Local convergence of Levenberg–Marquardt methods under Hölder metric subregularity

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Abstract

We describe and analyse Levenberg–Marquardt methods for solving systems of nonlinear equations. More specifically, we first propose an adaptive formula for the Levenberg–Marquardt parameter and analyse the local convergence of the method under Hölder metric subregularity. We then introduce a bounded version of the Levenberg–Marquardt parameter and analyse the local convergence of the modified method under the Łojasiewicz gradient inequality. We finally report encouraging numerical results confirming the theoretical findings for the problem of computing moiety conserved steady states in biochemical reaction networks. This problem can be cast as finding a solution of a system of nonlinear equations, where the associated mapping satisfies the Hölder metric subregularity assumption.

1 Introduction

For a given continuously differentiable mapping \( h : \mathbb{R}^m \to \mathbb{R}^m \), we consider the problem of finding a solution of the system of nonlinear equations

\[ h(x) = 0, \quad x \in \mathbb{R}^m. \tag{1} \]

We denote by \( \Omega \) the set of solutions of this problem, which is assumed to be nonempty. Systems of nonlinear equations of type (1) frequently appear in the mathematical modelling of many real-world applications in the fields of solid-state physics [8], quantum field theory, optics, plasma physics [20], fluid

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mechanics [42], chemical kinetics [1, 2], and applied mathematics including the
discretisation of ordinary and partial differential equations [38].

A classical approach for finding a solution of (1) is to search for a minimiser
of the nonlinear least-squares problem

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

where $\| \cdot \|$ denotes the Euclidean norm. This is a well-studied topic and there
are many iterative schemes with fast local convergence rates (e.g., superlinear or
quadratic) such as Newton, quasi-Newton, Gauss–Newton, adaptive regularised
methods, and Levenberg–Marquardt methods. To guarantee fast local conver-
gence, these methods require an initial point $x_0$ to be sufficiently close to a
solution $x^*$, and the gradient of $h$ at $x^*$, denoted by $\nabla h(x^*)$, to be nonsingular,
cf. [4, 13, 37, 38, 44].

Levenberg–Marquardt methods are standard techniques used to solve non-
linear system (1), each of which is a combination of the gradient descent and the
Gauss–Newton methods. More precisely, in each step, for a positive parameter
$\mu_k$, the convex subproblem

$$\min_{d \in \mathbb{R}^m} \phi_k(d),$$

with $\phi_k : \mathbb{R}^m \to \mathbb{R}$ given by

$$\phi_k(d) := \|\nabla h(x_k)^T d + h(x_k)\|^2 + \mu_k \|d\|^2, \quad (3)$$

is solved to compute a direction $d_k$, which is the unique solution to the system
of linear equations

$$\left(\nabla h(x_k)\nabla h(x_k)^T + \mu_k I\right) d_k = -\nabla h(x_k) h(x_k), \quad (4)$$

where $I \in \mathbb{R}^{m \times m}$ denotes the identity matrix. By choosing a suitable parameter
$\mu_k$, the Levenberg–Marquardt method acts like the gradient descent method
whenever the current iteration is far from a solution $x^*$, and behaves similar
to the Gauss–Newton method if the current iteration is close to $x^*$. The param-
eter $\mu_k$ helps to overcome problematic cases where $\nabla h(x_k)\nabla h(x_k)^T$ is singular,
or nearly singular, and thus ensures the existence of a unique solution to (4),
or avoids very large steps, respectively. The Levenberg–Marquardt method is
known to be quadratically convergent to a solution of (1) if $\nabla h(x^*)$ is nonsin-
gular. In fact, the nonsingularity assumption implies that the solution to the
minimization problem (2) must be locally unique, see [5, 25, 43]. However,
assuming local uniqueness of the solution might be restrictive for many applic-
ations.

The notion of (local) error bound usually plays a key role in establishing the
rate of convergence of the sequence of iterations generated by a given algorithm.
This condition guarantees that the distance from the current iteration $x_k$ to the
solution set $\Omega$, denoted by $\text{dist}(x_k, \Omega) = \inf_{y \in \Omega} \|x_k - y\|$, is less than the value of
a residual function $R : \mathbb{R}^m \to \mathbb{R}_+$ at that point ($R(x_k)$). If one considers
$R(x_k) \leq \epsilon$ as a stopping criterion for an iterative scheme, then $\text{dist}(x_k, \Omega) \leq R(x_k) \leq \epsilon$ implies that $x_k$ is an approximate solution to the problem.
The earliest publication using error bounds for solving a linear inequality system is
due to Hoffman [21], which was followed by many other authors, especially in
optimisation. For more information about error bonds, we recommend the nice survey [39].

For the particular case of nonlinear systems of equations, Yamashita and Fukushima [43] proved the local quadratic convergence of the Levenberg–Marquardt method with $\mu_k = \|h(x_k)\|^2$ assuming a local error bound condition. More precisely, they assumed the existence of some constant $\beta > 0$ such that

$$\beta \ dist(x, \Omega) \leq \|h(x)\|, \quad \forall x \in B(x^*, r), \quad (5)$$

where $B(x^*, r)$ denotes the closed ball centered at $x^*$ with radius $r > 0$. In this case, the residual function is given by $R(x) := \|h(x)\|$. The condition $\|h(x)\| \leq \varepsilon$ can be used as a stopping criterion for an iterative scheme, as it entails that the iterations must be close to a solution of (1).

Let us emphasise that the nonsingularity of $\nabla h(x^*)$ implies that $x^*$ is locally unique, and that the local error bound condition (5) holds [7, 33]. However, the latter does not imply the nonsingularity assumption and allows the solution set $\Omega$ to be locally nonunique (see Section 2), which frequently happens in many applications, e.g., Section 4. This means that the local error bound condition is a weaker assumption than the nonsingularity. The successful use of the local error bound has motivated many researchers to investigate, under this assumption (5), the local convergence of trust-region methods [9], adaptive regularised methods [5], and Levenberg–Marquardt methods [3, 10, 11], among other iterative schemes.

In Example 1, we show that the Powell singular function, which is a classical test function for nonlinear system of equations (cf. [35]), does not satisfy the local error bound condition (5). This motivates our quest to develop an adaptive Levenberg–Marquardt method where the underlying mapping $h$ is Hölder metrically subregular (see Definition 1), which is a weaker assumption than the local error bound condition (5) and is thus satisfied by a broader set of functions. The local convergence of a Levenberg–Marquardt method under Hölder metric subregularity has been recently studied in [17, 45]. As explained in Remark 2, our results broadly encompass those results.

From the definition of the Levenberg–Marquardt direction in (4), we observe that a key factor in the performance of the Levenberg–Marquardt method is the choice of the parameter $\mu_k$, cf. [24, 27]. Several parameters have been proposed to improve the efficiency of the method. For example, Yamashita and Fukushima [43] took $\mu_k = \|h(x_k)\|^2$, Fischer [12] used $\mu_k = \|\nabla h(x_k)h(x_k)\|$, while Fan and Yuan [11] proposed $\mu_k = \|h(x_k)\|^\eta$ with $\eta \in [1, 2]$. Inspired by these works, and assuming that the function $h$ is Hölder metrically subregular of order $\delta \in ]0, 1]$, we define an adaptive parameter

$$\mu_k := \xi_k \|h(x_k)\|^\eta + \omega_k \|\nabla h(x_k)h(x_k)\|^\eta, \quad (6)$$

where $\eta \in ]0, 4\delta[$, $\xi_k \in [\xi_{\min}, \xi_{\max}]$ and $\omega_k \in [0, \omega_{\max}]$, for some positive constants $\xi_{\min}$, $\xi_{\max}$ and $\omega_{\max}$. Thus, if the point $x_k$ is close to a solution, then the parameter $\mu_k$ will be small, in which case the Levenberg–Marquardt method will behave like the Gauss–Newton method, and a fast local convergence can be expected.

The main motivation for this paper comes from a nonlinear system of equations, the solution of which corresponds to a steady state of a given biochemical
reaction network, which plays a crucial role in the modeling of biochemical reaction systems. During our study of the properties of this problem, we were not able to show that the local error bound (5) is satisfied. However, taking standard biochemical assumptions [2], we show that the corresponding mapping is Hölder metrically subregular and that the merit function is real analytic. As a consequence, with the iteration generated by our proposed algorithm, we can ensure local convergence to a solution of (1) for all such networks. To the best of our knowledge, this is the first such algorithm able to reliably handle these nonlinear systems arising in the study of biological networks. We numerically apply the proposed algorithms to nonlinear systems derived from many real biological networks representative of a diverse set of biological species.

The remainder of this paper is organised as follows. In the next section, we particularise the Hölder metric subregularity for nonlinear equations and recall the Lojasiewicz inequalities. In Section 3, we develop a Levenberg–Marquardt method and investigate its local convergence. In Section 4, we report encouraging numerical results where nonlinear systems, arising from biochemical reaction networks, were solved. Finally, we deliver some conclusions in Section 5.

2 Hölder metric subregularity and Lojasiewicz inequalities

Let us begin this section by recalling the notion of Hölder metric subregularity, which can be also defined in a similar manner for set-valued mappings (see, e.g., [29]).

Definition 1. A mapping $h : \mathbb{R}^m \to \mathbb{R}^n$ is said to be Hölder metrically subregular of order $\delta \in [0, 1]$ at $(x, y)$ with $y = h(x)$ if there exist some constants $r > 0$ and $\beta > 0$ such that

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

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

$$ \beta \text{dist}(x, \Omega) \leq \|h(x)\|^{\delta}, \quad \forall x \in B(x^*, r). \quad (7) $$

Therefore, this property provides an upper bound for the distance from any point sufficiently close to the solution $x^*$ to the nearest zero of the function.

Hölder metric subregularity at $(x^*, 0)$ is also called Hölderian local error bound [36, 41]. It is known that Hölder metric subregularity is closely related to the Lojasiewicz inequalities, which are defined as follows.

Definition 2. 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 nonempty.

(i) The function $\psi$ is said to satisfy the Lojasiewicz inequality if for every compact subset $K \subset U$, there exist positive constants $\varrho$ and $\gamma$ such that

$$ \text{dist}(x, \Omega)^{\gamma} \leq \varrho |\psi(x)|, \quad \forall x \in K. $$

(8)
(ii) The function ψ is said to satisfy the Lojasiewicz gradient inequality if for any critical point π, there exist constants κ > 0, ε > 0 and θ ∈ [0, 1) such that

$$|ψ(x) - ψ(π)|^θ ≤ κ∥∇ψ(x)||, \quad ∀x ∈ B(π, ε),$$  \hspace{1cm} (9)

Stanislaw Lojasiewicz proved that every real analytic function satisfies these properties [32]. Recall that a function ψ : \mathbb{R}^m → \mathbb{R} is said to be real analytic if it can be represented by a convergent power series. Fortunately, real analytic functions frequently appear in real world application problems. A relevant example in biochemistry is presented in Section 4.

Fact 1 ([32, pp. 62 and 67]). Every real analytic function ψ : \mathbb{R}^m → \mathbb{R} satisfies both the Lojasiewicz inequality and the Lojasiewicz gradient inequality.

Clearly, if the merit function ψ(·) = \frac{1}{2}∥h(·)∥^2 satisfies the Lojasiewicz inequality (8), then the mapping h satisfies (7) with β := (2/ρ)^{1/θ} and δ := 2/γ; i.e., h is Hölder metrically subregular at (x^*, 0) of order 2/γ. In addition, if ψ(·) satisfies the Lojasiewicz gradient inequality (9), then for any π ∈ Ω and x ∈ B(π, ε), it holds

$$\frac{1}{θ} \text{dist}(x, Ω)^{γ} ≤ |ψ(x)| ≤ κ^{1/θ}∥∇ψ(x)||^{1/θ} = κ^{1/θ}∥∇h(x)h(x)||^{1/θ}.$$

In some cases, for example when ψ is a polynomial with an isolated zero at the origin, the order of the Hölder metric subregularity is known [18, 30, 31].

Fact 2 ([18, Theorem 1.5]). Let ψ : \mathbb{R}^m → \mathbb{R} be a polynomial function with an isolated zero at the origin. Then ψ is Hölder metrically subregular at (0, 0) of order (deg ψ − 1)^m + 1, where deg ψ denotes the degree of the polynomial function ψ.

Let us emphasise that the Hölder metric subregularity property of the function h at (x^*, 0) is weaker than the local error bound assumption (5), which in turns is implied by the nonsingularity of ∇h(x^*). Indeed, by the Lyusternik–Graves theorem (see e.g., [7, Theorem 5D.5] or [33, Theorem 1.57]), the nonsingularity of ∇h(x^*) is equivalent to the metric regularity of h around (x^*, 0), which entails the existence of some positive constants β, r and s such that

$$β \text{dist}(x, h^{-1}(y)) ≤ ∥y - h(x)||, \quad ∀x ∈ B(x^*, r), ∀y ∈ B(0, s).$$

Fixing y = 0, we obtain the metric subregularity condition (5). Furthermore, by making r smaller if needed so that ∥h(x)∥ < 1, we see that (5) implies (7), since δ ∈ (0, 1].

Example 1. The Powell singular function [35], which is the function h : \mathbb{R}^4 → \mathbb{R}^4 given by

$$h(x_1, x_2, x_3, x_4) := \left( x_1 + 10x_2, \sqrt{5}(x_3 - x_4), (x_2 - 2x_3)^2, \sqrt{10}(x_1 - x_4)^2 \right),$$

is Hölder metrically subregular at (x^*, 0) but does not satisfy the local error bound condition (5). We have Ω = {0} and ∇h(0) is singular; thus, h is not metrically
is Hölder metrically subregular if needed so that (7) holds and
\[ \text{dist}(x_k, \Omega) = \|x_k\| = \frac{\sqrt{7}}{k} = O(k^{-1}). \]

Since \( \|h(x_k)\| = \frac{\sqrt{70}}{k} = O(k^{-2}) \), we conclude that (5) does not hold.

Consider the polynomial function \( \psi(x) := \frac{1}{2}\|h(x)\|^2 \) of degree 4, which satisfies \( \psi^{-1}(0) = 0 \). It follows from Fact 2 that there exist some constants \( \beta > 0 \) and \( r > 0 \) such that
\[ \frac{1}{2}\|h(x)\|^2 = \psi(x) \geq \beta\|x\|^{(4-1)\delta+1} = \beta\|x\|^{8\delta}, \quad \forall x \in B(0, r). \]
This implies that \( h \) is Hölder metrically subregular of order \( \delta = \frac{1}{44} \) at \( (0, 0) \).

There are many examples of smooth functions that are Hölder metrically subregular of order \( \delta \) at some zero of the function and whose gradient is singular at that point, cf. [22, 23]. Nonetheless, the following result restricts this set of functions: if \( x^* \) is an isolated solution in \( \Omega \) (i.e., the function is Hölder strongly metrically subregular at \( x^* \), cf. [34]), then one must have \( \delta \in (0, 1/2] \).

**Proposition 1.** Let \( h : \mathbb{R}^m \to \mathbb{R}^m \) be a continuously differentiable function that is Hölder metrically subregular of order \( \delta \) at some isolated solution \( x^* \in \Omega = \{ x \in \mathbb{R}^m : h(x) = 0 \} \). Assume further that \( \nabla h \) is Lipschitz continuous around \( x^* \) and that \( \nabla h(x^*) \) is not full rank. Then, it holds that \( \delta \in (0, 1/2] \).

**Proof.** Because of the Lipschitz continuity assumption (and the mean value theorem), there are some positive constants \( L \) and \( r \) such that
\[ \|h(y) - h(x) - \nabla h(x)^T(y - x)\| \leq L\|y - x\|^2, \quad \forall x, y \in B(x^*, r). \]
By using the fact that \( x^* \) is an isolated solution, it is possible to make \( r \) smaller if needed so that (7) holds and
\[ \|x - x^*\| = \text{dist}(x, \Omega), \quad \forall x \in B(x^*, r). \]
Since \( \nabla h(x^*) \) is not full rank, there exists some \( z \neq 0 \) such that \( \nabla h(x^*)^T z = 0 \). Consider now the points
\[ w_k := x^* + \frac{r}{k\|z\|} z, \quad \text{with } k = 1, 2, \ldots. \]
Observe that
\[ \nabla h(x^*)^T(w_k - x^*) = \frac{r}{k\|z\|} \nabla h(x^*)^T z = 0. \]
As \( w_k \in B(x^*, r) \) for all \( k \), we deduce
\[ \beta\|w_k - x^*\| = \beta\text{dist}(w_k, \Omega) \leq \|h(w_k)\|^{\delta} \]
\[ = \|h(w_k) - h(x^*) - \nabla h(x^*)(w_k - x^*)\|^{\delta} \leq L\|w_k - x^*\|^{2\delta}. \]
Thus, we get
\[ \|w_k - x^*\|^{2\delta - 1} \geq \frac{\beta}{L^{\delta}}, \]
which implies that \( \delta \in (0, 1/2] \), since \( w_k \to x^* \), as claimed. \( \square \) \( \square \)
Locally convergent Levenberg–Marquardt methods

In this section, to solve a nonlinear system of the form (1), we develop adaptive Levenberg–Marquardt methods and investigate their local convergence near a solution under the assumption that the underlying function $h$ is Hölder metrically subregular. Specifically, we consider the following Levenberg–Marquardt algorithm.

Algorithm LLM: (Locally convergent Levenberg–Marquardt)

| Input: $x_0 \in \mathbb{R}^m$, $\eta > 0$, $\xi_0 \in [\xi_{\min}, \xi_{\max}]$, $\omega_0 \in [0, \omega_{\max}]$; |
|---|
| begin |
| $k := 0$; $\mu_0 := \xi_0 \|h(x_0)\|^{\eta} + \omega_0 \|\nabla h(x_0)h(x_0)\|^{\eta}$; |
| while $\|h(x_{k+1})\| > 0$ do |
| solve the linear system (4) to specify the direction $d_k$; |
| $x_{k+1} = x_k + d_k$; update $\xi_k$, $\omega_k$ and $\mu_k$ with (6); |
| end |
| end |

In order to prove the local convergence of algorithm LLM to some solution $x^* \in \Omega$, we assume that the next conditions hold:

(A1) The mapping $h$ is continuously differentiable and Hölder metrically subregular of order $\delta \in [0, 1]$ at $(x^*, 0)$; i.e., there exist some constants $\beta > 0$ and $r > 0$ such that (7) holds. We will assume that $r < 1$.

(A2) $\nabla h$ is Lipschitz continuous on some neighbourhood of $x^* \in \Omega$.

By making $r$ smaller if needed, note that from (A2) and the mean value theorem, there exists a positive constant $L$ such that,

$$\|h(y) - h(x) - \nabla h(x)^T (y - x)\| \leq L \|y - x\|^2, \quad \forall x, y \in B(x^*, r), \quad (11)$$

and

$$\|h(x) - h(y)\| \leq L \|x - y\|, \quad \forall x, y \in B(x^*, r). \quad (12)$$

We begin our study with an analysis inspired by [43] and [17]. The following result provides a bound for the norm of the direction $d_k$ based on the distance of the current iteration $x_k$ to the solution set $\Omega$. This will be useful later for deducing the rate of convergence of LLM.

Proposition 2. Let $x_k \notin \Omega$ be an iteration generated by LLM with $\eta \in [0, 4\delta]$ and such that $x_k \in B(x^*, r/2)$. Then, the direction $d_k$ given by (4) satisfies

$$\|d_k\| \leq \beta_1 \text{dist} (x_k, \Omega)^{\delta_1}, \quad (13)$$

where

$$\beta_1 := \sqrt{L^2 \xi_{\min}^{-1} \beta^{-\frac{\delta}{2}} + 1} \quad \text{and} \quad \delta_1 := \min \left\{ 2 - \frac{\eta}{2\delta}, 1 \right\}.$$
Proof. For all $k$, we will denote by $\mathbf{r}_k$ a vector in $\Omega$ such that $\|x_k - \mathbf{r}_k\| = \text{dist}(x_k, \Omega)$. Since $x_k \in \mathcal{B}(x^*, r/2)$, we have

$$\|\mathbf{r}_k - x^*\| \leq \|\mathbf{r}_k - x_k\| + \|x_k - x^*\| \leq 2\|x^* - x_k\| \leq r,$$

which implies $\mathbf{r}_k \in \mathcal{B}(x^*, r)$. Further,

$$\|\mathbf{r}_k - x^*\| = \text{dist}(x_k, \Omega) \leq \|x_k - x^*\| \leq \frac{r}{2} < 1. \quad (14)$$

Observe that $\phi_k$ is strongly convex and the global minimiser of $\phi_k$ is given by (4). Then, we have

$$\phi_k(d_k) \leq \phi_k(\mathbf{r}_k - x_k). \quad (15)$$

From the definition of $\phi_k$ in (3), by (11), (15) and (A2), we deduce

$$\|d_k\|^2 \leq \frac{1}{\mu_k} \phi_k(d_k) \leq \frac{1}{\mu_k} \phi_k(\mathbf{r}_k - x_k)$$

$$= \frac{1}{\mu_k} \left( \|\nabla h(x_k)^T(\mathbf{r}_k - x_k) + h(x_k)\|^2 + \mu_k \|\mathbf{r}_k - x_k\|^2 \right)$$

$$= \frac{1}{\mu_k} \left( \|\nabla h(x_k)^T(\mathbf{r}_k - x_k) + h(x_k) - h(\mathbf{r}_k)\|^2 + \mu_k \|\mathbf{r}_k - x_k\|^2 \right)$$

$$\leq \frac{1}{\mu_k} \left( L^2 \|\mathbf{r}_k - x_k\|^2 + \mu_k \|\mathbf{r}_k - x_k\|^2 \right). \quad (16)$$

It follows from the definition of $\mu_k$ in (6) and (7) that

$$\mu_k \geq \xi_k \|h(x_k)\|^n \geq \xi_{\text{min}}\|h(x_k)\|^n \geq \xi_{\text{min}} \beta^2 \|x_k - \mathbf{r}_k\|^2 = \xi_{\text{min}} \beta^2 \|\mathbf{r}_k - x_k\|^2,$$

leading to

$$\|d_k\|^2 \leq L^2 \xi_{\text{min}}^{-1} \beta^{-2} \|\mathbf{r}_k - x_k\|^{4 - \frac{2}{\beta}} + \|\mathbf{r}_k - x_k\|^2. \quad (17)$$

Let us consider two cases: (i) $0 < \eta/\delta < 2$; (ii) $2 \leq \eta/\delta < 4$. In Case (i), we have

$$\|d_k\|^2 \leq \left( L^2 \xi_{\text{min}}^{-1} \beta^{-2} + 1 \right) \|\mathbf{r}_k - x_k\|^2. \quad (17)$$

In Case (ii), we have

$$\|d_k\|^2 \leq \left( L^2 \xi_{\text{min}}^{-1} \beta^{-2} + 1 \right) \|\mathbf{r}_k - x_k\|^{4 - \frac{2}{\beta}}. \quad (18)$$

Because of (14), the inequalities (17) and (18) imply (13), and this completes the proof. \qed

The next result provides an upper bound for the distance of $x_{k+1}$ to the solution set $\Omega$ based on the distance of $x_k$ to $\Omega$.

**Proposition 3.** Let $x_k \notin \Omega$ and $x_{k+1}$ be two consecutive iterations generated by LLM with $\eta \in [0, 4\delta]$ and such that $x_k, x_{k+1} \in \mathcal{B}(x^*, r/2)$. Then, we have

$$\text{dist}(x_{k+1}, \Omega) \leq \beta_2 \text{dist}(x_k, \Omega)^{\delta_2}, \quad (19)$$

where $\beta_2$ is a positive constant and $\delta_2 := \min \left\{ \delta + \frac{\delta}{2}, 4\delta - \eta \right\}$. 

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Proof. Let \( \overline{\pi}_k \in \Omega \) be such that \( \|x_k - \overline{\pi}_k\| = \text{dist}(x_k, \Omega) \). From the definition of \( \phi_k \) in (3) and the reasoning in (16), we obtain

\[
\|\nabla h(x_k)^T d_k + h(x_k)\| \leq \phi_k(d_k) \leq L^2\|\overline{\pi}_k - x_k\|^4 + \mu_k\|\overline{\pi}_k - x_k\|^2.
\]

It follows from (A2) that there exists some constant \( \hat{L} \) such that \( \|\nabla h(x)\| \leq \hat{L} \) for all \( x \in B(x^*, r) \). Then, by the definition of \( \mu_k \) in (6) and (12), we have that

\[
\mu_k = \xi_k\|h(x_k)\|^\eta + \omega_k\|\nabla h(x_k)h(x_k)\|^\eta \\
\leq \xi_{\max}\|h(x_k)\|^\eta + \omega_{\max}\hat{L}^\eta\|h(x_k)\|^\eta \\
= \left(\xi_{\max} + \omega_{\max}\hat{L}^\eta\right)\|h(x_k) - h(\overline{\pi}_k)\|^\eta \\
\leq \left(\xi_{\max} + \omega_{\max}\hat{L}^\eta\right)\hat{L}^\eta\|x_k - \overline{\pi}_k\|^\eta,
\]

which implies, thanks to (14),

\[
\|\nabla h(x_k)^T d_k + h(x_k)\|^2 \leq L^2\|\overline{\pi}_k - x_k\|^4 + \left(\xi_{\max} + \omega_{\max}\hat{L}^\eta\right)\hat{L}^\eta\|x_k - \overline{\pi}_k\|^2 + \eta
\]

\[
\leq \left(\xi_{\max} + \omega_{\max}\hat{L}^\eta\right)\hat{L}^\eta\|x_k - \overline{\pi}_k\|^\eta,
\]

where \( \zeta := \min\{4, 2 + \eta\} \). By (7), (11), the latter inequality and Proposition 2, we get

\[
(\beta_{\text{dist}}(x_{k+1}, \Omega))^{\frac{1}{2}} \leq \|x_k + d_k\| \\
\leq \|\nabla h(x_k)^T d_k + h(x_k)\| \\
+ \|h(x_k + d_k) - h(x_k) - \nabla h(x_k)^T d_k\| \\
\leq \|\nabla h(x_k)^T d_k + h(x_k)\| + L\|d_k\|^2 \\
\leq \left(\xi_{\max} + \omega_{\max}\hat{L}^\eta\right)\hat{L}^\eta\|x_k - \overline{\pi}_k\|^\frac{2}{3} \\
+ L\beta_2^2\text{dist}(x_k, \Omega)^{2\delta_1}
\]

\[
\leq \left(\sqrt{L^2 + L^\eta\xi_{\max} + \hat{L}^\eta\omega_{\max}} + L\beta_1^2\right)\text{dist}(x_k, \Omega)^{\delta_1},
\]

where \( \delta_1 := \min\left\{\frac{2}{3}, 2\delta_1\right\} = \min\left\{2, 1 + \frac{2}{3}, 4 - \frac{2}{3}\right\} = \min\left\{1 + \frac{2}{3}, 4 - \frac{2}{3}\right\}. \) Therefore,

\[
\text{dist}(x_{k+1}, \Omega) \leq \beta_2\text{dist}(x_k, \Omega)^{\delta_1} = \beta_2\text{dist}(x_k, \Omega)^{\delta_2},
\]

with \( \beta_2 := \frac{1}{\beta_1^2}\left(\sqrt{L^2 + L^\eta\xi_{\max} + \hat{L}^\eta\omega_{\max}} + L\beta_1^2\right)^{\frac{1}{2}} \), giving the result. \( \square \)

The following proposition is a modification of [17, Lemma 4.4] that gives a different value of the exponent in (19).

**Proposition 4.** Assume \( \delta \geq \frac{1}{2} \), and let \( \tilde{\sigma} := \min\left\{\frac{1}{2}, \left(\frac{\beta_2^2}{\beta_1^2}\right)^{\frac{1}{4+\delta}}\right\} \). Let \( x_k \notin \Omega \) and \( x_{k+1} \) be two consecutive iterations generated by LLM with \( \eta \in [0, 4\delta_1] \) and such that \( x_k, x_{k+1} \in B(x^*, \tilde{\sigma}) \). Then, we have

\[
\text{dist}(x_{k+1}, \Omega) \leq \beta_3\text{dist}(x_k, \Omega)^{\delta_3},
\]

where \( \beta_3 \) is a positive constant and \( \delta_3 := \frac{1}{2+\delta} \min\{4\delta - \eta, (\eta + 1)\delta, 2\delta\} \).
Proof. Let \( \overline{x}_k, \overline{x}_{k+1} \in \Omega \) be such that \( \|x_k - \overline{x}_k\| = \text{dist}(x_k, \Omega) \) and \( \|x_{k+1} - \overline{x}_{k+1}\| = \text{dist}(x_{k+1}, \Omega) \). Assume that \( x_{k+1} \notin \Omega \) (otherwise, the inequality trivially holds). By (11), we have
\[
\|h(x_{k+1}) + \nabla h(x_{k+1})^T (\overline{x}_{k+1} - x_{k+1})\|^2 \leq L^2 \|\overline{x}_{k+1} - x_{k+1}\|^4
= L^2 \text{dist}(x_{k+1}, \Omega)^4.
\]
Thus, by the Cauchy–Schwarz inequality and (7), we get
\[
-\|\nabla h(x_{k+1}) h(x_{k+1})\| \text{dist}(x_{k+1}, \Omega) \leq h(x_{k+1})^T \nabla h(x_{k+1})^T (\overline{x}_{k+1} - x_{k+1})
\leq \frac{L^2}{2} \text{dist}(x_{k+1}, \Omega)^4 - \frac{1}{2} \|h(x_{k+1})\|^2
- \frac{1}{2} \|\nabla h(x_{k+1})^T (\overline{x}_{k+1} - x_{k+1})\|^2
\leq \frac{L^2}{2} \text{dist}(x_{k+1}, \Omega)^4 - \frac{\beta^2}{2} \text{dist}(x_{k+1}, \Omega)^\frac{\beta}{2},
\]
that is,
\[
\frac{\beta^2}{2} \text{dist}(x_{k+1}, \Omega)^\frac{\beta}{2} - \frac{L^2}{2} \text{dist}(x_{k+1}, \Omega)^4 \leq \|\nabla h(x_{k+1}) h(x_{k+1})\| \text{dist}(x_{k+1}, \Omega).
\tag{22}
\]
Now, by (4), we have
\[
\|\nabla h(x_{k+1}) h(x_{k+1})\|
= \|\nabla h(x_{k+1}) h(x_{k+1}) - \nabla h(x_k) (h(x_k) + \nabla h(x_k)^T d_k) - \mu_k d_k\|
\leq \|\nabla h(x_{k+1}) - \nabla h(x_k)\| \|h(x_{k+1})\|
+ \|\nabla h(x_k)\| \|h(x_{k+1}) - h(x_k) - \nabla h(x_k)^T (x_{k+1} - x_k)\| + \mu_k \|d_k\|
\leq L \|d_k\| \|h(x_{k+1})\| + \|\nabla h(x_k)\| L \|d_k\|^2 + \mu_k \|d_k\|.
\tag{23}
\]
By (12) and Proposition 2, it holds,
\[
\|h(x_{k+1})\| = \|h(x_{k+1}) - h(\overline{x}_k)\| \leq L \|x_{k+1} - \overline{x}_k\|
\leq L (\|x_{k+1} - x_k\| + \|x_k - \overline{x}_k\|)
\leq L (\beta_1 \text{dist}(x_k, \Omega)^{\delta_1} + \text{dist}(x_k, \Omega))
\leq L (\beta_1 + 1) \text{dist}(x_k, \Omega)^{\delta_1}.
\]
It follows from (A2) that there exists some constant \( \widehat{L} \) such that \( \|\nabla h(x)\| \leq \widehat{L} \) for all \( x \in \mathbb{B}(x^*, r) \). Then, by the definition of \( \mu_k \) in (6) and (12), we get (20). Hence, by (23) and Proposition 2, we deduce
\[
\|\nabla h(x_{k+1}) h(x_{k+1})\| \leq L^2 \beta_1 (\beta_1 + 1) \text{dist}(x_k, \Omega)^{2\delta_1} + \widehat{L} \beta_1^2 \text{dist}(x_k, \Omega)^{2\delta_1}
+ \left( \xi_{\max} + \omega_{\max} \widehat{L} \right) L^\eta \beta_1 \text{dist}(x_k, \Omega)^{\eta + \delta_1}
\leq \beta_3 \text{dist}(x_k, \Omega)^{\delta_3},
\]
where \( \beta_3 := L^2 \beta_1 (\beta_1 + 1) + \widehat{L} \beta_1^2 + \left( \xi_{\max} + \omega_{\max} \widehat{L} \right) L^\eta \beta_1 \) and \( \delta_3 := \min\{\eta + \delta_1, 2\delta_1\} \). Therefore, by (22),
\[
\frac{\beta_3}{2} \text{dist}(x_{k+1}, \Omega)^{\frac{\beta}{2}} - \frac{L^2}{2} \text{dist}(x_{k+1}, \Omega)^4 \leq \tilde{\beta}_3 \text{dist}(x_k, \Omega)^{\delta_3} \text{dist}(x_{k+1}, \Omega).
\tag{24}
\]
Finally, since $\delta \geq \frac{1}{2}$, we have
\[
L^2_2 \operatorname{dist}(x_{k+1}, \Omega)^{4-\frac{q}{2}} \leq L^2_2 \|x_{k+1} - x^*\|^{4-\frac{q}{2}} \leq \frac{L^2_2}{2} R^{4-\frac{q}{2}} \leq \frac{\beta^2}{4},
\]
where the last inequality follows from the definition of $\beta$. Then, by (24), we deduce
\[
\frac{\beta^2}{4} \operatorname{dist}(x_{k+1}, \Omega)^{\frac{q}{2}-1} \leq \beta_3 \operatorname{dist} (x_k, \Omega)^{\delta_3},
\]
whence,
\[
\operatorname{dist}(x_{k+1}, \Omega) \leq \beta_3 \operatorname{dist} (x_k, \Omega)^{\delta_3},
\]
where $\beta_3 := \frac{2\beta}{\beta^2}$ and $\delta_3 := \frac{\delta + \delta \eta}{2 - \delta} = \frac{1}{2-\delta} \min \{4\delta - \eta, (\eta + 1)\delta, 2\delta\}$. \qed \qed

In Figure 1, we plot the values of $\delta_2$ in Proposition 3 and $\delta_3$ in Proposition 4. The bounds given by (19) and (21) are usually employed to analyse the rate of convergence of the sequence $\{x_k\}$ generated by LLM. A larger value of $\delta_2$ or $\delta_3$ would serve us to derive a better rate of convergence. To deduce a convergence result from Proposition 3, one needs to have $\delta_2 \geq 1$, which holds if and only if $\eta \in \left[\frac{2}{3} - 2, 4\delta - 1\right]$. This imposes the requirement that $\delta \geq \frac{-1 + \sqrt{33}}{8}$. On the other hand, to guarantee that $\delta_3 \geq 1$, a stronger requirement would be needed, namely, $\delta \geq \frac{1}{2}$ and $\eta \in \left[\frac{2}{3} - 2, 5\delta - 2\right] \subset \left[\frac{2}{3} - 2, 4\delta - 1\right]$. Nonetheless, if $\eta \in \left[\frac{2}{3} - 2, \frac{2\delta}{2-\delta}\right]$, it holds that $1 < \delta_2 < \delta_3$. In fact, it is important to emphasise that if $\delta = 1$ and $\eta \in [1, 2]$, then $\delta_3 = 2$, and we can derive from Proposition 4 the quadratic convergence of the sequence, which can only be guaranteed for $\eta = 2$ by Proposition 3.

![Figure 1: Plot of $\delta_2 = \min \left\{ \delta + \frac{\delta \eta}{2}, 4\delta - \eta \right\}$ (in blue) and $\delta_3 = \min \left\{ \frac{4\delta - \eta}{2 - \delta}, \frac{(\eta + 1)\delta}{2 - \delta}, \frac{4\delta}{2 - \delta} \right\}$ (in red) for $\delta \in \left[\frac{1}{2}, 1\right]$ and $\eta \in [0, 4\delta]$.](image)

**Remark 1.** In light of Proposition 1, the extent of the results that can be derived from Propositions 3 and 3 is rather reduced when $\nabla h(x^*)$ is not full rank, since $\delta \geq \frac{-1 + \sqrt{33}}{8} > \frac{1}{2}$. In fact, we have not been able to find any function that satisfies the hypothesis of Proposition 1 with $\delta > \frac{1}{2}$ and such that $\nabla h(x^*)$ is not full rank (remember that, as explained in Section 2, if $\nabla h(x^*)$ is full rank,
one can take $\delta = 1$ in (7)). Note that the function $F_S$ given as example in [17, Section 5] is Hölder metrically subregular of order $\delta = \frac{2}{3} > 0.5$, but $\nabla F_S$ is not Lipschitz continuous around any zero of the function, so it does not satisfy (A2) (and, therefore, it does not satisfy [17, Assumption 4.1] either). However, with an additional assumption that the Lojasiewicz gradient inequality (9) holds, we will obtain other local convergence results for all $\delta \in [0, 1]$, see Subsection 3.1.

In spite of Remark 1, we proceed to derive the main result of this section from Propositions 3 and 4. We show that, as long as $\delta > \frac{1-\sqrt{33}}{8}$, it is possible to choose a parameter $\eta$ such that superlinear convergence is attained.

**Theorem 1.** Assume that $\delta \in \left[\frac{1-\sqrt{33}}{8}, 1\right]$ and $\eta \in \left[\frac{3}{2} - 2, 4\delta - 1\right]$. Then, there exists some $\tau > 0$ such that for every sequence $\{x_k\}$ generated by LLM with $x_0 \in B(x^*, \tau)$, one has that $\{\text{dist}(x_k, \Omega)\}$ converges to 0 at least superlinearly, with order no less than $\delta_2 := \min \left\{\delta + \frac{\delta\eta}{2}, 4\delta - \eta\right\}$. Moreover, the sequence $\{x_k\}$ converges to a solution $x^* \in \Omega \cap B(x^*, r/2)$, and if $\eta \leq 2\delta$, the rate of convergence is also superlinear and no less than $\delta_2$. Furthermore, if $\delta \in \left[\frac{3}{2}, 1\right]$ and $\eta \in \left[\frac{3}{2} - 2, \frac{24}{25}\right]$, all the latter holds with order no less than $\delta_3 := \min \left\{\frac{4\delta - \eta}{2 - \delta}, \frac{(\delta + 1)\delta}{2 - \delta}, \frac{24}{25}\right\} > \delta_2$.

**Proof.** Let $\delta_1, \beta_1, \delta_2$ and $\beta_2$ be defined as in Proposition 2 and in Proposition 3. Since $\delta_2 > 1$, we have that $\delta_1 \delta_2 > i$ for all $i$ sufficiently large. As $\sum_{i=1}^{\infty} (\frac{1}{2})^i = 1$, we deduce that

$$\sigma := \sum_{i=1}^{\infty} \left(\frac{1}{2}\right)^{\delta_i \delta_2^i} < \infty$$

Define

$$\tau := \min \left\{\frac{1}{2} (\beta_2)^{1-\frac{1}{\delta_2^1}}, \left(\frac{r}{2 (1 + \beta_1 + 2\delta_1 \sigma)}\right)^{\frac{1}{\delta_1}}\right\}.$$ 

Note that $\tau \in [0, r/2]$, because $r \in [0, 1]$ and $\delta_1 \leq 1$.

Pick any $x_0 \in B(x^*, \tau)$ and let $\{x_k\}$ be an infinite sequence generated by LLM. First, we will show by induction that $x_k \in B(x^*, r/2)$. It follows from $\tau < 1$ and (13) that

$$\|x_1 - x^*\| = \|x_0 + d_0 - x^*\| \leq \|x_0 - x^*\| + \|d_0\| \leq \tau + \beta_1 \text{dist}(x_0, \Omega)^{\delta_1} \leq \tau^{\delta_1} + \beta_1 \|x_0 - x^*\|^\delta_1 \leq (1 + \beta_1)\tau^{\delta_1} \leq r/2.$$ (26)

Let us assume now that $x_i \in B(x^*, r/2)$ for $i = 1, 2, \ldots, k$. Then, from Proposition 3 and the definition of $\tau$, we have

$$\text{dist}(x_i, \Omega) \leq \beta_2 \text{dist}(x_{i-1}, \Omega)^{\delta_2} \leq \beta_2^{1+\delta_2} \text{dist}(x_{i-2}, \Omega)^{\delta_2} \leq \ldots \leq \beta_2^{\sum_{j=0}^{i-1} \delta_2^j} \text{dist}(x_0, \Omega)^{\delta_2} \leq \beta_2^{\sum_{j=0}^{i-1} \delta_2^j} \|x_0 - x^*\|^{\delta_2} = \beta_2^{\sum_{j=0}^{i-1} \delta_2} \|x_0 - x^*\|^{\delta_2} \leq \left(\frac{1}{2^\tau}\right)^{\delta_2^{\delta_2^{i-1}}} = 2^\tau \left(\frac{1}{2}\right)^{\delta_2^i}.$$
which yields
\[
\text{dist}(x_i, \Omega)^{\delta_i} \leq (2\sigma)^{\delta_i} \left(\frac{1}{2}\right)^{\delta_i}\delta_i^2.
\] (27)

The latter inequality, together with (13), (25) and (26), implies
\[
\|x_{k+1} - x^*\| \leq \|x_i - x^*\| + \sum_{i=1}^{k} \|d_i\| \leq (1 + \beta_1)\sigma^{\delta_i} + \beta_1 \sum_{i=1}^{k} \text{dist}(x_i, \Omega)^{\delta_i}
\]
\[
\leq (1 + \beta_1)\sigma^{\delta_i} + \beta_1 (2\sigma)^{\delta_i} \sum_{i=1}^{k} \left(\frac{1}{2}\right)^{\delta_i}\delta_i^2
\]
\[
\leq (1 + \beta_1)\sigma^{\delta_i} + \beta_1 (2\sigma)^{\delta_i} \sum_{i=1}^{\infty} \left(\frac{1}{2}\right)^{\delta_i}\delta_i^2
\]
\[
= (1 + \beta_1)\sigma^{\delta_i} + \beta_1 (2\sigma)^{\delta_i} \sigma = (1 + \beta_1 + 2\beta_1\sigma) \sigma^{\delta_i} \leq \frac{r}{2},
\]
which completes the induction. Thus, we have \(x_k \in B(x^*, r/2)\) for all \(k\), as claimed.

From Proposition 3, we obtain that \(\{\text{dist}(x_k, \Omega)\}\) converges to 0 at least superlinearly. Further, it follows from (13) and (27) that
\[
\sum_{i=1}^{\infty} \|d_i\| \leq \beta_1 \sum_{i=1}^{\infty} \text{dist}(x_i, \Omega)^{\delta_i} \leq \beta_1 \sigma \sigma^{\delta_i} < +\infty.
\]
Denoting by \(s_k := \sum_{i=1}^{k} \|d_i\|\), we have that \(\{s_k\}\) is a Cauchy sequence. Then, for any \(k, p \in \mathbb{N} \cup \{0\}\), we have
\[
\|x_{k+p} - x_k\| \leq \|d_{k+p-1}\| + \|x_{k+p-1} - x_k\|
\]
\[
\leq \cdots \leq \sum_{i=k}^{k+p-1} \|d_i\| = s_{k+p-1} - s_{k-1},
\] (28)
which implies that \(\{x_k\}\) is also a Cauchy sequence. Thus, the sequence \(\{x_k\}\) converges to some \(\tilde{x}\). Since \(x_k \in B(x^*, r/2)\) for all \(k\) and \(\{\text{dist}(x_k, \Omega)\}\) converges to 0, we have \(\tilde{x} \in \Omega \cap B(x^*, r/2)\).

Further, if \(\eta \leq 2\delta\) we have \(\delta_1 = 1\) in Proposition 2, and by letting \(p \to \infty\) in (28), we deduce
\[
\|\tilde{x} - x_k\| \leq \sum_{i=k}^{\infty} \|d_i\| \leq \beta_1 \sum_{i=k}^{\infty} \text{dist}(x_i, \Omega).
\]
Since \(\text{dist}(x_i, \Omega)\) is superlinearly convergent to zero, for all \(k\) sufficiently large, it holds \(\text{dist}(x_{k+1}, \Omega) \leq \frac{1}{2}\text{dist}(x_k, \Omega)\). Therefore, for \(k\) sufficiently large, we have
\[
\|x_k - \tilde{x}\| \leq \beta_1 \sum_{i=k}^{\infty} \frac{1}{2^{i-k}} \text{dist}(x_k, \Omega) \leq 2\beta_1 \text{dist}(x_k, \Omega) \leq 2\beta_1 \beta_2 \text{dist}(x_{k-1}, \Omega)^{\delta_2}
\]
\[
\leq 2\beta_1 \beta_2 \|x_{k-1} - \tilde{x}\|^2,
\]
which proves the superlinear convergence of \(x_k\) to \(\tilde{x}\) with rate \(\delta_2\).

Finally, the last assertion follows by the same argumentation, using \(\tilde{r}, \delta_3\) and Proposition 4 instead of \(r, \delta_2\) and Proposition 3, respectively. \(\square\)
Remark 2.

(i) Our results above generalise the results in [17, 45], because the parameter $\mu_k$ considered by these authors is equal to $\xi \|h(x_k)\|^\alpha$. Furthermore, in their convergence results, cf. [17, Theorem 4.1 and Theorem 4.2] and [45, Theorem 2.1 and Theorem 2.2], the authors assume $\delta > \max \left\{ \frac{1}{3}, \frac{2+\eta}{3} \right\}$ and $\delta > \max \left\{ \frac{\sqrt{8+4\eta+4}}{8}, \frac{1}{2+\eta} + \frac{\eta+1}{4} \right\} > \sqrt{\frac{5}{2}}$, respectively, which both entail $\delta > \frac{1}{\alpha} + \sqrt{\frac{33}{8}}$, so we have slightly improved the lower bound on $\delta$ for the superlinear convergence in Theorem 1.

(ii) The values of $\delta_2$ and $\delta_3$ are maximised when $\eta = \frac{64}{8+2}$ and $\eta \in [1, 2\delta]$, respectively, in which case $\delta_2 = \frac{4\delta^2+2\delta}{8+2\delta}$ and $\delta_3 = \frac{2\delta}{2-\delta}$, and $\delta_2 \leq \delta_3$.

As a direct consequence of Theorem 1, we can derive quadratic convergence of the sequence generated by LLM whenever $\delta = 1$ and $\eta \in [1, 2]$.

Corollary 1. Assume that $\delta = 1$ and $\eta \in [1, 2]$. Then, there exists $\tau > 0$ such that for every sequence $\{x_k\}$ generated by LLM with $x_0 \in B(x^*, \tau)$, one has that $\{\text{dist}(x_k, \Omega)\}$ converges to 0 at least quadratically. Moreover, the sequence $\{x_k\}$ converges quadratically to a solution $x^* \in \Omega \cap B(x^*, \tau/2)$.

The question of whether the sequence $\{\text{dist}(x_k, \Omega)\}$ converges to 0 when $\delta < \frac{1}{\alpha} + \sqrt{\frac{33}{8}}$ remains open. However, with the additional assumption that $\psi$ satisfies the Lojasiewicz gradient inequality (which holds for real analytic functions) and a slight modification of $\mu_k$, we can prove that the sequences $\{\text{dist}(x_k, \Omega)\}$ and $\{\psi(x_k)\}$ converge to 0 for all $\delta \in (0, 1]$, and we can also provide a rate of convergence that depends on the exponent of the Lojasiewicz gradient inequality. This is the subject of the next subsection.

3.1 Convergence analysis under the Lojasiewicz gradient inequality

In this subsection, under the assumption that the Lojasiewicz gradient inequality holds, we prove that the sequences $\{\text{dist}(x_k, \Omega)\}$ and $\{\psi(x_k)\}$ converge to 0 for all $\delta \in [0, 1]$. To do that, we make use the following two lemmas.

Lemma 1. Let $\{s_k\}$ be a sequence in $\mathbb{R}_+$ and let $\alpha, \nu$ be some nonnegative constants. Suppose that $s_k \to 0$ and that the sequence satisfies

$$s_k^\alpha \leq \nu(s_k - s_{k+1}), \quad \text{for all } k \text{ sufficiently large.} \quad (29)$$

Then

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

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

(iii) if $\alpha > 1$, there exists $\varsigma > 0$ such that

$$s_k \leq \varsigma k^{-\frac{\alpha}{\alpha-1}}, \quad \text{for all } k \text{ sufficiently large.}$$

Proof. See [2, Lemma 1].

□ □
Lemma 2. The sequence \( \{x_k\} \) generated by LLM satisfies
\[
\|d_k\| \leq \frac{1}{2\sqrt{\mu_k}}\|h(x_k)\|,
\]
and
\[
\|h(x_{k+1})\|^2 \leq \|h(x_k)\|^2 + \frac{L^2}{4}\|d_k\|^2 + L\|h(x_k)\| - \mu_k. \tag{30}
\]

Proof. See [26, Theorem 2.5 and Lemma 2.3].

In our main result of this subsection, we prove the convergence to 0 of the sequences \( \{\text{dist}(x_k, \Omega)\} \) and \( \{\psi(x_k)\} \) as long as the parameter \( \mu_k \) in LLM is updated in such a way that \( \mu_k \in [\mu_{\text{min}}, \mu_{\text{max}}] \) for all \( k \), where \( \mu_{\text{min}} \) and \( \mu_{\text{max}} \) are some positive constants.

Theorem 2. Suppose that \( \psi \) satisfies the Lojasiewicz gradient inequality (9) with exponent \( \theta \in [0, 1] \). Assume that the updating rule for \( \mu_k \) is defined in such a way that for every bounded sequence \( \{x_k\} \) generated by LLM, there exist some positive constants \( \mu_{\text{min}} \) and \( \mu_{\text{max}} \) such that \( \mu_k \in [\mu_{\text{min}}, \mu_{\text{max}}] \) for all \( k \).

Then, there exist positive constants \( s \) and \( \bar{s} \) such that, for every \( x_0 \in B(x^*, s) \) and every sequence \( \{x_k\} \) generated by LLM, one has \( \{x_k\} \subset B(x^*, \bar{s}) \) and the two sequences \( \{\psi(x_k)\} \) and \( \{\text{dist}(x_k, \Omega)\} \) converge to 0. Moreover, the following holds:

(i) if \( \theta = 0 \), the sequences \( \{\psi(x_k)\} \) and \( \{\text{dist}(x_k, \Omega)\} \) converge to 0 in a finite number of steps;

(ii) if \( \theta \in [0, \frac{1}{2}] \), the sequences \( \{\psi(x_k)\} \) and \( \{\text{dist}(x_k, \Omega)\} \) converge linearly to 0;

(iii) if \( \theta \in \left[\frac{1}{2}, 1\right] \), there exist some positive constants \( \varsigma_1 \) and \( \varsigma_2 \) such that, for all large \( k \),
\[
\psi(x_k) \leq \varsigma_1 k^{-\frac{\theta}{2\theta - 1}} \quad \text{and} \quad \text{dist}(x_k, \Omega) \leq \varsigma_2 k^{-\frac{\theta}{2\theta - 1}}.
\]

Proof. The proof has three key parts.

In the first part of the proof, we will set the values of \( s \) and \( \bar{s} \). Let \( \varepsilon > 0 \) and \( \kappa > 0 \) be such that (9) holds. Let \( \bar{s} := \min\{r, \varepsilon\} > 0 \). Then, by the assumption on the updating rule for \( \mu_k \) and by Assumption (A2), there exist some positive constants \( v_{\text{min}} \) and \( v_{\text{max}} \) such that
\[
\mu_k \geq v_{\text{min}} \quad \text{and} \quad \|
abla h(x_k)\| + \mu_k \leq v_{\text{max}}, \quad \text{whenever} \ x_k \in B(x^*, \bar{s}). \tag{31}
\]

Make \( \bar{s} \) smaller if needed so that
\[
v_{\text{min}} \geq \frac{2 + \sqrt{5}}{4} L\|h(x)\|, \quad \forall x \in B(x^*, \bar{s}). \tag{32}
\]

For all \( x \in B(x^*, \bar{s}) \), one has by (12) that
\[
\psi(x) = \frac{1}{2}\|h(x) - h(x^*)\|^2 \leq \frac{L^2}{2}\|x - x^*\|^2 \leq \frac{L^2}{2}\|x - x^*\|, \tag{33}
\]
since \( \bar{s} \leq r < 1 \). Let
\[
\Delta := \frac{2^{\theta} KL^2 (1-\theta) v_{\max}}{(1-\theta) v_{\min}} \quad \text{and} \quad s := \left( \frac{\bar{s}}{1+\Delta} \right)^{1/\bar{s}}.
\]

Then, since \( \bar{s} < 1 \) and \( \theta \in [0, 1] \), we have \( s \leq \bar{s} \).

Pick any \( x_0 \in \mathbb{B}(x^*, \bar{s}) \) and let \( \{x_k\} \) be the sequence generated by LLM. It follows from Lemma 2 that
\[
\psi(x_{k+1}) \leq \psi(x_k) - \frac{1}{2} d_k^T H_k d_k + \frac{\|d_k\|^2}{2\mu_k} \left( \frac{L^2}{16} \|h(x_k)\|^2 + L\mu_k \|h(x_k)\| - \mu_0^2 \right),
\]
for all \( k \), where \( H_k = \nabla h(x_k) \nabla h(x_k)^T + \mu_k I \), since \( d_k = -H_k^{-1} \nabla h(x_k) h(x_k) \).

In the second part of the proof, we will prove by induction that
\[
x_i \in \mathbb{B}(x^*, \bar{s}) \quad \text{and} \quad \|d_{i-1}\| \leq \frac{2^{\theta} \mu_{\max}}{(1-\theta) v_{\min}} \left( \psi(x_{i-1})^{1-\theta} - \psi(x_i)^{1-\theta} \right)
\]
for all \( i = 1, 2, \ldots \). Since \( x_0 \in \mathbb{B}(x^*, \bar{s}) \), we have by (32) that
\[
\mu_0 \geq v_{\min} \geq \frac{2 + \sqrt{5}}{4} L\|h(x_0)\|,
\]
which implies
\[
\frac{L^2}{16} \|h(x_0)\|^2 + L\mu_0 \|h(x_0)\| - \mu_0^2 \leq 0.
\]
Therefore, from (34), we get
\[
\psi(x_1) \leq \psi(x_0) - \frac{1}{2} d_0^T H_0 d_0 \leq \psi(x_0) - \frac{v_{\min}}{2} \|d_0\|^2.
\]

Observe that the convexity of the function \( \varphi(t) := -t^{1-\theta} \) with \( t > 0 \) yields
\[
\psi(x)^{1-\theta} - \psi(y)^{1-\theta} \geq (1-\theta)(\psi(x)^{\theta} - \psi(y)^{\theta}), \quad \forall x,y \in \mathbb{R}^m \setminus \Omega.
\]

By combining (36) with (37), we deduce
\[
\psi(x_0)^{1-\theta} - \psi(x_1)^{1-\theta} \geq \frac{(1-\theta) v_{\min}}{2} \psi(x_0)^{-\theta} \|d_0\|^2
\]
Since \( x_0 \in \mathbb{B}(x^*, s) \) \( \subseteq \mathbb{B}(x^*, \bar{s}) \), we have by (31) that \( \|H_0\| \leq v_{\max} \). Further, from the Łojasiewicz gradient inequality (9), it holds
\[
\psi(x_0)^{\theta} \leq \kappa \|\nabla \psi(x_0)\| \leq \kappa \|H_0\||d_0\| \leq \kappa v_{\max} ||d_0||.
\]

From the last inequality, together with (38) and then (33), we obtain
\[
\|d_0\| \leq \frac{2^{\theta} \mu_{\max}}{(1-\theta) v_{\min}} \psi(x_0)^{1-\theta} \psi(x_1)^{1-\theta}
\]
Therefore, \( x_1 \in \mathbb{B}(x^*, \overline{\tau}) \). Assume now that (35) holds for all \( i = 1, \ldots, k \). Since \( x_k \in \mathbb{B}(x^*, \overline{\tau}) \), by the assumption on \( \mu_k \) and (32), we have

\[
\mu_k \geq \nu_{\min} \geq \frac{2 + \sqrt{5}}{4} L \|h(x_k)\|,
\]

which implies

\[
\frac{L^2}{16} \|h(x_k)\|^2 + L \mu_k \|h(x_k)\| - \mu_k^2 \leq 0.
\]

Therefore, by (34), we get

\[
\psi(x_{k+1}) \leq \psi(x_k) - \frac{1}{2} d_k^T H_k d_k \leq \psi(x_k) - \frac{\nu_{\min}}{2} \|d_k\|^2.
\]

Combining the latter inequality with (37), we deduce

\[
\psi(x_k)^{1-\theta} - \psi(x_{k+1})^{1-\theta} \geq \frac{(1 - \theta) \nu_{\min}}{2} \|d_k\|^2 \quad (40)
\]

Further, since \( x_k \in \mathbb{B}(x^*, \overline{\tau}) \), from the Łojasiewicz gradient inequality (9) and (31), it holds

\[
\psi(x_k)^{\theta} \leq \kappa \|\nabla \psi(x_k)\| \leq \kappa \|H_k\| \|d_k\| \leq \kappa \nu_{\max} \|d_k\|.
\]

From the last inequality and (40), we deduce

\[
\|d_k\| \leq \frac{2 \kappa \nu_{\max}}{(1 - \theta) \nu_{\min}} (\psi(x_k)^{1-\theta} - \psi(x_{k+1})^{1-\theta}),
\]

which proves the second assertion in (35) for \( i = k + 1 \). Hence, by (33), we have

\[
\|x_{k+1} - x^*\| \leq \|x_0 - x^*\| + \sum_{i=0}^k \|d_i\|
\]

\[
\leq \|x_0 - x^*\| + \frac{2 \kappa \nu_{\max}}{(1 - \theta) \nu_{\min}} \sum_{i=0}^k (\psi(x_i)^{1-\theta} - \psi(x_{i+1})^{1-\theta})
\]

\[
= \|x_0 - x^*\| + \frac{2 \kappa \nu_{\max}}{(1 - \theta) \nu_{\min}} (\psi(x_0)^{1-\theta} - \psi(x_{k+1})^{1-\theta})
\]

\[
\leq \|x_0 - x^*\| + \frac{2 \kappa \nu_{\max}}{(1 - \theta) \nu_{\min}} \psi(x_0)^{1-\theta}
\]

\[
\leq (1 + \Delta) \|x_0 - x^*\|^{1-\theta} \leq (1 + \Delta) s^{1-\theta} = \overline{\tau},
\]

which proves the first assertion in (35) for \( i = k + 1 \). This completes the second part of the proof.

In the third part of the proof, we will finally show the assertions in the statement of the theorem. From the second part of the proof we know that \( x_k \in \mathbb{B}(x^*, \overline{\tau}) \) for all \( k \). This, together with the assumption on \( \mu_k \) and (31), implies that \( \|H_k\| \leq \nu_{\max} \) for all \( k \). Thus,

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

Therefore, by (39), we have

\[
\psi(x_{k+1}) \leq \psi(x_k) - \frac{1}{2 \nu_{\max}} \|\nabla \psi(x_k)\|^2.
\]
It follows from the Łojasiewicz gradient inequality (9) and the last inequality that
\[ \psi(x_{k+1}) \leq \psi(x_k) - \frac{1}{2\kappa^2 \upsilon_{\text{max}}} \psi(x_k)^{2\theta}. \]
This implies that \( \{\psi(x_k)\} \) converges to 0. By applying Lemma 1 with \( s_k := \psi(x_k), \nu := 2\kappa^2 \upsilon_{\text{max}} \) and \( \alpha := 2\theta \), we conclude that the rate of convergence depends on \( \theta \) as claimed in (i)-(iii). Finally, observe that \( \{\text{dist}(x_k, \Omega)\} \) converges to 0 with the rate stated in (i)-(iii) thanks to the Hölder metric subregularity of \( h \).

\[ \square \]

**Remark 3.** Theorem 2 covers many possibilities for updating the parameter \( \mu_k \):

(i) The constant sequence \( \mu_k := \mu > 0 \) for all \( k \) clearly satisfies the updating assumption for \( \mu_k \) in Theorem 2, and thus, LLM with \( \mu_k = \mu \) instead of (6) gives rise to a convergent sequence satisfying Theorem 2.

(ii) If instead of using \( \mu_k \) defined in (6), we use
\[ \mu_k := \max\{\mu_{\text{min}}, \xi_k\|h(x_k)\|^\eta + \omega_k\|\nabla h(x_k)h(x_k)\|^\eta\}, \]
where \( \mu_{\text{min}} \) is a small positive number, then Theorem 2 holds, as (41) satisfies the updating assumption for \( \mu_k \) because of (A2) and the fact that \( \xi_k \leq \xi_{\text{max}} \) and \( \omega_k \leq \omega_{\text{max}} \).

In our second main result of this subsection, for a sequence generated by LLM with \( \mu_k \) updated by (6), we prove the convergence of \( \{\psi(x_k)\} \) and \( \{\text{dist}(x_k, \Omega)\} \) to 0, as long as the entire sequence \( \{x_k\} \) remains sufficiently close to the solution \( x^\ast \).

**Theorem 3.** Suppose that \( \psi \) satisfies the Łojasiewicz gradient inequality (9) with exponent \( \theta \in [0, 1] \). Then, there exists a positive constant \( s \) such that, for every sequence \( \{x_k\} \) generated by LLM with \( \mu_k \) updated by (6), \( \eta \in [0, 1] \) and \( x_k \in B(x^\ast, s) \) for all \( k \), one has that the two sequences \( \{\psi(x_k)\} \) and \( \{\text{dist}(x_k, \Omega)\} \) converge to 0. Moreover, the statements (i)-(iii) in Theorem 2 hold.

**Proof.** Since \( \eta \in [0, 1] \), there exists a positive constant \( s \leq \min\{r, \varepsilon\} \) such that
\[ \xi_{\text{min}}\|h(x)\|^\eta \geq \frac{2 + \sqrt{5}}{4} L\|h(x)\|, \quad \forall x \in B(x^\ast, s). \]
Let \( \{x_k\} \) be a sequence generated by LLM be such that \( x_k \in B(x^\ast, s) \), for all \( k \). It follows from Lemma 2 that (34) holds. By the definition of \( \mu_k \) in (6) and (42), we have
\[ \mu_k \geq \xi_{\text{min}}\|h(x_k)\|^\eta \geq \frac{2 + \sqrt{5}}{4} L\|h(x_k)\|, \]
which implies
\[ \frac{L^2}{16} \|h(x_k)\|^2 + L\mu_k\|h(x_k)\| - \mu_k^2 \leq 0. \]
Therefore,
\[ \psi(x_{k+1}) \leq \psi(x_k) - \frac{1}{2} d_k^2 H_k d_k. \]
Further, since \( x_k \in B(x^\ast, s) \), there exists \( \lambda_{\text{max}} \) such that \( \|H_k\| \leq \lambda_{\text{max}} \) for all \( k \). The rest of the proof is the same as in Theorem 2.

\[ \square \]
Example 2. Let $h : \mathbb{R} \to \mathbb{R}$ be defined by $h(x) := |x|^\alpha$ with $\alpha \in [2, +\infty[$. Then, one has that $h'(x) = \alpha \text{sign}(x)|x|^{\alpha-1}$ is locally Lipschitz continuous around the unique solution $x^* = 0$. Moreover, the Hölder metric subregularity condition (7) holds with $\beta = 1$ and $\delta = \frac{\alpha}{\pi}$, and the Lojasiewicz gradient inequality (9) holds for $\psi(x) = \frac{1}{2}|x|^{2\alpha}$ with exponent $\theta = 1 - \frac{1}{2\alpha}$. Theorem 2 guarantees the local convergence of the sequence $\{x_k\}$ generated by LLM, as long as the starting point $x_0$ is chosen sufficiently close to 0. Nevertheless, as $\theta > \frac{1}{2}$, linear convergence is not guaranteed. The sequence is given by

$$x_{k+1} = x_k - \frac{\alpha \text{sign}(x_k)|x_k|^{2\alpha-1}}{\alpha^2 \text{sign}(x_k)|x_k|^{2\alpha-2} + \mu_k} = \left(1 - \frac{\alpha}{\alpha^2 \text{sign}(x_k)|x_k|^{2\alpha-2} + \mu_k}\right) x_k.$$

Pick any initial point $x_0 > 0$. Then, one has

$$x_{k+1} = \left(1 - \frac{\alpha}{\alpha^2 + \mu_k|x_k|^{2-2\alpha}}\right) x_k \in ]0, x_k[ , \quad \forall k.$$

If $\mu_k > \mu_{\text{min}} > 0$ for all $k$, we deduce from (44) that $\{x_k\}$ is sublinearly convergent to 0, in accordance with Theorem 2.

Consider now $\mu_k$ given by (6) with $\xi_k = \omega_k = \frac{1}{2}$ and $\eta = \frac{6\alpha}{\delta + 2} = \frac{6}{1+2\alpha}$. Then,

$$\mu_k = \frac{1}{2}x_k^{\frac{6\alpha}{1+2\alpha}} + \frac{\alpha^\eta}{2} x_k^{\frac{6(2\alpha-1)}{1+2\alpha}},$$

and we get

$$x_{k+1} = \left(1 - \frac{\alpha}{\alpha^2 + \frac{6\alpha}{1+2\alpha} + \frac{\alpha\eta}{2} x_k^{\frac{6(2\alpha-1)}{1+2\alpha}+2-2\alpha}}\right) x_k,$$

leading to $x_k \to 0$. To analyse the rate of convergence of this sequence, we need to distinguish three different cases, depending on the value of $\alpha$:

(i) If $\alpha \in \left[2, 1 + \frac{\sqrt{5}}{2}\right]$, then $0 < \frac{6\alpha}{1+2\alpha} + 2 - 2\alpha < \frac{6(2\alpha-1)}{1+2\alpha} + 2 - 2\alpha$, i.e.,

$$\lim_{k \to \infty} \frac{x_{k+1}}{x_k} = \lim_{k \to \infty} \left(1 - \frac{\alpha}{\alpha^2 + \frac{1}{2} x_k^{\frac{6\alpha}{1+2\alpha}+2-2\alpha} + \frac{\alpha^\eta}{2} x_k^{\frac{6(2\alpha-1)}{1+2\alpha}+2-2\alpha}}\right) = 1 - \frac{1}{\alpha} < 1,$$

implying that $\{x_k\}$ converges to 0 linearly.

(ii) If $\alpha = 1 + \frac{\sqrt{5}}{2}$, then $0 = \frac{6\alpha}{1+2\alpha} + 2 - 2\alpha < \frac{6(2\alpha-1)}{1+2\alpha} + 2 - 2\alpha$, i.e.,

$$\lim_{k \to \infty} \frac{x_{k+1}}{x_k} = \lim_{k \to \infty} \left(1 - \frac{\alpha}{\alpha^2 + \frac{1}{2} + \frac{\alpha^\eta}{2} x_k^{\frac{6(2\alpha-1)}{1+2\alpha}+2-2\alpha}}\right) = 1 - \frac{\alpha}{\alpha^2 + 1} < 1,$$

implying that $\{x_k\}$ converges to 0 linearly.
(iii) If \( \alpha \in \left[1 + \frac{\sqrt{5}}{2}, +\infty\right] \), then \( \frac{6\alpha}{2 + 2\alpha} + 2 - 2\alpha < 0 \), i.e.,

\[
\lim_{k \to \infty} \frac{x_{k+1}}{x_k} = 1,
\]

which means that \( \{x_k\} \) converges to 0 sublinearly.

Observe that \( \alpha \geq 2 \) corresponds with \( \frac{\sqrt{5}}{2} \leq \frac{1}{\alpha} \leq \frac{1}{2} \). Theorem 1 cannot be applied to the function \( h \) (unless \( \alpha = 1 \)). On one hand, \( h' \) is not locally Lipschitz around the origin when \( \alpha \in [0, 1] \cup [1, 2] \). On the other hand, superlinear convergence is only guaranteed by Theorem 1 for values of \( \delta \) greater than \( \frac{1}{1+\sqrt{33}} \approx 0.5931 \), which correspond with values of \( \alpha \) smaller than \( \frac{8}{1+\sqrt{33}} \approx 1.6861 \).

Example 3. Let us investigate the rate of convergence of the sequence \( \{x_k\} \) generated by LLM for the Powell singular function (10) and the Rosenbrock function \( h : \mathbb{R}^2 \to \mathbb{R}^2 \), which is given by

\[
h(x_1, x_2) = (10(x_2 - x_1^2), 1 - x_1). \]

It is clear that the solutions of the nonlinear system (1) for the Powell singular and the Rosenbrock functions are unique and given by \( x^* = (0, 0, 0, 0) \) and \( x^* = (1, 1) \), respectively. Since the solution for both problems is unique, we have \( \text{dist}(x_k, \Omega) = \|x_k - x^*\| \). We run LLM with \( \eta = 1.2 \) and \( \xi_k = \omega_k = 0.5 \) for both functions, using as starting points \( x_0 = (0.5, -0.5, 1, 0.3) \) and \( x_0 = (0.6, 1.4) \) for the Powell singular and the Rosenbrock functions, respectively. In order to analyse the convergence rate of the sequence \( \{x_k\} \), we consider the ratio

\[
\Delta_q(x_k, x^*) := \frac{\|x_{k+1} - x^*\|}{\|x_k - x^*\|^q}, \quad \text{with } q \in [1, 2].
\]

In Figure 2, we draw \( \Delta_q(x_k, x^*) \) for \( q \in \{1, 1.25, 1.5, 1.75, 2\} \), where \( q = 1 \) stands for the linear convergence, \( q \in \{1.25, 1.5, 1.75\} \) stand for the superlinear convergence, and \( q = 2 \) stands for the quadratic convergence.

(a) Powell singular function

(b) Rosenbrock function

Figure 2: Plots of the ratios \( \Delta_q(x_k, x^*) \) for the Powell singular and Rosenbrock functions, where the Powell singular function attains the linear convergence and the Rosenbrock function obtains the quadratic convergence.
From Figure 2(a), it can be seen that the ratio $\Delta q(x_k, x^*)$ with $q = 1$ is convergent to a point in the interval $[0, 1]$, while the other ratios for $q \neq 1$ are divergent, which occurs when the sequence $\{x_k\}$ generated by LLM is linearly convergent. We can deduce the convergence of $\{\text{dist}(x_k, \Omega)\} = \{|x_k|\}$ to 0 from Theorem 2(iii). Unfortunately, linear convergence cannot be guaranteed because the Lojasiewicz gradient inequality (9) does not hold for $\theta = \frac{1}{2}$. Indeed, for any $\kappa > 0$, one has

$$|\psi(10x_1, -x_1, x_1, x_1) - \psi(0)| - \kappa^2 \|\nabla \psi(10x_1, -x_1, x_1, x_1)\|^2 = 65691x_1^4 - 1700669520\kappa^2 x_1^6,$$

which is positive when $x_1$ is sufficiently small.

Figure 2(b) shows the ratios $\Delta_q(x_k, x^*)$ for the Rosenbrock mapping. One can see that $\Delta_1(x_k, x^*)$ is convergent to 0, which happens when the rate of convergence is superlinear. Since $\Delta_q(x_k, x^*)$ for $q \in \{1.25, 1.5, 1.75, 2\}$ are decreasing and bounded above by 10, the rate of convergence seems to be quadratic. Indeed, this is the case: Corollary 1 guarantees the quadratic convergence for all $\eta \in [1, 2]$, because $\nabla h(0, 0)$ is nonsingular (in which case (7) is valid with $\delta = 1$).

4 Application to biochemical reaction networks

In this section, we introduce first a class of nonlinear equations arising in the study of biochemistry, cf. [14]. After that, we compare the performance of LLM with some state-of-the-art algorithms for finding steady states of nonlinear systems of biochemical networks on 21 different real data biological models.

4.1 Nonlinear systems in biochemical reaction networks

Consider a biochemical 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, that is, there exists at least one positive vector $l \in \mathbb{R}^m_{++}$ satisfying $(R - F)^T l = 0$, cf. [16]. The matrix $N := R - F$ represents net reaction stoichiometry and may be viewed as the incidence matrix of a directed hypergraph, see [28]. We assume that there are less molecular species than there are net reactions, that is $m < n$. 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 particular sparsity pattern depends on the particular biochemical network being modeled. Moreover, we also assume that rank$([F, R]) = m$, which is a requirement for kinetic consistency, cf. [15].

Let $c \in \mathbb{R}^m_{++}$ denote a variable vector of molecular species concentrations. Assuming constant nonnegative elementary kinetic parameters $k_f, k_r \in \mathbb{R}^n_{+}$, we

\(^1\)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.
assume 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., [2, 15]. Then, the deterministic dynamical equation for time evolution of molecular species concentration is given by

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

A vector \( c^* \) is a steady state if and only if it satisfies

\[
f(c^*) = 0.
\]

Note that a vector \( c^* \) 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 \( \mathcal{N}(N) \) denotes the null space of \( N \). Therefore, the set of steady states \( \Omega = \{ c \in \mathbb{R}_m^+, f(c) = 0 \} \) is unchanged if we replace the matrix \( N \) 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 rank \((\tilde{N}) = \text{rank}(N) =: r \). If one replaces \( N \) by \( \tilde{N} \) and transforms (45) to 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 (45) is equal to the function

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

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

Let \( L \in \mathbb{R}^{m-r, m} \) denote a basis for the left nullspace of \( N \), which implies \( LN = 0 \). We have \( \text{rank}(L) = m - r \). We say that 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 network, cf. [19]. The problem of finding the moiety conserved steady state of a biochemical reaction network is equivalent to solving the nonlinear equation (1) with

\[
h(x) := \begin{pmatrix}
\tilde{f}(x) \\
L \exp(x) - l_0
\end{pmatrix}.
\]
Let \( A := [\bar{N}, -\bar{N}] \) and \( B := [F, R]^T \). Then we can write
\[
\psi(x) = \frac{1}{2} \|h(x)\|^2 = \frac{1}{2} h(x)^T h(x)
\]
\[
= \frac{1}{2} \exp(k + Bx)^T A^T A \exp(k + Bx)
+ \frac{1}{2} (L \exp(x) - l_0)^T (L \exp(x) - l_0)
\]
\[
= \exp(k + Bx)^T Q \exp(k + Bx) + \frac{1}{2} (L \exp(x) - l_0)^T (L \exp(x) - l_0)
\]
\[
= \sum_{p,q=1}^{2n} Q_{p,q} \exp \left( k_p + k_q + \sum_{i=1}^{m} (B_{pi} + B_{qi}) x_i \right)
\]
\[
+ \frac{1}{2} (L \exp(x) - l_0)^T (L \exp(x) - l_0),
\]
where \( Q = A^T A \). Since \( B_{ij} \) are nonnegative integers for all \( i \) and \( j \), we conclude that the function \( \psi \) is real analytic (see Proposition 2.2.2 and Proposition 2.2.8 in [40]). It follows from Fact 1 and the discussion after it in Section 2 that the mapping \( h \) is Hölder metrically subregular at \( (x^*, 0) \).

### 4.2 Computational experiments

In this subsection, we first tune the parameter \( \eta \) for LLM and then compare it with some state-of-the-art Levenberg–Marquard methods for solving the nonlinear system (1) with \( h \) defined by (47).

In our comparison, \( N_f \) and \( T \) denote the total number of function evaluations and the running time, respectively. To illustrate the results, we used the Dolan and Moré performance profile [6] 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 the performance index, which is used in the definition of the performance ratio
\[
r_{p,s} := \min \left\{ t_{p,s} : s \in S \right\}.
\]
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 (48). 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 3 and 4, 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.

Let us now apply LLM to the system of nonlinear equations (47). In a first step, we tuned the parameter $\eta$ to get the best performance of LLM. To this end, we apply five versions of LLM associated to the parameter $\eta \in \{0.6, 0.8, 1.0, 1.2, 1.4\}$ to the nonlinear system (47) defined by 21 biological models. The results of this comparison are summarised in Table 1 and Figure 3. From Table 1, it can be seen that LLM with $\eta = 1.2$ outperforms the others with respect to the number of function evaluations and the running time. Figure 3 displays the performance profiles for the number of function evaluations and the running time. It shows that best results are attained for $\eta = 1.2$.

We now compare LLM with the following Levenberg–Marquard methods:

- LLM-YF: with $\mu_k = \|h(x_k)\|^2$, given by Yamashita and Fukushima [43];
- LLM-FY: with $\mu_k = \|h(x_k)\|$, given by Fan and Yuan [11];
- LLM-F: with $\mu_k = \|\nabla h(x_k)h(x_k)\|$, given by Fischer [12].

It is clear that all of these three methods are special case of LLM by selecting suitable parameters $\xi_k$, $\omega_k$, and $\eta$. In our implementation, all codes were written in MATLAB and runs were performed on a Dell Precision Tower 7000 Series 7810 (Dual Intel Xeon Processor E5-2620 v4 with 32 GB RAM). The algorithms were stopped whenever either

$$\|h(x_k)\| \leq \max \{10^{-6}, 10^{-12}\|h(x_0)\|\} \quad \text{or} \quad \|\nabla \psi(x_k)\| \leq \max \{10^{-6}, 10^{-12}\|\nabla \psi(x_0)\|\}$$

is satisfied, cf. [4]. On the basis of our experiments with the mapping (47), we set $\omega_k := 1 - \xi_k$ and

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

Figure 3: Performance profile the number of function evaluations ($N_f$) and the running time ($T$) of LLM to tune the parameter $\eta$, with $\eta \in \{0.6, 0.8, 1.0, 1.2, 1.4\}$, where the best performance attained by $\eta = 1.2$. 

![Graph showing performance profiles](image.png)
The initial point is set to $x_0 = 0$. We stop the algorithms if either (49) holds or the maximum number of iterations (say 100,000) is reached. The results of our implementation are summarised in Table 2 and Figure 4. In Figures 4(a) and 4(b), we see that LLM attains the most wins, by about 86% and 87%, for the number of function evaluations and the running time, respectively. Moreover, while LLM-F outperforms LLM-YF and LLM-FY, we find that LLM-YF obtains better results than LLM-FY for the considered problems.

![Figure 4: Performance profiles for the number of function evaluations ($N_f$) and the running time ($T$) of LLM-YF, LLM-FY, LLM-F, and LLM on a set of 21 biological models for the mapping (47) in which LLM outperforms the others significantly.](image)

In order to see the evolution of the merit function, we illustrate its value with respect to the number of iterations in Figure 5 for the mapping (47) with the biological models iAF692 and iNJ661. We limit the maximum number of iterations to 1,000. Clearly, LLM attains the best results, followed by LLM-F. Both methods are competitive and seem to be more suited to biological problems than LLM-YF and LLM-FY.
Figure 5: Value of the merit function with respect to the number of iterations for the methods LLM-YF, LLM-FY, LLM-F, and LLM, when applied to the mapping (47) defined by the biological models iAF692 and iNJ661, where LLM performs better than the others.

5 Conclusion and further research

We have presented novel adaptive Levenberg–Marquardt methods for solving systems of nonlinear equations. We have analysed their local convergence under Hölder metric subregularity and the Lojasiewicz gradient inequality of the underlying function. These properties hold in many applied problems, as they are satisfied by any real analytic function. One of these applications is computing a solution to a system of nonlinear equations arising in biochemical reaction networks. We showed that such systems satisfy the Hölder metric subregularity assumption and we obtained superior performance, compared to existing Levenberg–Marquardt methods, for 21 different biological networks.

Several extensions to the present study are possible. It would be desirable to develop some Levenberg–Marquardt methods with faster local convergence under Hölder metric subregularity, as in [10]. A study of the local convergence of adaptive regularisation and trust-region methods [4, 5] would be of particular interest for Hölder metrically subregular mappings. Finally, a globally convergent version of the proposed Levenberg–Marquardt method would be desirable. One approach, which is currently being investigated, would be to combine the scheme with an Armijo-type line search and a trust-region technique. This will be reported in a separate article.

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Appendix

See Tables 1 and 2 for the summary results of the comparisons.
Table 1: The summary results of tuning the parameter $\eta$ for LLM with $\eta \in \{0.6, 0.8, 1.0, 1.2, 1.4\}$ to solve (47) with 21 biological models. For each model, the best number of function evaluations ($N_f$) and the best running time ($T$) are displayed in bold.

| Model                  | $\eta = 0.6$ | $\eta = 0.8$ | $\eta = 1.0$ | $\eta = 1.2$ | $\eta = 1.4$ |
|------------------------|--------------|--------------|--------------|--------------|--------------|
| Ecoli-core             | 402          | 493          | 689          | 689          | 689          |
| Ecoli                    | 1520         | 1193         | 1639         | 1656         | 1700         |
| Escherichia              | 193          | 1167         | 1427         | 1510         | 1577         |
| ImageNet                | 415          | 558          | 237          | 229          | 234          |
| ImageNet2               | 404          | 428          | 295          | 300          | 300          |
| iAF692                  | 614          | 669          | 2669         | 2669         | 2669         |
| iAF1260                 | 1520         | 1193         | 1639         | 1656         | 1700         |
| iBsu1103                | 1654         | 2102         | 2102         | 2102         | 2102         |
| iCB925                  | 524          | 595          | 233          | 220          | 220          |
| iIT341                  | 597          | 757          | 297          | 289          | 289          |
| iJN678                  | 524          | 595          | 233          | 220          | 220          |
| iJN746                  | 597          | 757          | 297          | 289          | 289          |
| iJO1366                 | 524          | 595          | 233          | 220          | 220          |
| iJR904                  | 524          | 595          | 233          | 220          | 220          |
| iMB745                  | 524          | 595          | 233          | 220          | 220          |
| iNJ661                  | 524          | 595          | 233          | 220          | 220          |
| iRsp1095                | 524          | 595          | 233          | 220          | 220          |
| iSB619                  | 524          | 595          | 233          | 220          | 220          |
| iTZ479                  | 524          | 595          | 233          | 220          | 220          |
| iYL1228                 | 524          | 595          | 233          | 220          | 220          |
| Lactococcus MG1363     | 483          | 491          | 228          | 228          | 228          |
| Lactobacillus BioNet    | 483          | 491          | 228          | 228          | 228          |
| Staphylococcus           | 483          | 491          | 228          | 228          | 228          |
| Streptococcus            | 483          | 491          | 228          | 228          | 228          |
| Average                 | 483          | 491          | 228          | 228          | 228          |
Table 2: The summary results of LLM-YF, LLM-FY, LLM-F, and LLM for solving (47) with 21 biological models. For each model, the best number of function evaluations (\(N_f\)) and the best running time (\(T\)) are displayed in bold.

| Model               | \(m\) | \(n\) | \(r\) | LLM-YF   | LLM-FY   | LLM-F   | LLM   |
|---------------------|-------|-------|-------|----------|----------|---------|-------|
|                     | \(N_f\) | \(T\) | \(N_f\) | \(T\)    | \(N_f\) | \(T\)   | \(N_f\) | \(T\)   |
| Ecoli core          | 72     | 73    | 11    | 424      | 0.19     | 4533    | 2.11   | 95      | 0.05     | 128   | 0.05 |
| iAF692              | 462    | 493   | 32    | 1345     | 15.86    | 1449    | 17.10  | 215     | 2.44     | 185   | 2.11 |
| iAF1260             | 1520   | 1193  | 63    | 7325     | 1327.24  | 10729   | 1911.56| 435     | 77.72    | 407   | 73.11|
| iBsu103             | 993    | 1167  | 36    | 2314     | 152.88   | 7864    | 503.77 | 244     | 15.76    | 207   | 12.99|
| iCB925              | 415    | 558   | 29    | 809      | 9.53     | 7693    | 90.06  | 214     | 2.50     | 186   | 2.05 |
| iT341               | 424    | 428   | 32    | 1125     | 9.48     | 12615   | 103.32 | 222     | 1.90     | 178   | 1.45 |
| iJN678              | 641    | 669   | 52    | 1842     | 39.13    | 16123   | 346.28 | 320     | 6.80     | 239   | 4.95 |
| iJN746              | 727    | 797   | 27    | 2822     | 88.19    | 13991   | 419.20 | 260     | 7.91     | 216   | 6.50 |
| iJO1366             | 1654   | 2102  | 72    | 7720     | 1809.60  | 36534   | 8488.88| 359     | 83.59    | 283   | 64.73|
| iJP815              | 524    | 595   | 23    | \(4\)    | 0.05     | 100000  | 1976.03| 100000  | 1984.57  | 100000 | 1594.01|
| iJR904              | 597    | 757   | 33    | 2585     | 59.41    | 30172   | 688.88 | 282     | 6.31     | 212   | 4.82 |
| iMB745              | 525    | 598   | 35    | 640      | 10.86    | 13878   | 237.95 | 199     | 3.10     | 184   | 3.06 |
| iNJ661              | 651    | 764   | 47    | 2327     | 57.20    | 13383   | 329.42 | 331     | 8.17     | 225   | 5.63 |
| iRsp1095            | 966    | 1042  | 45    | 3779     | 232.80   | 25324   | 1531.54| 383     | 23.65    | 305   | 18.90|
| iSB619              | 462    | 508   | 27    | 1657     | 19.49    | 15049   | 166.39 | 201     | 2.24     | 180   | 1.96 |
| iT3466              | 583    | 606   | 54    | 1666     | 30.85    | 15504   | 291.13 | 249     | 4.54     | 200   | 3.71 |
| iTZ479\_v2          | 435    | 476   | 20    | 992      | 10.03    | 217     | 2.22  | 143     | 1.42     | 131   | 1.39 |
| iYL1228             | 1350   | 1695  | 69    | 5325     | 760.99   | 43410   | 6231.59| 422     | 60.86    | 282   | 41.79|
| L_lactis_MG1363     | 483    | 491   | 54    | 1501     | 18.34    | 13442   | 150.58 | 182     | 1.99     | 174   | 2.05 |
| Sc\_thermophilis\_rBioNet | 348    | 365   | 28    | 2559     | 15.73    | 100000  | 619.32 | 286     | 1.71     | 207   | 1.25 |
| T_Maritima          | 434    | 470   | 20    | 775      | 7.99     | 221     | 2.14  | 115     | 1.02     | 119   | 1.06 |
| **Average**         |        |       |       | 2359     | 222.66   | 22959   | 1148.07| 5007    | 109.44   | **4964** | **87.98** |
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