)}{\tau} \right)^T h(x)
\]

\[
= \lim_{\tau \to 0} \left( \frac{-h(x) + h(x - \tau (-h(x)))}{\tau} \right)^T (-h(x)) > 0, \quad \forall x \in \mathbb{R}^m, \quad \tau \in (0, \bar{\tau}].
\]

The result follows from the last two inequalities at \(x = x^*, (30),\) and (58).

Note that the strict monotonicity of \(h\) does not imply the positive definiteness of \(\nabla h(x)\).

Therefore the results of Theorem 4.2 (i) is not a trivial consequence of Theorem 4.1 (i).

5. **Application to biochemical reaction networks**

In this section, we use the following notation: \(\mathbb{Z}_{m \times n}^+:= \{A \in \mathbb{Z}_{m \times n} \mid A_{ij} \geq 0, \quad i = 1, \ldots, m, \quad j = 1, \ldots, n\}, \mathbb{R}_+^m := \{a \in \mathbb{R}^m \mid a_i \geq 0, \quad i = 1, \ldots, m\}, \text{and } \mathbb{R}^m_+ := \{a \in \mathbb{R}^m \mid a_i > 0, \quad i = 1, \ldots, m\}.\) Let us consider a biochemical reaction network with \(m\) molecular species and \(n\) reversible elementary reactions.\(^1\) We define *forward* and *reverse* stoichiometric matrices, \(F, R \in \mathbb{Z}_{m \times n}^+,\) respectively, where \(F_{ij}\) denotes the stoichiometry\(^2\) of the \(i\)th molecular species in the \(j\)th forward reaction and \(R_{ij}\) denotes the stoichiometry of the \(i\)th molecular species in the \(j\)th reverse reaction. We assume that every reaction conserves mass, i.e. there exists at least a positive vector \(l \in \mathbb{R}^m_+\) such that \((R - F)^T l = 0;\) cf. \cite{21}. The matrix \(N := R - F\) represents net reaction stoichiometry and may be viewed as
an incidence matrix of a directed hypergraph; see [32]. In practice, there are less molecular species than net reactions \((m < n)\). We assume the cardinality of each row of \(F\) and \(R\) is at least one, and the cardinality of each column of \(R - F\) is at least two. The matrices \(F\) and \(R\) are sparse and the sparsity pattern depends on the particular biochemical reaction network being modelled. It is here assumed that \(\text{rank}([F, R]) = m\), which is a requirement for kinetic consistency; cf. [20].

Let \(c \in \mathbb{R}_+^m\) be a vector of molecular species concentrations. For non-negative elementary kinetic parameters \(k_f, k_r \in \mathbb{R}_+^n\), elementary reaction kinetics for forward and reverse elementary reaction rates as \(s(k_f, c) := \exp(\ln(k_f) + F^T \ln(c))\) and \(r(k_r, c) := \exp(\ln(k_r) + R^T \ln(c))\), respectively, where \(\exp(\cdot)\) and \(\ln(\cdot)\) denote the respective componentwise functions; see, e.g. [7,20]. Then, the system of differential equations

\[
\frac{dc}{dt} = N(s(k_f, c) - r(k_r, c)) = N (\exp(\ln(k_f) + F^T \ln(c)) - \exp(\ln(k_r) + R^T \ln(c))) =: -f(c).
\]

\[ (81) \]

shows the deterministic dynamical equation for time evolution of molecular species concentration. A vector \(c^*\) is called a steady state if and only if \(f(c^*) = 0\). Hence, \(c^*\) is a steady state of the biochemical system if and only if

\[ s(k_f, c^*) - r(k_r, c^*) \in \mathcal{N}(N), \]

where \(\mathcal{N}(N)\) stands for the null space of \(N\). The set of steady states \(\Omega_1 = \{c \in \mathbb{R}_+^m, f(c) = 0\}\) will be unchanged if \(N\) is replaced by a matrix \(\tilde{N}\) with the same kernel. Suppose that \(\tilde{N} \in \mathbb{Z}^{r \times n}\) is the submatrix of \(N\) whose rows are linearly independent, then \(\text{rank}(\tilde{N}) = \text{rank}(N) =: r\). If one replaces \(N\) by \(\tilde{N}\) and transforms \((81)\) into logarithmic scale, by letting \(x := \ln(c) \in \mathbb{R}^m, k := [\ln(k_f)^T, \ln(k_r)^T]^T \in \mathbb{R}^{2n}\), then the right-hand side of \((81)\) can be translated to

\[
\tilde{f}(x) := [\tilde{N}, -\tilde{N}] \exp \left( k + [F, R]^T x \right),
\]

\[ (82) \]

where \([\cdot, \cdot, \cdot]\) stands for the horizontal concatenation operator.

Let \(L \in \mathbb{R}^{m-r, m}\) be a basis for the left nullspace of \(N\), i.e. \(L^T N = 0\), where \(\text{rank}(N) = r\) and \(\text{rank}(L) = m - r\). The system satisfies moiety conservation if for any initial concentration \(c_0 \in \mathbb{R}_+^m\), it holds

\[ L c = L \exp(x) = l_0, \]

where \(l_0 \in \mathbb{R}_+^m\). It is possible to compute \(L\) such that each corresponds to a structurally identifiable conserved moiety in a biochemical reaction network; cf. [24]. Therefore, finding the moiety conserved steady state of a biochemical reaction network is equivalent to finding a zero of the mapping

\[
h : \mathbb{R}^m \rightarrow \mathbb{R}^m \quad \text{with} \quad h(x) := \left( \frac{\tilde{f}(x)}{L \exp(x) - l_0} \right).
\]

\[ (83) \]

It was shown by the authors in Section 4.1 of [4] that the merit function \(\psi\) satisfies Łojasiewicz gradient inequality (with an exponent \(\theta \in [0, 1]\)) and the mapping \(h\) is Hölder metrically subregular at \((x^*, 0)\).
Table 1. The list of 21 biological models, where the stoichiometric matrix $N$ is $m \times n$ and rank is the rank of the matrix $N$.

| Model          | $m$ | $n$ | rank |
|----------------|-----|-----|------|
| Ecoli_core     | 72  | 73  | 61   |
| iAF692         | 462 | 493 | 430  |
| iAF1260        | 1520| 1931| 1456 |
| iBSU1103       | 993 | 1167| 956  |
| iCB925         | 415 | 558 | 386  |
| iEcoli        | 924 | 1289| 956  |
| iCB925         | 415 | 558 | 386  |
| iIT341         | 641 | 699 | 589  |
| iJN678         | 727 | 795 | 700  |
| iJR904         | 597 | 757 | 564  |

5.1. Computational results

We find zeros of the mapping (83) with a set of real-world biological data using LMLS and LMQR. In details, we compare the performance of LMLS and LMQR with some state-of-the-art algorithms on a set of 21 biochemical reaction networks given in Table 1. We applied the gradient descent, Gauss–Newton, and trust-region methods to (2) with the mapping (83); however, their performances were poor for this problem, i.e. we did not include them in our comparison with LMLS and LMQR. In Section 4.2 of [4], it is computationally shown that $\nabla h$ is rank-deficient or ill-conditioned at zeros of the mapping $h$ (83) for these biological models. This clearly justifies the reason of unsuccessful performances of mentioned algorithms and vindicates the development of the two adaptive Levenberg–Mardquart methods (LMLS and LMQR) for such difficult problems.

All codes are written in MATLAB and runs are performed on a Dell Precision Tower 7000 Series 7810 (Dual Intel Xeon Processor E5-2620 v4 with 32 GB RAM). We compare LMLS and LMQR with:

- LM-YF: a Levenberg–Marquard line search method with $\mu_k = \|h(x_k)\|^2$, given by Yamashita and Fukushima [48];
- LM-FY: a Levenberg–Marquard line search method with $\mu_k = \|h(x_k)\|$, given by Fan and Yuan [18];
- LevMar: a Levenberg–Marquard trust-region method with $\mu_k = \|\nabla h(x_k)h(x_k)\|$, given by Ipsen et al. [26].

The codes of LMLS and LMQR are publicly available as a part of the COBRA Toolbox v3.0 [25] and a user guide is given in https://opencobra.github.io/cobratoolbox/latest/tutorials/tutorialVariationalKinetics.html. Users can pass the solver name to the parameter structure of the MATLAB function optimizeVKmodels.m. For both LMLS and LMQR, on the basis of our experiments with the mapping (83), we set $\omega_k := 1 - \xi_k$ and

$$\xi_k := \begin{cases} 
0.95 & \text{if } (0.95)^k > 10^{-2}, \\
\max \left( (0.95)^k, 10^{-10} \right) & \text{otherwise},
\end{cases}$$

(84)
implying $\xi_k \in [10^{-10}, 0.95]$. We here use the starting point $x_0 = 0$ and consider the stopping criterion
\[ \|h(x_k)\| \leq \max(10^{-6}, 10^{-12}\|h(x_0)\|) \quad \text{or} \quad \|\nabla \psi(x_k)\| \leq \max(10^{-6}, 10^{-12}\|\nabla \psi(x_0)\|), \]
\[
\text{cf. [9]. We stop the algorithms if either (85) holds or the maximum number of iterations (say 10,000 for tuning $\eta$ and 100,000 for the comparison) is reached. While LMLS uses the parameters}
\[
\bar{\alpha} = 1, \quad \rho = 0.5, \quad \sigma = 10^{-2}, \quad \theta_{\min} = 0, \quad \theta_{\max} = 0.95, \quad \theta_k = 0.95,
\]
\[
\text{LMQR employs the parameters}
\]
\[
\rho_1 = 2, \quad \rho_2 = 0.5, \quad \upsilon_1 = 10^{-4}, \quad \upsilon_1 = 0.9, \quad \lambda_0 = 10^{-2},
\]
\[
\mu_{\min} = 10^{-8}, \theta_{\min} = 0, \quad \theta_{\max} = 0.95, \quad \theta_k = 0.95.
\]
In our comparison, $N_i$, $N_f$ and $T$ denote the total number of iterations, the total number of function evaluations, and the running time, respectively. To illustrate the results, we used the Dolan and Moré performance profile [17] with the performance measures $N_f$ and $T$. In this procedure, the performance of each algorithm is measured by the ratio of its computational outcome versus the best numerical outcome of all algorithms. This performance profile offers a tool to statistically compare the performance of algorithms. Let $S$ be a set of all algorithms and $\mathcal{P}$ be a set of test problems. For each problem $p$ and algorithm $s$, $t_{p,s}$ denotes the computational outcome with respect to a performance index (e.g. the total number of iterations or function evaluations), which is used in the definition of the performance ratio
\[
r_{p,s} := \frac{t_{p,s}}{\min\{t_{p,s} : s \in S\}}.
\]
If an algorithm $s$ fails to solve a problem $p$, the procedure sets $r_{p,s} := r_{\text{failed}}$, where $r_{\text{failed}}$ should be strictly larger than any performance ratio (86). Let $n_p$ be the number of problems in the experiment. For any factor $\tau \in \mathbb{R}$, the overall performance of an algorithm $s$ is given by
\[
\rho_s(\tau) := \frac{1}{n_p} \text{size}\{p \in \mathcal{P} : r_{p,s} \leq \tau\}.
\]
Here, $\rho_s(\tau)$ is the probability that a performance ratio $r_{p,s}$ of an algorithm $s \in S$ is within a factor $\tau$ of the best possible ratio. The function $\rho_s(\tau)$ is a distribution function for the performance ratio. In particular, $\rho_s(1)$ gives the probability that an algorithm $s$ wins over all other considered algorithms, and $\lim_{\tau \to r_{\text{failed}}} \rho_s(\tau)$ gives the probability that algorithm $s$ solves all considered problems. Therefore, this performance profile can be considered as a measure of efficiency among all considered algorithms. In Figures 1 and 3, the number $\tau$ is represented in the $x$-axis, while $P(r_{p,s} \leq \tau : 1 \leq s \leq n_s)$ is shown in the $y$-axis.

First, let us tune the parameter $\eta$ to get the best performance of MLS and LMQR. To do so, we consider several versions of these algorithms corresponding to several levels of the parameter $\eta (\eta = 0.6, 0.8, 1.0, 1.2, 1.4)$ and compare the results in Figure 1. From this
Figure 1. Performance profile for the number of iterations ($N_i$), the number of function evaluations ($N_f$), and the running time ($T$) of LMLS and LMQR to tune the parameter $\eta$, with $\eta \in \{0.6, 0.8, 1.0, 1.2, 1.4\}$. The best performance is attained by $\eta = 1.2$ for both methods. (a) LMLS, the number of iterations $N_i$. (b) LMQR, the number of function evaluations $N_f$. (c) LMLS, the number of function evaluations $N_f$. (d) LMQR, the number of function evaluations $N_f$. (e) LMLS, the running time $T$. (f) LMQR, the running time $T$. 
Figure 2. Performance profiles for the number of iterations and the running time of LM-YF, LM-FY, LevMar, LMLS, and LMQR on a set of 21 biological models for the mapping (83), where LMLS and LMQR outperform the others substantially. (a) the number of iterations \( N_i \), (b) the number of function evaluations \( N_f \), (c) the mixed measure \( 3N_i + N_f \), (d) the running time \( T \).

figure, it is clear that \( \eta = 1.2 \) attains the best results for both LMLS and LMQR. Therefore, we use \( \eta = 1.2 \) for finding a zero of the mapping \( h \) defined in (83); however, to solve a different mappings, one may tune this parameter carefully before any practical usage.

Next, we report the results of a comparison among LM-YF, LM-FY, LevMar, LMLS, and LMQR for finding a zero of \( h \) (83) with respect to the total number of iterations \( (N_i) \), the total number of function evaluations \( (N_f) \), the mixed measure \( N_f + 3N_i \), and the running time \( (T) \) in Figure 2. From this figure, it can be seen that LMLS and LMQR outperform the others substantially with respect to all considered measures. Moreover, LMQR solves the problems even faster than LMLS; however, the slope of curve of LMLS indicates that its performance is much better than LM-YF, LM-FY, and LevMar, and its performance is close to the performance of LMQR. Surprisingly, both LMLS and LMQR are convergent to a zero of the mapping \( h \) (83) not to a stationary point of the merit function \( \psi \) given by (2). This clearly show the potential of LMLS and LMQR for finding the moiety conserved steady state of biochemical reaction networks.
Figure 3. Value of the merit function with respect to the number of iterations for LM-YF, LM-FY, Lev-Mar, LMLS and LMQR, when applied to the mapping (83) defined by the biological models iBsu1103 and iSB619. LMLS and LMQR require much less iterations than the others to achieve the accuracy given in (85). (a) iBsu1103. (b) iSB619.

Finally, we conclude this section by displaying the evolution of the merit function values during run of the considered algorithms. To this end, we illustrate the function values $\psi$ versus iterations in Figure 3 for the mapping (83) with the biological models iBsu1103 and iSB619. Here, we limit the maximum number of iterations to 1000. From Figure 3, it can be seen that LMLS and LMQR perform much better than the others; however, the best performance is attained by LMQR.

6. Conclusion and further research

We have employed two globalization techniques for Levenberg-Marquardt methods for finding a zero of Hölder metrically subregular mappings. First, we combined the Levenberg–Marquardt direction with a non-monotone Armijo-type line search. Then, we modified the Levenberg–Marquardt parameter and combined the corresponding direction with a non-monotone quadratic regularization technique. Next, we studied the global convergence and the worst-case global and evaluation complexities of both methods, which are of the order $O(\varepsilon^{-2})$. The worst-case behaviour of the proposed methods, up to a factor, are equivalent to that of the steepest descent method for unconstrained optimization, cf. [12,39], which is not the best-known global complexity for non-convex problems, cf. [13,42]; however, practical usage of these methods show much better performance than the worst-case complexity, giving scope for future establishment of tighter complexity bounds. Finally, we have studied some special mappings that satisfy certain conditions for a stationary point to correspond to a zero of a mapping, when obtained with the proposed methods.

We also investigate finding zeros of Hölder metrically subregular mappings that appear in modelling of biochemical reaction networks. Our numerical experiments establish the suitability of the proposed methods for a range of medium- and large-scale biochemical
network problems. Nevertheless, biochemical reaction networks on the order of tens of millions of dimensions already exist [37], and the projection is for even larger models in the future. Therefore, considerable scope exists for development of accelerated solution methods.

Notes

1. An elementary reaction is a chemical reaction for which no intermediate molecular species need to be postulated in order to describe the chemical reaction on a molecular scale.
2. Reaction stoichiometry is a quantitative relationship between the relative quantities of molecular species involved in a single chemical reaction.

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