



Convergence and evaluation-complexity analysis of a regularized tensor-Newton method for solving nonlinear least-squares problems

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Abstract

Given a twice-continuously differentiable vector-valued function $r(x)$, a local minimizer of $\|r(x)\|_2$ is sought. We propose and analyse tensor-Newton methods, in which $r(x)$ is replaced locally by its second-order Taylor approximation. Convergence is controlled by regularization of various orders. We establish global convergence to a first-order critical point of $\|r(x)\|_2$, and provide function evaluation bounds that agree with the best-known bounds for methods using second derivatives. Numerical experiments comparing tensor-Newton methods with regularized Gauss–Newton and Newton methods demonstrate the practical performance of the newly proposed method.

Keywords Nonlinear least-squares · Levenberg Marquardt · Trust region methods · Data fitting

1 Introduction

Consider a given, smooth, vector-valued residual function $r : \mathbb{R}^n \rightarrow \mathbb{R}^m$, and let $\|\cdot\|$ be the Euclidean norm. Our goal is to design effective methods for finding values of $x \in \mathbb{R}^n$ for which $\|r(x)\|$ is (locally) as small as possible. Since $\|r(x)\|$ is generally

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non smooth, it is common to consider the equivalent problem of minimizing

$$\Phi(x) := \frac{1}{2} \|r(x)\|^2, \quad (1.1)$$

and to tackle the resulting problem using a generic method for unconstrained optimization, or one that exploits the special structure of Φ .

To put our proposal into context, arguably the most widely used method for solving nonlinear least-squares problems is the Gauss–Newton method and its variants. These iterative methods all build locally-linear (Taylor) approximations to $r(x_k + s)$ about x_k , and then minimize the approximation as a function of s in the least-squares sense to derive the next iterate $x_{k+1} = x_k + s_k$ [21,22,24]. The iteration is usually stabilized either by imposing a trust-region constraint on the permitted s , or by including a quadratic regularization term [3,23]. While these methods are undoubtedly popular in practice, they often suffer when the optimal value of the norm of the residual is large. To counter this, regularized Newton methods for minimizing (1.1) have also been proposed [7,16,17]. Although this usually provides a cure for the slow convergence of Gauss–Newton-like methods on non-zero-residual problems, the global behaviour is sometimes less attractive; we attribute this to the Newton model not fully reflecting the sum-of-squares nature of the original problem.

With this in mind, we consider instead the obvious nonlinear generalization of Gauss–Newton in which a locally quadratic (Taylor) “tensor-Newton” approximation to the residuals is used instead of a locally linear one. Of course, the resulting least-squares model is now quartic rather than quadratic (and thus in principle is harder to solve), but our experiments [19] have indicated that this results in more robust global behaviour than Newton-type methods and an improved performance on non-zero-residual problems than seen for Gauss–Newton variants. Our intention here is to explore the convergence behaviour of a tensor-Newton approach.

We mention in passing that we are not the first authors to consider higher-order models for least-squares problems. The earliest approach we are aware of [4,5] uses a quadratic model of $r(x_k + s)$ in which the Hessian of each residual is approximated by a low-rank matrix that is intended to compensate for any small singular values of the Jacobian. Another approach, known as geodesic acceleration [29,30], aims to modify Gauss–Newton-like steps with a correction that allows for higher-order derivatives. More recently, derivative-free methods that aim to build quadratic models of $r(x_k + s)$ by interpolation/regression of past residual values have been proposed [31,32], although these ultimately more resemble Gauss–Newton variants. While each of these methods has been shown to improve performance relative to Gauss–Newton-like approaches, none makes full use of the residual Hessians. Our intention is thus to investigate the convergence properties of methods based on the tensor-Newton model.

There has been a long-standing interest in establishing the global convergence of general smooth unconstrained optimization methods, that is, in ensuring that a method for minimizing a function $f(x)$ starting from an arbitrary initial guess ultimately delivers an iterate for which a measure of optimality is small. A more recent concern has focused on *how many* evaluations of $f(x)$ and its derivatives are necessary to reduce the optimality measure below a specified (small) $\epsilon > 0$ from the initial guess. If the measure is $\|g(x)\|$, where $g(x) := \nabla_x f(x)$, it is known that some well-known

schemes (including steepest descent and generic second-order trust-region methods) may require $\Theta(\epsilon^{-2})$ evaluations under standard assumptions [6], while this may be improved to $\Theta(\epsilon^{-3/2})$ evaluations for second-order methods with cubic regularization or using specialised trust-region tools [8,15,26]. Here and hereafter $O(\cdot)$ indicates a term that is of at worst a multiple of its argument, while $\Theta(\cdot)$ indicates additionally there are instances for which the bound holds.

For the problem we consider here, an obvious approach is to apply any of the aforementioned algorithms to minimize (1.1), and to terminate as soon as

$$\|\nabla_x \Phi(x)\| \leq \epsilon, \text{ where } \nabla_x \Phi(x) = J^T(x)r(x) \text{ and } J(x) := \nabla_x r(x). \tag{1.2}$$

However, it has been argued [9] that this ignores the possibility that it may suffice to stop instead when $r(x)$ is small, and that a more sensible criterion is to terminate when

$$\|r(x)\| \leq \epsilon_p \text{ or } \|g_r(x)\| \leq \epsilon_d, \tag{1.3}$$

where $\epsilon_p > 0$ and $\epsilon_d > 0$ are required accuracy tolerances and $g_r(x)$ is the scaled gradient given by

$$g_r(x) := \begin{cases} \frac{J^T(x)r(x)}{\|r(x)\|}, & \text{whenever } r(x) \neq 0; \\ 0, & \text{otherwise.} \end{cases} \tag{1.4}$$

We note that $g_r(x)$ in (1.4) is precisely the gradient of $\|r(x)\|$ whenever $r(x) \neq 0$, while if $r(x) = 0$, we are at the global minimum of r and so $g_r(x) = 0 \in \partial(\|r(x)\|)$, the sub-differential of $r(x)$. Furthermore $\|g_r(x)\|$ is less sensitive to scaling than $\|J^T(x)r(x)\|$. It has been shown that a second-order method based on cubic regularization will satisfy (1.3) after $O(\max(\epsilon_d^{-3/2}, \epsilon_p^{-1/2}))$ evaluations [9, Theorem 3.2]. One of our aims here is to show similar bounds for the tensor-Newton method we are advocating. We propose a regularized tensor-Newton method in Sect. 2, and analyse both its global convergence and its evaluation complexity in Sect. 3. The regularization order, r , permitted by the algorithm proposed in Sect. 2 is restricted to be no larger than 3, and so in Sect. 4 we introduce a modified algorithm for which $r > 3$ is possible. We make further comments and draw general conclusions in Sect. 6.

2 The tensor-Newton method

Suppose that $r(x) \in C^2$ has components $r_i(x)$ for $i = 1, \dots, m$. Let $t(x, s)$ be the vector whose components are

$$t_i(x, s) := r_i(x) + s^T \nabla_x r_i(x) + \frac{1}{2} s^T \nabla_{xx} r_i(x) s \tag{2.1}$$

for $i = 1, \dots, m$. We build the *tensor-Newton* approximation

$$m(x, s) := \frac{1}{2} \|t(x, s)\|^2 \quad (2.2)$$

of $\Phi(x + s)$, and define the regularized model

$$m^R(x, s, \sigma) := m(x, s) + \frac{1}{r} \sigma \|s\|^r, \quad (2.3)$$

where $r \geq 2$ is given. Note that

$$\nabla_s m^R(x, s, \sigma) = \nabla_s m(x, s) + \sigma \|s\|^{r-2} s. \quad (2.4)$$

We consider the following algorithm (Algorithm 2.1) to find a critical point of $\Phi(x)$.

Algorithm 2.1 Adaptive Tensor-Newton Regularization.

A starting point x_0 , an initial and a minimal regularization parameter $\sigma_0 \geq \sigma_{\min} > 0$ and algorithmic parameters $\theta > 0$, $\gamma_3 \geq \gamma_2 > 1 > \gamma_1 > 0$ and $1 > \eta_2 \geq \eta_1 > 0$, are given. Evaluate $\Phi(x_0)$. For $k = 0, 1, \dots$, until **termination**, do:

1. If the termination test has not been satisfied, compute derivatives of $r(x)$ at x_k .
2. Compute a step s_k by approximately minimizing $m^R(x_k, s, \sigma_k)$ so that

$$m^R(x_k, s_k, \sigma_k) < m^R(x_k, 0, \sigma_k) \quad (2.5)$$

and

$$\|\nabla_s m^R(x_k, s_k, \sigma_k)\| \leq \theta \|s_k\|^{r-1}. \quad (2.6)$$

3. Set $\widehat{x}_k = x_k + s_k$ and compute $\Phi(\widehat{x}_k)$ and

$$\rho_k = \frac{\Phi(x_k) - \Phi(\widehat{x}_k)}{m(x_k, 0) - m(x_k, s_k)}. \quad (2.7)$$

4. Set

$$\sigma_{k+1} \in \begin{cases} [\max(\sigma_{\min}, \gamma_1 \sigma_k), \sigma_k] & \text{if } \rho_k \geq \eta_2 & \text{[very successful iteration]} \\ [\sigma_k, \gamma_2 \sigma_k] & \text{if } \eta_1 \leq \rho_k < \eta_2 & \text{[successful iteration]} \\ [\gamma_2 \sigma_k, \gamma_3 \sigma_k] & \text{otherwise} & \text{[unsuccessful iteration]}, \end{cases} \quad (2.8)$$

5. If $\rho_k \geq \eta_1$, set $x_{k+1} = \widehat{x}_k$. Otherwise go to Step 2.

At the very least, we insist that (trivial) termination should occur in Step 1 of Algorithm 2.1 if $\|\nabla_x \Phi(x_k)\| = 0$, but in practice a rule such as (1.2) or (1.3) at $x = x_k$ will be preferred.

At the heart of Algorithm 2.1 is the need (Step 2) to find a vector s_k that both reduces $m^R(x_k, s, \sigma_k)$ and satisfies $\|\nabla_s m^R(x_k, s_k, \sigma_k)\| \leq \theta \|s_k\|^{r-1}$ (see, e.g., [1]).

Since $m^R(x_k, s, \sigma_k)$ is bounded from below (and grows as s approaches infinity), we may apply any descent-based local optimization method that is designed to find a critical point of $m^R(x_k, s, \sigma_k)$, starting from $s = 0$, as this will generate an s_k that is guaranteed to satisfy both Step 2 stopping requirements. Crucially, such a minimization is on the model $m^R(x_k, s, \sigma_k)$, not the true objective, and thus involves no true objective evaluations. We do not claim that this calculation is trivial, but it might, for example, be achieved by applying a safeguarded Gauss–Newton method to the least-squares problem involving the extended residuals $(t(x_k, s), \sqrt{\sigma_k} \|s\|^{r-2}s)$.

We define the index set of successful iterations, in the sense of (2.8), up to iteration k to be $\mathcal{S}_k := \{0 \leq l \leq k \mid \rho_l \geq \eta_1\}$ and let $\mathcal{S} := \{k \geq 0 \mid \rho_k \geq \eta_1\}$ be the set of all successful iterations.

3 Convergence analysis

We make the following blanket assumption:

AS.1 each component $r_i(x)$ and its first two derivatives are Lipschitz continuous on an open set containing the intervals $[x_k, x_k + s_k]$ generated by Algorithm 2.1 (or its successor).

It has been shown [10, Lemma 3.1] that AS.1 implies that $\Phi(x)$ and its first two derivatives are Lipschitz on $[x_k, x_k + s_k]$.

We define

$$H(x, y) := \sum_{i=1}^m y_i \nabla_{xx} r_i(x)$$

and let $q(x, s)$ be the vector whose i th component is

$$q_i(x, s) := s^T \nabla_{xx} r_i(x) s$$

for $i = 1, \dots, m$. In this case

$$t(x, s) = r(x) + J(x)s + \frac{1}{2}q(x, s).$$

Since $m(x_k, s)$ is a second-order accurate model of $\Phi(x_k + s)$, we expect bounds of the form

$$|\Phi(x_k + s_k) - m(x_k, s_k)| \leq L_f \|s_k\|^3 \tag{3.1}$$

and

$$|\nabla_x \Phi(x_k + s_k) - \nabla_s m(x_k, s_k)| \leq L_g \|s_k\|^2 \tag{3.2}$$

for some $L_f, L_g > 0$ and all $k \geq 0$ for which $\|s_k\| \leq 1$ (see ‘‘Appendix A’’).

Also, since $\|r(x)\|$ decreases monotonically,

$$\|J^T(x_k)r(x_k)\| \leq \|J^T(x_k)\|\|r(x_k)\| \leq L_J\|r(x_0)\| \quad (3.3)$$

and

$$\|H(x_k, r(x_k))\| \leq L_H\|r(x_k)\| \leq L_H\|r(x_0)\| \quad (3.4)$$

for some $L_J, L_H > 0$ and all $k \geq 0$ (again, see ‘‘Appendix A’’).

Our first result derives simple conclusions from the basic requirement that the step s_k in our algorithm is chosen to reduce the regularized model.

Lemma 3.1 *Algorithm 2.1 ensures that*

$$m(x_k, 0) - m(x_k, s_k) > \frac{1}{r}\sigma_k\|s_k\|^r \quad (3.5)$$

In addition, if $r = 2$, at least one of

$$\sigma_k < 2\|H(x_k, r(x_k))\| \quad (3.6)$$

or

$$\sigma_k\|s_k\| < 4\|J^T(x_k)r(x_k)\| \quad (3.7)$$

holds, while if $r > 2$,

$$\|s_k\| < \max\left(\left(\frac{r\|H(x_k, r(x_k))\|}{\sigma_k}\right)^{1/(r-1)}, \left(\frac{2r\|J^T(x_k)r(x_k)\|}{\sigma_k}\right)^{1/(r-2)}\right). \quad (3.8)$$

Proof It follows from (2.5), (2.3) and (2.2) that

$$\begin{aligned} 0 &> 2\left(m(x_k, s_k) + \frac{1}{r}\sigma_k\|s_k\|^r - m(x_k, 0)\right) \\ &= \|r(x_k) + J(x_k)s_k + \frac{1}{2}q(x_k, s_k)\|^2 + \frac{2}{r}\sigma_k\|s_k\|^r - \|r(x_k)\|^2 \\ &= \|J(x_k)s_k + \frac{1}{2}q(x_k, s_k)\|^2 + 2r^T(x_k)\left(J(x_k)s_k + \frac{1}{2}q(x_k, s_k)\right) + \frac{2}{r}\sigma_k\|s_k\|^r \\ &= \|J(x_k)s_k + \frac{1}{2}q(x_k, s_k)\|^2 + 2s_k^T J^T(x_k)r(x_k) + s_k^T H(x_k, r(x_k))s_k + \frac{2}{r}\sigma_k\|s_k\|^r \\ &\geq \|J(x_k)s_k + \frac{1}{2}q(x_k, s_k)\|^2 - 2\|J^T(x_k)r(x_k)\|\|s_k\| \\ &\quad - \|H(x_k, r(x_k))\|\|s_k\|^2 + \frac{2}{r}\sigma_k\|s_k\|^r. \end{aligned} \quad (3.9)$$

Inequality (3.5) follows immediately from the first inequality in (3.9). When $r = 2$, inequality (3.9) becomes

$$\begin{aligned} 0 &> \|J(x_k)s_k + \frac{1}{2}q(x_k, s_k)\|^2 \\ &\quad + \left(\frac{1}{2}\sigma_k\|s_k\| - 2\|J^T(x_k)r(x_k)\|\right)\|s_k\| + \left(\frac{1}{2}\sigma_k - \|H(x_k, r(x_k))\|\right)\|s_k\|^2. \end{aligned}$$

In order for this to be true, it must be that at least one of the last two terms is negative, and this provides the alternatives (3.6) and (3.7). By contrast, when $r > 2$, inequality (3.9) becomes

$$0 > \|J(x_k)s_k + \frac{1}{2}q(x_k, s_k)\|^2 + \left(\frac{1}{r}\sigma_k \|s_k\|^{r-1} - 2\|J^T(x_k)r(x_k)\|\right) \|s_k\| + \left(\frac{1}{r}\sigma_k \|s_k\|^{r-2} - \|H(x_k, r(x_k))\|\right) \|s_k\|^2,$$

and this implies that

$$\frac{1}{r}\sigma_k \|s_k\|^{r-1} < 2\|J^T(x_k)r(x_k)\| \text{ or } \frac{1}{r}\sigma_k \|s_k\|^{r-2} < \|H(x_k, r(x_k))\|$$

(or both), which gives (3.8). □

Our next task is to show that σ_k is bounded from above. Let

$$\mathcal{B}_\gamma := \left\{j \geq 0 \mid \sigma_j \geq \gamma r \max\left(\|H(x_j, r(x_j))\|, 2\|J^T(x_j)r(x_j)\|\right)\right\}$$

and

$$\mathcal{B} := \mathcal{B}_1,$$

and note that Lemma 3.1 implies that

$$\|s_k\| \leq 1 \text{ if } k \in \mathcal{B}_\gamma \text{ when } \gamma \geq 1,$$

and in particular

$$\|s_k\| \leq 1 \text{ for all } k \in \mathcal{B}. \tag{3.10}$$

We consider first the special case for which $r = 2$.

Lemma 3.2 *Suppose that AS.1 holds, $r = 2$, $k \in \mathcal{B}$ and*

$$\sigma_k \geq \sqrt{\frac{8L_f L_j \|r(x_0)\|}{1 - \eta_2}}. \tag{3.11}$$

Then iteration k of Algorithm 2.1 is very successful.

Proof Since $k \in \mathcal{B}$, Lemma 3.1 implies that (3.7) and (3.10) hold. Then (2.7), (3.1) and (3.5) give that

$$|\rho_k - 1| = \frac{|\Phi(x_k + s_k) - m(x_k, s_k)|}{m(x_k, 0) - m(x_k, s_k)} \leq \frac{2L_f \|s_k\|}{\sigma_k}$$

and hence

$$|\rho_k - 1| \leq \frac{8L_f \|J^T(x_k)r(x_k)\|}{\sigma_k^2} \leq \frac{8L_f L_J \|r(x_0)\|}{\sigma_k^2} \leq 1 - \eta_2$$

from (3.3), (3.7) and (3.11). Thus it follows from (2.8) that the iteration is very successful. \square

Lemma 3.3 *Suppose that AS.1 holds and $r = 2$. Then Algorithm 2.1 ensures that*

$$\sigma_k \leq \sigma_{\max} := \gamma_3 \max \left(\sqrt{\frac{8L_f L_J \|r(x_0)\|}{1 - \eta_2}}, \sigma_0, 2 \max(L_H, 2L_J) \|r(x_0)\| \right) \quad (3.12)$$

for all $k \geq 0$.

Proof Let

$$\sigma_{\max}^B = \gamma_3 \max \left(\sqrt{\frac{8L_f L_J \|r(x_0)\|}{1 - \eta_2}}, \sigma_0 \right).$$

Suppose that $k + 1 \in \mathcal{B}_{\gamma_3}$ is the first iteration for which $\sigma_{k+1} \geq \sigma_{\max}^B$. Then, since $\sigma_k < \sigma_{k+1}$, iteration k must have been unsuccessful, $x_k = x_{k+1}$ and (2.8) gives that $\sigma_{k+1} \leq \gamma_3 \sigma_k$. Thus

$$\begin{aligned} \gamma_3 \sigma_k &\geq \sigma_{k+1} \geq 2\gamma_3 \max(\|H(x_{k+1}, r(x_{k+1}))\|, 2\|J^T(x_{k+1})r(x_{k+1})\|) \\ &= 2\gamma_3 \max(\|H(x_k, r(x_k))\|, 2\|J^T(x_k)r(x_k)\|) \end{aligned}$$

since $k + 1 \in \mathcal{B}_{\gamma_3}$, which implies that $k \in \mathcal{B}$. Furthermore,

$$\gamma_3 \sigma_k \geq \sigma_{k+1} \geq \sigma_{\max}^B \geq \gamma_3 \sqrt{\frac{8L_f L_J \|r(x_0)\|}{1 - \eta_2}},$$

which implies that (3.11) holds. But then Lemma 3.2 implies that iteration k must be very successful. This contradiction ensures that

$$\sigma_k < \sigma_{\max}^B \quad (3.13)$$

for all $k \in \mathcal{B}_{\gamma_3}$. For all other iterations, we have that $k \notin \mathcal{B}_{\gamma_3}$, and for these the definition of \mathcal{B}_{γ_3} , and the bounds (3.3) and (3.4) give

$$\sigma_k < 2\gamma_3 \max(\|H(x_k, r(x_k))\|, 2\|J^T(x_k)r(x_k)\|) \leq 2\gamma_3 \max(L_H, 2L_J) \|r(x_0)\|. \quad (3.14)$$

Combining (3.13) and (3.14) gives (3.12). \square

We now turn to the general case for which $2 < r \leq 3$.

Lemma 3.4 *Suppose that AS.1 holds, $2 < r \leq 3$, $k \in \mathcal{B}$ and*

$$\sigma_k \geq \max \left(\left(\frac{rL_f(rL_H\|r(x_0)\|)^{\frac{3-r}{r-1}}}{1-\eta_2} \right)^{\frac{r-1}{2}}, \left(\frac{rL_f(2rL_J\|r(x_0)\|)^{\frac{3-r}{r-2}}}{1-\eta_2} \right)^{r-2} \right) \tag{3.15}$$

Then iteration k of Algorithm 2.1 is very successful.

Proof Since $k \in \mathcal{B}$, it follows from (2.7), (3.10), (3.1), (3.5), (3.8), (3.3), (3.4) and (3.15) that

$$\begin{aligned} |\rho_k - 1| &= \frac{|\Phi(x_k + s_k) - m(x_k, s_k)|}{m(x_k, 0) - m(x_k, s_k)} \leq \frac{rL_f\|s_k\|^{3-r}}{\sigma_k} \\ &< rL_f \max \left((r\|H(x_k, r(x_k))\|)^{(3-r)/(r-1)} \sigma_k^{-2/(r-1)}, \right. \\ &\quad \left. (2r\|J^T(x_k)r(x_k)\|)^{(3-r)/(r-2)} \sigma_k^{-1/(r-2)} \right) \\ &\leq rL_f \max \left((rL_H\|r(x_0)\|)^{(3-r)/(r-1)} \sigma_k^{-2/(r-1)}, \right. \\ &\quad \left. (2rL_J\|r(x_0)\|)^{(3-r)/(r-2)} \sigma_k^{-1/(r-2)} \right) \\ &\leq 1 - \eta_2. \end{aligned} \tag{3.16}$$

As before, (2.8) then ensures that the iteration is very successful. □

Lemma 3.5 *Suppose that AS.1 holds and $2 < r \leq 3$. Then Algorithm 2.1 ensures that*

$$\sigma_k \leq \sigma_{\max} := \gamma_3 \max \left(\left(\frac{rL_f(pL_H\|r(x_0)\|)^{\frac{3-r}{r-1}}}{1-\eta_2} \right)^{\frac{r-1}{2}}, \left(\frac{rL_f(2rL_J\|r(x_0)\|)^{\frac{3-r}{r-2}}}{1-\eta_2} \right)^{r-2}, \sigma_0, r \max(L_H, 2L_J)\|r(x_0)\| \right) \tag{3.17}$$

for all $k \geq 0$.

Proof The proof mimics that of Lemma 3.3. First, suppose that $k \in \mathcal{B}_{\gamma_3}$ and that iteration $k + 1$ is the first for which

$$\sigma_{k+1} \geq \sigma_{\max}^B := \gamma_3 \max \left(\left(\frac{rL_f(rL_H\|r(x_0)\|)^{\frac{3-r}{r-1}}}{1-\eta_2} \right)^{\frac{r-1}{2}}, \left(\frac{rL_f(2rL_J\|r(x_0)\|)^{\frac{3-r}{r-2}}}{1-\eta_2} \right)^{r-2}, \sigma_0 \right).$$

Then, since $\sigma_k < \sigma_{k+1}$, iteration k must have been unsuccessful and (2.8) gives that

$$\gamma_3\sigma_k \geq \sigma_{k+1} \geq \sigma_{\max}^B,$$

which implies that $k \in \mathcal{B}$ and (3.15) holds. But then Lemma 3.4 implies that iteration k must be very successful. This contradiction provides the first three terms in the bound (3.17), while the others arise as for the proof of Lemma 3.3 when $k \notin \mathcal{B}_{\gamma_3}$. \square

Next, we bound the number of iterations in terms of the number of successful ones.

Lemma 3.6 [8, Theorem 2.1]. *The adjustment (2.8) in Algorithm 2.1 ensures that*

$$k \leq \kappa_u |\mathcal{S}_k| + \kappa_s, \quad \text{where } \kappa_u := \left(1 - \frac{\log \gamma_1}{\log \gamma_2}\right), \kappa_s := \frac{1}{\log \gamma_2} \log \left(\frac{\sigma_{\max}}{\sigma_0}\right), \quad (3.18)$$

and σ_{\max} is any known upper bound on σ_k .

Our final ingredient is to find a useful bound on the smallest model decrease as the algorithm proceeds. Let $\mathcal{L} := \{k \mid \|s_k\| \leq 1\}$, and let $\mathcal{G} := \{k \mid \|s_k\| > 1\}$ be its complement. We then have the following crucial bounds.

Lemma 3.7 *Suppose that AS.1 holds and $2 \leq r \leq 3$. Then Algorithm 2.1 ensures that*

$$m(x_k, 0) - m(x_k, s_k) \geq \begin{cases} \frac{1}{r} \sigma_{\min} \left(\frac{\|\nabla_x \Phi(x_k + s_k)\|}{L_g + \theta + \sigma_{\max}} \right)^{\frac{r}{r-1}} & \text{if } k \in \mathcal{L} \\ \frac{1}{r} \sigma_{\min} & \text{if } k \in \mathcal{G}. \end{cases} \quad (3.19)$$

Proof Consider $k \in \mathcal{L}$. The Cauchy-Schwarz inequality and (2.4) reveal that

$$\begin{aligned} \|\nabla_x \Phi(x_k + s_k)\| &= \|(\nabla_x \Phi(x_k + s_k) - \nabla_s m(x_k, s_k)) \\ &\quad + (\nabla_s m(x_k, s_k) + \sigma_k \|s_k\|^{r-2} s_k) - \sigma_k \|s_k\|^{r-2} s_k\| \\ &\leq \|\nabla_x \Phi(x_k + s_k) - \nabla_s m(x_k, s_k)\| \\ &\quad + \|\nabla_s m^R(x_k, s_k, \sigma_k)\| + \sigma_k \|s_k\|^{r-1}. \end{aligned} \quad (3.20)$$

Combining (3.20) with (3.2), (2.6), (3.12), (3.17) and $\|s_k\| \leq 1$ we have

$$\|\nabla_x \Phi(x_k + s_k)\| \leq L_g \|s_k\|^2 + \theta \|s_k\|^{r-1} + \sigma_{\max} \|s_k\|^{r-1} \leq (L_g + \theta + \sigma_{\max}) \|s_k\|^{r-1}$$

and thus that

$$\|s_k\| \geq \left(\frac{\|\nabla_x \Phi(x_k + s_k)\|}{L_g + \theta + \sigma_{\max}} \right)^{\frac{1}{r-1}}.$$

But then, combining this with (3.5), the lower bound

$$\sigma_k \geq \sigma_{\min} \quad (3.21)$$

imposed by Algorithm 2.1 and (3.5) provides the first possibility in (3.19).

By contrast, if $k \in \mathcal{G}$, (3.5), $\|s_k\| > 1$ and (3.21) ensure the second possibility in (3.19). \square

Corollary 3.8 *Suppose that AS.1 holds and $2 \leq r \leq 3$. Then Algorithm 2.1 ensures that*

$$\Phi(x_k) - \Phi(x_{k+1}) \geq \begin{cases} \frac{1}{r} \eta_1 \sigma_{\min} \left(\frac{\|\nabla_x \Phi(x_k + s_k)\|}{L_g + \theta + \sigma_{\max}} \right)^{\frac{r}{r-1}} & \text{if } k \in \mathcal{L} \cap \mathcal{S} \\ \frac{1}{r} \eta_1 \sigma_{\min} & \text{if } k \in \mathcal{G} \cap \mathcal{S}. \end{cases} \quad (3.22)$$

Proof The result follows directly from and (2.7) and (3.19). □

We now provide our three main convergence results. Firstly, we establish the global convergence¹ of our algorithm to first-order critical points of $\Phi(x)$.

Theorem 3.9 *Suppose that AS.1 holds and $2 \leq r \leq 3$. Then the iterates $\{x_k\}$ generated by Algorithm 2.1 satisfy*

$$\lim_{k \rightarrow \infty} \|\nabla_x \Phi(x_k)\| = 0 \quad (3.23)$$

if no non-trivial termination test is provided.

Proof Suppose that $\epsilon > 0$, and consider any successful iteration for which

$$\|\nabla_x \Phi(x_k)\| \geq \epsilon > 0. \quad (3.24)$$

Then it follows from (3.22) that

$$\Phi(x_k) - \Phi(x_{k+1}) \geq \delta := \frac{\eta_1 \sigma_{\min}}{r} \min \left(\left(\frac{\epsilon}{L_g + \theta + \sigma_{\max}} \right)^{\frac{r}{r-1}}, 1 \right) > 0. \quad (3.25)$$

Consider the set $\mathcal{U}_\epsilon = \{k \in \mathcal{S} \mid \|\nabla_x \Phi(x_k)\| \geq \epsilon\}$, suppose that \mathcal{U}_ϵ is infinite, and let k_i be the i -th entry of \mathcal{U}_ϵ . Now consider

$$i_\epsilon = \lceil \frac{1}{2} \|r(x_0)\|^2 / \delta \rceil + 1.$$

Thus summing (3.25) over successful iterations, recalling that $\Phi(x_0) = \frac{1}{2} \|r(x_0)\|^2$, $\Phi(x_k) \geq 0$, and that Φ decreases monotonically and using (3.25), we have that

$$\frac{1}{2} \|r(x_0)\|^2 \geq \Phi(x_0) - \Phi(x_{k_{i_\epsilon}+1}) \geq \sum_{k \in \mathcal{U}_\epsilon, k \leq k_{i_\epsilon}} \Phi(x_k) - \Phi(x_{k+1}) \geq i_\epsilon \delta > \frac{1}{2} \|r(x_0)\|^2. \quad (3.26)$$

This contradiction shows that \mathcal{U}_ϵ is finite for any $\epsilon > 0$, and therefore (3.23) holds. □

Secondly, we provide an evaluation complexity result based on the stopping criterion (1.2).

¹ Our proof avoids the traditional route via a lim inf result, and is indebted to [14].

Theorem 3.10 *Suppose that AS.1 holds and $2 \leq r \leq 3$. Then Algorithm 2.1 requires at most*

$$\left\lceil \frac{\kappa_u \|r(x_0)\|^2 r (L_g + \theta + \sigma_{\max})^{\frac{r}{r-1}}}{2\eta_1 \sigma_{\min}} \epsilon^{-\frac{r}{r-1}} \right\rceil + \kappa_s + 1 \quad (3.27)$$

evaluations of $r(x)$ and its derivatives to find an iterate x_k for which the termination test

$$\|\nabla_x \Phi(x_k)\| \leq \epsilon$$

is satisfied for given $0 < \epsilon < 1$, where κ_u and κ_s are defined in (3.18).

Proof If the algorithm has not terminated, (3.24) holds, so summing (3.25) as before

$$\frac{1}{2} \|r(x_0)\|^2 \geq \Phi(x_0) - \Phi(x_{k+1}) \geq |\mathcal{S}_k| \delta = |\mathcal{S}_k| \frac{\eta_1 \sigma_{\min}}{r} \left(\frac{\epsilon}{L_g + \theta + \sigma_{\max}} \right)^{\frac{r}{r-1}} \quad (3.28)$$

since $\epsilon < 1$, and thus that

$$|\mathcal{S}_k| \leq \frac{\|r(x_0)\|^2 (L_g + \theta + \sigma_{\max})^{\frac{r}{r-1}}}{2\eta_1 \sigma_{\min}} \epsilon^{-\frac{r}{r-1}}.$$

Combining this with (3.18) and remembering that we need to evaluate the function and gradient at the final x_{k+1} yields the bound (3.27). \square

Notice how the evaluation complexity improves from $O(\epsilon^{-2})$ evaluations with quadratic ($r = 2$) regularization to $O(\epsilon^{-3/2})$ evaluations with cubic ($r = 3$) regularization. It is not clear if these bounds are sharp.

Finally, we refine this analysis to provide an alternative complexity result based on the stopping rule (1.3). The proof of this follows similar arguments in [9, §3.2], [11, §3] and crucially depends upon the following elementary result.

Lemma 3.11 *Suppose that $a > b \geq 0$. Then*

$$a^2 - b^2 \geq c \text{ implies that } a^{1/2^i} - b^{1/2^i} \geq \frac{c}{2^{i+1} a^{\frac{2^{i+1}-1}{2^i}}}$$

for all integers $i \geq -1$.

Proof The result follows directly by induction using the identity $A^2 - B^2 = (A - B)(A + B)$ with $A = a^{1/2^j} > B = b^{1/2^j}$ for increasing $j \leq i$. \square

Theorem 3.12 *Suppose that AS.1 holds, $2 < r \leq 3$ and that the integer*

$$i \geq i_0 := \left\lceil \log_2 \left(\frac{r-1}{r-2} \right) \right\rceil \tag{3.29}$$

is given. Then Algorithm 2.1 requires at most

$$\left\lceil \kappa_u \max \left(\kappa_c^{-1}, \kappa_g^{-1} \epsilon_d^{-r/(r-1)}, \kappa_r^{-1} \epsilon_p^{-1/2^i} \right) \right\rceil + \kappa_s + 1 \tag{3.30}$$

evaluations of $r(x)$ and its derivatives to find an iterate x_k for which the termination test

$$\|r(x_k)\| \leq \epsilon_p \quad \text{or} \quad \|g_r(x_k)\| \leq \epsilon_d, \tag{3.31}$$

is satisfied for given $\epsilon_p > 0$ and $\epsilon_d > 0$, where κ_u and κ_s are defined in (3.18), κ_c , κ_g and κ_r are given by

$$\begin{aligned} \kappa_c &:= \frac{1}{2}^{i+1} \frac{\eta_1 \sigma_{\min}}{r} \|r(x_0)\|^{-(2^{i+1}-1)/2^i}, \\ \kappa_g &:= \frac{\frac{1}{2}^i \eta_1 \sigma_{\min} \beta^{r/(r-1)}}{r(L + \theta + \sigma_{\max})^{r/(r-1)}} \|r(x_0)\|^{(r/(r-1)-(2^{i+1}-1)/2^i)} \\ \text{and } \kappa_r &:= \frac{1 - \beta^{1/2^i}}{\beta^{1/2^i}}, \end{aligned} \tag{3.32}$$

and $\beta \in (0, 1)$ is a fixed problem-independent constant.

Proof Consider $\mathcal{S}_\beta := \{l \in \mathcal{S} \mid \|r(x_{l+1})\| > \beta \|r(x_l)\|\}$, and let i be the smallest integer for which

$$\frac{2^{i+1} - 1}{2^i} \geq \frac{r}{r-1}, \tag{3.33}$$

that is i satisfies (3.29).

First, consider $l \in \mathcal{G} \cap \mathcal{S}$. Then (3.22) gives that

$$\|r(x_l)\|^2 - \|r(x_{l+1})\|^2 \geq \frac{\eta_1 \sigma_{\min}}{r}$$

and, since

$$\|r(x_{l+1})\| < \|r(x_l)\| \leq \|r(x_0)\| \tag{3.34}$$

for all $l \in \mathcal{S}$, Lemma 3.11 implies that

$$\begin{aligned} \|r(x_l)\|^{1/2^i} - \|r(x_{l+1})\|^{1/2^i} &\geq \frac{1}{2}^{i+1} \frac{\eta_1 \sigma_{\min}}{r} \|r(x_l)\|^{-(2^{i+1}-1)/2^i} \\ &\geq \frac{1}{2}^{i+1} \frac{\eta_1 \sigma_{\min}}{r} \|r(x_0)\|^{-(2^{i+1}-1)/2^i}. \end{aligned} \tag{3.35}$$

By contrast, for $l \in \mathcal{L} \cap \mathcal{S}$, (3.22) gives that

$$\begin{aligned} \|r(x_l)\|^2 - \|r(x_{l+1})\|^2 &\geq \kappa \|J^T(x_{l+1})r(x_{l+1})\|^{r/(r-1)}, \quad \text{where} \\ \kappa &= \frac{2\eta_1\sigma_{\min}}{r(L + \theta + \sigma_{\max})^{r/(r-1)}}. \end{aligned} \quad (3.36)$$

If additionally $l \in \mathcal{S}_\beta$, (3.36) may be refined as

$$\begin{aligned} \|r(x_l)\|^2 - \|r(x_{l+1})\|^2 &\geq \kappa \left(\frac{\|J^T(x_{l+1})r(x_{l+1})\|}{\|r(x_{l+1})\|} \right)^{r/(r-1)} \|r(x_{l+1})\|^{r/(r-1)} \\ &\geq \kappa \left(\frac{\|J^T(x_{l+1})r(x_{l+1})\|}{\|r(x_{l+1})\|} \right)^{r/(r-1)} \|r(x_{l+1})\|^{r/(r-1)} \\ &\geq \kappa \beta^{r/(r-1)} \|g_r(x_{l+1})\|^{r/(r-1)} \|r(x_l)\|^{r/(r-1)} \end{aligned} \quad (3.37)$$

from (1.4) and the requirement that $\|r(x_{l+1})\| > \beta \|r(x_l)\|$. Using (3.37), (3.34), Lemma 3.11 and (3.33), we then obtain the bound

$$\begin{aligned} \|r(x_l)\|^{1/2^i} - \|r(x_{l+1})\|^{1/2^i} &\geq \frac{1}{2}^{i+1} \kappa \beta^{r/(r-1)} \|g_r(x_{l+1})\|^{r/(r-1)} \\ &\quad \|r(x_l)\|^{(r/(r-1) - (2^{i+1} - 1)/2^i)} \\ &\geq \frac{1}{2}^{i+1} \kappa \beta^{r/(r-1)} \|r(x_0)\|^{(r/(r-1) - (2^{i+1} - 1)/2^i)} \\ &\quad \|g_r(x_{l+1})\|^{r/(r-1)} \end{aligned} \quad (3.38)$$

for all $l \in \mathcal{L} \cap \mathcal{S}_\beta$. Finally, consider $l \in \mathcal{S} \setminus \mathcal{S}_\beta$, for which $\|r(x_{l+1})\| \leq \beta \|r(x_l)\|$ and hence $\|r(x_{l+1})\|^{1/2^i} \leq \beta^{1/2^i} \|r(x_l)\|^{1/2^i}$. Thus we have that

$$\begin{aligned} \|r(x_l)\|^{1/2^i} - \|r(x_{l+1})\|^{1/2^i} &\geq (1 - \beta^{1/2^i}) \|r(x_l)\|^{1/2^i} \\ &\geq \frac{1 - \beta^{1/2^i}}{\beta^{1/2^i}} \|r(x_{l+1})\|^{1/2^i} \end{aligned} \quad (3.39)$$

for all $l \in \mathcal{L} \cap (\mathcal{S} \setminus \mathcal{S}_\beta)$. Thus, combining (3.35), (3.38) and (3.39), we have that

$$\|r(x_l)\|^{1/2^i} - \|r(x_{l+1})\|^{1/2^i} \geq \min \left(\kappa_c, \kappa_g \|g_r(x_{l+1})\|^{r/(r-1)}, \kappa_r \|r(x_{l+1})\|^{1/2^i} \right), \quad (3.40)$$

for κ_c, κ_g and κ_r given by (3.32), for all $l \in \mathcal{S}$.

Now suppose that the stopping rule (3.31) has not been satisfied up until the start of iteration $k + 1$, and thus that

$$\|r(x_{l+1})\| > \epsilon_p \quad \text{and} \quad \|g_r(x_{l+1})\| > \epsilon_d \quad (3.41)$$

for all $l \in \mathcal{S}_k$. Combining this with (3.40), we have that

$$\|r(x_l)\|^{1/2^i} - \|r(x_{l+1})\|^{1/2^i} \geq \min\left(\kappa_c, \kappa_g \epsilon_d^{r/(r-1)}, \kappa_r \epsilon_p^{1/2^i}\right),$$

and thus, summing over $l \in \mathcal{S}_k$ and using (3.34),

$$\|r(x_0)\|^{1/2^i} \geq \|r(x_0)\|^{1/2^i} - \|r(x_{k+1})\|^{1/2^i} \geq |\mathcal{S}_k| \min\left(\kappa_c, \kappa_g \epsilon_d^{r/(r-1)}, \kappa_r \epsilon_p^{1/2^i}\right).$$

As before, combining this with (3.18) and remembering that we need to evaluate the function and gradient at the final x_{k+1} yields the bound (3.30). \square

If $i < i_0$, a weaker bound that includes $r = 2$ is possible. The key is to note that the purpose of (3.33) is to guarantee the second inequality in (3.38). Without this, we have instead

$$\|r(x_l)\|^{1/2^i} - \|r(x_{l+1})\|^{1/2^i} \geq \frac{1}{2}^{i+1} \kappa \beta^{r/(r-1)} \|g_r(x_{l+1})\|^{r/(r-1)} \|r(x_{l+1})\|^{(r/(r-1)-(2^{i+1}-1)/2^i)} \tag{3.42}$$

for all $l \in \mathcal{L} \cap \mathcal{S}_\beta$, and this leads to

$$\|r(x_l)\|^{1/2^i} - \|r(x_{l+1})\|^{1/2^i} \geq \min\left(\kappa_c, \kappa_g \epsilon_d^{r/(r-1)} \epsilon_p^{(r/(r-1)-(2^{i+1}-1)/2^i)}, \kappa_r \epsilon_p^{1/2^i}\right),$$

where

$$\kappa_g' := \frac{\frac{1}{2}^i \eta_1 \sigma_{\min} \beta^{r/(r-1)}}{r(L_g + \theta + \sigma_{\max})^{r/(r-1)}}.$$

if (3.41) holds. This results in a bound of $O\left(\max(1, \epsilon_d^{r/(r-1)} \cdot \epsilon_p^{(r/(r-1)-(2^{i+1}-1)/2^i)}, \epsilon_p^{1/2^i})\right)$ function evaluations, which approaches that in (3.30) as i increases to infinity when $r = 2$.

4 A modified algorithm for cubic-and-higher regularization

For the case where $r > 3$, the proof of Lemma 3.4 breaks down as there is no obvious bound on the quantity $\|s_k\|^{3-r}/\sigma_k$. One way around this defect is to modify Algorithm 2.1 so that such a bound automatically occurs. We consider the following variant; our development follows very closely that in [12], itself inspired by [20]. For completeness, we allow $r = 3$ in this new framework since it is trivial to do so.

Algorithm 4.1 Adaptive Tensor-Newton Regularization when $r \geq 3$.

A starting point x_0 , an initial regularization parameter $\sigma_0 > 0$ and algorithmic parameters $\theta > 0, \alpha \in (0, \frac{1}{3}], \gamma_3 \geq \gamma_2 > 1 > \gamma_1 > 0$ and $1 > \eta_2 \geq \eta_1 > 0$, are given. Evaluate $\Phi(x_0)$, and test for termination at x_0 .

For $k = 0, 1, \dots$, until **termination**, do:

1. Compute derivatives of $r(x)$ at x_k .
2. Compute a step s_k by approximately minimizing $m^R(x_k, s, \sigma_k)$ so that

$$m^R(x_k, s_k, \sigma_k) < m^R(x_k, 0, \sigma_k)$$

and

$$\|\nabla_s m^R(x_k, s_k, \sigma_k)\| \leq \theta \|s_k\|^2 \quad (4.1)$$

hold.

3. Set $\hat{x}_k = x_k + s_k$, and test for termination at \hat{x}_k .
4. Compute $\Phi(\hat{x}_k)$ and

$$\rho_k = \frac{\Phi(x_k) - \Phi(\hat{x}_k)}{m(x_k, 0) - m(x_k, s_k)}.$$

If $\rho_k \geq \eta_1$ and

$$\sigma_k \|s_k\|^{r-1} \geq \alpha \|\nabla_x \Phi(\hat{x}_k)\|, \quad (4.2)$$

set $x_{k+1} = \hat{x}_k$.

5. Set

$$\sigma_{k+1} \in \begin{cases} [\gamma_1 \sigma_k, \sigma_k] & \text{if } \rho_k \geq \eta_2 \text{ and (4.2) holds} \\ [\sigma_k, \gamma_2 \sigma_k] & \text{if } \eta_1 \leq \rho_k < \eta_2 \text{ and (4.2) holds} \\ [\gamma_2 \sigma_k, \gamma_3 \sigma_k] & \text{if } \rho_k < \eta_1 \text{ or (4.2) fails,} \end{cases} \quad (4.3)$$

and go to Step 2 if $\rho_k < \eta_1$ or (4.2) fails.

It is important that termination is tested at Step 3 as deductions from computations in subsequent steps rely on this. We modify our definition of a successful step accordingly so that now $\mathcal{S}_k = \{0 \leq l \leq k \mid \rho_l \geq \eta_1 \text{ and (4.2) holds}\}$ and $\mathcal{S} = \{k \geq 0 \mid \rho_k \geq \eta_1 \text{ and (4.2) holds}\}$, and note in particular that Lemma 3.6 continues to hold in this case since it only depends on the adjustments in (4.3). Likewise, a very successful iteration is now one for which $\rho_k \geq \eta_2$ and (4.2) holds. Note that (4.3), unlike (2.8) in Algorithm 2.1, does not impose a nonzero lower bound on the generated regularization weight; this will be reflected in our derived complexity bound (cf Theorems 3.12 and 4.7).

As is now standard, our first task is to establish an upper bound on σ_k .

Lemma 4.1 *Suppose that AS.1 holds, $r \geq 3$ and*

$$\sigma_k \|s_k\|^{r-3} \geq \kappa_2, \quad \text{where } \kappa_2 := \frac{rL}{1 - \eta_2} \text{ and } L = \max(L_f, L_g, \theta). \quad (4.4)$$

Then iteration k of Algorithm 4.1 is very successful.

Proof It follows immediately from (2.7), (3.1), (3.5) and (4.4) that

$$|\rho_k - 1| = \frac{|\Phi(x_k + s_k) - m(x_k, s_k)|}{m(x_k, 0) - m(x_k, s_k)} \leq \frac{rL_f \|s_k\|^{3-r}}{\sigma_k} \leq \frac{rL \|s_k\|^{3-r}}{\sigma_k} \leq 1 - \eta_2,$$

and thus $\rho_k \geq \eta_2$. Observe that

$$\kappa_2 \geq L \tag{4.5}$$

since $1 - \eta_2 \leq 1$ and $r \geq 1$. We also have from (3.20), (3.2) and (4.1) that

$$\|\nabla_x \Phi(x_k + s_k)\| \leq L_g \|s_k\|^2 + \theta \|s_k\|^2 + \sigma_k \|s_k\|^{r-1} = \left(L_g + \theta + \sigma_k \|s_k\|^{r-3} \right) \|s_k\|^2 \tag{4.6}$$

and thus from (4.4), (4.5) and the algorithmic restriction $3 \leq 1/\alpha$ that

$$\begin{aligned} \|\nabla_x \Phi(x_k + s_k)\| &\leq \left(2L + \sigma_k \|s_k\|^{r-3} \right) \|s_k\|^2 \leq \left(3\sigma_k \|s_k\|^{r-3} \right) \|s_k\|^2 \\ &= 3\sigma_k \|s_k\|^{r-1} \leq \frac{\sigma_k}{\alpha} \|s_k\|^{r-1}. \end{aligned}$$

Thus (4.2) is also satisfied, and hence iteration k is very successful. □

Lemma 4.2 *Suppose that AS.1 holds, $r \geq 3$ and*

$$\sigma_k \geq \kappa_1 \|\nabla_s \Phi(x_k + s_k)\|^{(3-r)/2}, \quad \text{where } \kappa_1 := \kappa_2(3\kappa_2)^{(r-3)/2} \tag{4.7}$$

and κ_2 is defined in the statement of Lemma 4.1. Then iteration k of Algorithm 4.1 is very successful.

Proof It follows from Lemma 4.1 that it suffices to show that (4.7) implies (4.4). The result is immediate when $r = 3$ since then (4.4) is (4.7). Suppose therefore that $r > 3$ and that (4.4) is not true, that is

$$\sigma_k \|s_k\|^{r-3} < \kappa_2. \tag{4.8}$$

Then (4.6), (4.8) and (4.5) imply that

$$\|\nabla_x \Phi(x_k + s_k)\| \leq (2L + \kappa_2) \|s_k\|^2 < 3\kappa_2 \|s_k\|^2 < 3\kappa_2 \left(\frac{\kappa_2}{\sigma_k} \right)^{2/(r-3)}$$

which contradicts (4.7). Thus (4.4) holds. □

Unlike in our previous analysis of Algorithm 2.1 when $r \leq 3$, we are unable to deduce an upper bound on σ_k without further consideration. With this in mind, we now suppose that all the iterates $x_k + s_k$ generated by Algorithm 4.1 satisfy

$$\|\nabla_x \Phi(x_k + s_k)\| \geq \epsilon \tag{4.9}$$

for some $\epsilon > 0$ and all $0 \leq k \leq l$, and thus, from (4.2), that

$$\sigma_k \|s_k\|^{r-1} \geq \alpha \epsilon \quad (4.10)$$

for $k \in S_l$. In this case, we can show that σ_k is bounded from above.

Lemma 4.3 *Suppose that AS.1 holds and $r \geq 3$. Then provided that (4.9) holds for all $0 \leq k \leq l$, Algorithm 4.1 ensures that*

$$\sigma_k \leq \sigma_{\max} := \gamma_3 \max \left(\kappa_1 \epsilon^{(3-r)/2}, \sigma_0 \right) \quad (4.11)$$

and κ_1 is defined in the statement of Lemma 4.2.

Proof The proof is similar to the first part of that of Lemma 3.5. Suppose that iteration $k+1$ (with $k \leq l$) is the first for which $\sigma_{k+1} \geq \sigma_{\max}$. Then, since $\sigma_k < \sigma_{k+1}$, iteration k must have been unsuccessful and (4.3) gives that

$$\gamma_3 \sigma_k \geq \sigma_{k+1} \geq \sigma_{\max},$$

i.e., that

$$\sigma_k \geq \max \left(\kappa_1 \epsilon^{(3-r)/2}, \sigma_0 \right) \geq \kappa_1 \epsilon^{(3-r)/2} \geq \kappa_1 \|\nabla_x \Phi(x_k + s_k)\|^{(3-r)/2}$$

because of (4.9). But then Lemma 4.2 implies that iteration k must be very successful. This contradiction establishes (4.11). \square

We may also show that a successful step ensures a non-trivial reduction in $\Phi(x)$.

Lemma 4.4 *Suppose that AS.1 holds and $r \geq 3$. Suppose further that (4.9) holds for all $0 \leq k \leq l$. Then provided that (4.9) holds for all $0 \leq k \leq l$ and some $0 < \epsilon \leq 1$, Algorithm 4.1 guarantees that*

$$\Phi(x_k) - \Phi(x_{k+1}) \geq \kappa_4 \epsilon^{3/2} > 0 \quad (4.12)$$

for all $k \in S$, where

$$\kappa_4 := \frac{\eta \alpha^{r/(r-1)}}{r \kappa_3^{1/(r-1)}}, \quad \kappa_3 := \gamma_3 \max(\kappa_1, \sigma_0), \quad (4.13)$$

and κ_1 is defined in the statement of Lemma 4.2.

Proof Since $0 < \epsilon \leq 1$, (4.11) ensures that $\sigma_{\max} \leq \kappa_3 \epsilon^{(3-r)/2}$ and thus if $k \in \mathcal{S}$, it follows from (3.5) and (4.10) that

$$\begin{aligned} \Phi(x_k) - \Phi(x_{k+1}) &\geq \eta_1(m(x_k, 0) - m(x_k, s_k)) > \frac{\eta_1}{r} \sigma_k \|s_k\|^r \\ &= \frac{\eta_1}{r} (\sigma_k \|s_k\|^{r-1}) \|s_k\| \geq \frac{\eta_1}{r} \alpha \epsilon \frac{(\alpha \epsilon)^{1/(r-1)}}{\sigma_k^{1/(r-1)}} \geq \frac{\eta(\alpha \epsilon)^{r/(r-1)}}{r \sigma_{\max}^{1/(r-1)}} \\ &\geq \frac{\eta \alpha^{r/(r-1)}}{r \kappa_3^{1/(r-1)}} \frac{\epsilon^{r/(r-1)}}{(\epsilon^{(3-r)/2})^{1/(r-1)}} = \kappa_4 \epsilon^{3/2} > 0, \end{aligned}$$

as required. □

These introductory lemmas now lead to our main convergence results. First we establish global convergence to a critical point of $\Phi(x)$.

Theorem 4.5 *Suppose that AS.1 holds and $r \geq 3$. Then the iterates $\{x_k\}$ generated by Algorithm 4.1 satisfy*

$$\liminf_{k \rightarrow \infty} \|\nabla_x \Phi(x_k)\| = 0 \tag{4.14}$$

if no non-trivial termination test is provided.

Proof Suppose that (4.14) does not hold, in which case (4.9) holds for some $0 < \epsilon \leq 1$ and all $k \geq 0$. We then deduce by summing the reduction in $\Phi(x)$ guaranteed by Lemma 4.4 over successful iterations that

$$\frac{1}{2} \|r(x_0)\|^2 \geq \Phi(x_0) - \Phi(x_{k+1}) \geq |S_k| \kappa_4 \epsilon^{3/2}.$$

Just as in the proof of Theorem 3.10, this ensures that there are only a finite number of successful iterations. If iteration k is the last of these, all subsequent iterations are unsuccessful, and thus σ_k grows without bound. But as this contradicts Lemma 4.3, (4.9) cannot be true, and thus (4.14) holds. □

Next, we give an evaluation complexity result based on the stopping criterion (1.2).

Theorem 4.6 *Suppose that AS.1 holds and $r \geq 3$. Then Algorithm 4.1 requires at most*

$$\begin{aligned} &\left\lceil \kappa_u \frac{\|r(x_0)\|^2}{2\kappa_4} \epsilon^{-3/2} + \kappa_b \right\rceil + 1 && \text{if } r = 3, \\ &\left\lceil \kappa_u \frac{\|r(x_0)\|^2}{2\kappa_4} \epsilon^{-3/2} + \kappa_i + \kappa_e \log \epsilon^{-1} \right\rceil + 1 && \text{if } r > 3 \text{ and } \epsilon < \left(\frac{\kappa_1}{\sigma_0}\right)^{2/(r-3)}, \\ &\left\lceil \kappa_u \frac{\|r(x_0)\|^2}{2\kappa_4} \epsilon^{-3/2} + \kappa_a \right\rceil + 1 && \text{otherwise} \end{aligned} \tag{4.15}$$

evaluations of $r(x)$ and its derivatives to find an iterate x_k for which the termination test

$$\|\nabla_x \Phi(x_k)\| \leq \epsilon$$

is satisfied for given $0 < \epsilon < 1$, where

$$\kappa_b := \frac{\log(\kappa_3/\sigma_0)}{\log \gamma_2}, \quad \kappa_i := \frac{\log(\gamma_3 \kappa_1/\sigma_0)}{\log \gamma_2}, \quad \kappa_e := \frac{r-3}{2 \log \gamma_2} \quad \text{and} \quad \kappa_a := \frac{\log \gamma_3}{\log \gamma_2}, \quad (4.16)$$

κ_u is defined in (3.18), κ_1 in (4.7) and κ_3 in (4.13).

Proof If the algorithm has not terminated on or before iteration k , (4.9) holds, and so summing (4.12) over successful iterations and recalling that $\Phi(x_0) = \frac{1}{2} \|r(x_0)\|^2$ and $\Phi(x_k) \geq 0$, we have that

$$\frac{1}{2} \|r(x_0)\|^2 \geq \Phi(x_0) - \Phi(x_{k+1}) \geq |\mathcal{S}_k| \kappa_4 \epsilon^{3/2}.$$

Thus there at most

$$|\mathcal{S}_k| \leq \frac{\|r(x_0)\|^2}{2\kappa_4} \epsilon^{-3/2}$$

successful iterations. Combining this with Lemma 3.6, accounting for the max in (4.11) and remembering that we need to evaluate the function and gradient at the final x_{k+1} yields the bound (4.15). □

We note in passing that in order to derive Theorem 4.6, we could have replaced the test (4.2) in Algorithm 4.1 by the normally significantly-weaker requirement (4.10).

Our final result examines the evaluation complexity under the stopping rule (3.31).

Theorem 4.7 *Suppose that AS.1 holds, $r \geq 3$ and an $i \geq 1$ is given. Then Algorithm 4.1 requires at most*

$$\left[\kappa_u \|r(x_0)\|^{1/2^i} \max \left(\kappa_g^{-1} \epsilon_d^{-3/2}, \kappa_r^{-1} \epsilon_p^{-1/2^i} \right) + \kappa_b \right] + 1$$

when $r = 3$

$$\left[\kappa_u \|r(x_0)\|^{1/2^i} \max \left(\kappa_g^{-1} \epsilon_d^{-3/2}, \kappa_r^{-1} \epsilon_p^{-1/2^i} \right) + \kappa_i + \kappa_e (\log \epsilon_d^{-1} + \log \epsilon_p^{-1}) \right] + 1 \quad (4.17)$$

when $r > 3$ and $\epsilon_p \epsilon_d < \left(\frac{\kappa_1}{\sigma_0} \right)^{2/(r-3)}$, or otherwise

$$\left[\kappa_u \|r(x_0)\|^{1/2^i} \max \left(\kappa_g^{-1} \epsilon_d^{-3/2}, \kappa_r^{-1} \epsilon_p^{-1/2^i} \right) + \kappa_a \right] + 1,$$

evaluations of $r(x)$ and its derivatives to find an iterate x_k for which the termination test

$$\|r(x_k)\| \leq \epsilon_p \quad \text{or} \quad \|g_r(x_k)\| \leq \epsilon_d,$$

is satisfied for given $0 < \epsilon_p, \epsilon_d \leq 1$, where κ_u is defined in (3.18),

$$\kappa_g := \frac{\eta_1 \alpha^{r/(r-1)}}{2^i r \gamma_3^{1/(r-1)}} \min \left(\frac{1}{\kappa_1}, \frac{1}{\sigma_0} \right)^{1/(r-1)} \|r(x_0)\|^{(3/2 - (2^{i+1} - 1)/2^i)}, \quad \kappa_r := (1 - \beta^{1/2^i}), \tag{4.18}$$

κ_1 is defined in (4.7), $\kappa_b, \kappa_i, \kappa_e$ and κ_a in (4.16), and $\beta \in (0, 1)$ is a fixed problem-independent constant.

Proof As in the proof of Theorem 3.12, let $S_\beta := \{l \in \mathcal{S} \mid \|r(x_{l+1})\| > \beta \|r(x_l)\|\}$ for a given $\beta \in (0, 1)$. We suppose that Algorithm 4.1 has not terminated prior to iteration $l + 1$, and thus that

$$\|r(x_k)\| > \epsilon_p \quad \text{and} \quad \|g_r(x_k)\| > \epsilon_d \tag{4.19}$$

for all $k \leq l + 1$. If $l \in S_\beta$, it follows from (3.5), (4.2) and the definition (1.4) that

$$\begin{aligned} \|r(x_l)\|^2 - \|r(x_{l+1})\|^2 &\geq 2\eta_1(m(x_l, 0) - m(x_l, s_l)) > \frac{2\eta_1}{r} \sigma_l \|s_l\|^r \\ &= \frac{2\eta_1}{r} (\sigma_l \|s_l\|^{r-1}) \|s_l\| \geq \frac{2\eta_1}{r} \alpha^{r/(r-1)} \sigma_l^{-1/(r-1)} \|\nabla_x \Phi(x_{l+1})\|^{r/(r-1)} \\ &\geq \frac{2\eta_1}{r} \alpha^{r/(r-1)} \sigma_l^{-1/(r-1)} \|g_r(x_{l+1})\|^{r/(r-1)} \|r(x_{l+1})\|^{r/(r-1)} \\ &\geq \frac{2\eta_1}{r} \alpha^{r/(r-1)} \sigma_l^{-1/(r-1)} \|g_r(x_{l+1})\|^{r/(r-1)} \|r(x_l)\|^{r/(r-1)} \beta^{r/(r-1)} \end{aligned}$$

and thus applying Lemma 3.11 with $i \geq 1$,

$$\begin{aligned} &\|r(x_l)\|^{1/2^i} - \|r(x_{l+1})\|^{1/2^i} \\ &\geq \frac{\eta_1 \alpha^{r/(r-1)}}{2^i r} \beta^{r/(r-1)} \sigma_l^{-1/(r-1)} \|g_r(x_{l+1})\|^{r/(r-1)} \|r(x_l)\|^{(r/(r-1) - (2^{i+1} - 1)/2^i)} \\ &= \frac{\eta_1 \alpha^{r/(r-1)}}{2^i r} \beta^{r/(r-1)} \sigma_l^{-1/(r-1)} \|g_r(x_{l+1})\|^{r/(r-1)} \|r(x_l)\|^{(r/(r-1) - 3/2)} \\ &\quad \|r(x_l)\|^{(3/2 - (2^{i+1} - 1)/2^i)} \\ &\geq \kappa_d \sigma_l^{-1/(r-1)} \|g_r(x_{l+1})\|^{r/(r-1)} \|r(x_l)\|^{(r/(r-1) - 3/2)}, \end{aligned} \tag{4.20}$$

where $\kappa_d := \frac{\eta_1 \alpha^{r/(r-1)}}{2^i r} \beta^{r/(r-1)} \|r(x_0)\|^{(3/2 - (2^{i+1} - 1)/2^i)}$, as $3/2 \leq (2^{i+1} - 1)/2^i$ and (3.34) holds.

In particular (4.20) becomes

$$\|r(x_l)\|^{1/2^i} - \|r(x_{l+1})\|^{1/2^i} \geq \kappa_d \sigma_l^{-1/(r-1)} \epsilon_p^{(3-r)/2(r-1)} \epsilon_d^{r/(r-1)} \tag{4.21}$$

and (4.10) holds with $\epsilon = \epsilon_p \epsilon_d$, and so

$$\sigma_l \leq \sigma_{\max} := \gamma_3 \max \left(\kappa_1 \epsilon_p^{(3-r)/2} \epsilon_d^{(3-r)/2}, \sigma_0 \right) \tag{4.22}$$

from Lemma 4.3. Consider the possibility

$$\kappa_1 \epsilon_p^{(3-r)/2} \epsilon_d^{(3-r)/2} \geq \sigma_0. \tag{4.23}$$

In this case, (4.22) implies that

$$\sigma_l^{-1/(r-1)} \geq \frac{1}{(\gamma_3 \kappa_1)^{1/(r-1)}} \epsilon_p^{(r-3)/2(r-1)} \epsilon_d^{(r-3)/2(r-1)}$$

and hence combining with (4.21), we find that

$$\|r(x_l)\|^{1/2^i} - \|r(x_{l+1})\|^{1/2^i} \geq \frac{\kappa_d}{(\gamma_3 \kappa_1)^{1/(r-1)}} \epsilon_d^{3/2} \tag{4.24}$$

If (4.23) does not hold,

$$\sigma_l^{-1/(r-1)} \geq \frac{1}{(\gamma_3 \sigma_0)^{1/(r-1)}}$$

and thus (4.21) implies that

$$\begin{aligned} \|r(x_l)\|^{1/2^i} - \|r(x_{l+1})\|^{1/2^i} &\geq \frac{\kappa_d}{(\gamma_3 \sigma_0)^{1/(r-1)}} \epsilon_p^{(3-r)/2(r-1)} \epsilon_d^{r/(r-1)} \\ &\geq \frac{\kappa_d}{(\gamma_3 \sigma_0)^{1/(r-1)}} \epsilon_d^{3/2} \end{aligned} \tag{4.25}$$

since ϵ_p and $\epsilon_d \leq 1$ and $r \geq 3$. Hence (4.24) and (4.25) hold when $l \in \mathcal{S}_\beta$,

For $l \in \mathcal{S} \setminus \mathcal{S}_\beta$, for which $\|r(x_{l+1})\| \leq \beta \|r(x_l)\|$ and hence $\|r(x_{l+1})\|^{1/2^i} \leq \beta^{1/2^i} \|r(x_l)\|^{1/2^i}$. Thus in view of (4.19), we have that

$$\|r(x_l)\|^{1/2^i} - \|r(x_{l+1})\|^{1/2^i} \geq (1 - \beta^{1/2^i}) \|r(x_l)\|^{1/2^i} \geq (1 - \beta^{1/2^i}) \epsilon_p^{1/2^i} \tag{4.26}$$

for all $l \in \mathcal{S} \setminus \mathcal{S}_\beta$. Thus, combining (4.24), (4.25) and (4.26), we have that

$$\|r(x_l)\|^{1/2^i} - \|r(x_{l+1})\|^{1/2^i} \geq \min \left(\kappa_g \epsilon_d^{3/2}, \kappa_r \epsilon_p^{1/2^i} \right)$$

for all $l \in \mathcal{S}$, where κ_g and κ_r are given by (4.18). Summing over $l \in \mathcal{S}_k$ and using (3.34),

$$\|r(x_0)\|^{1/2^i} \geq \|r(x_0)\|^{1/2^i} - \|r(x_{k+1})\|^{1/2^i} \geq |\mathcal{S}_k| \min\left(\kappa_g \epsilon_d^{3/2}, \kappa_r \epsilon_p^{1/2^i}\right)$$

and thus that there are at most

$$|\mathcal{S}_k| \leq \|r(x_0)\|^{1/2^i} \max\left(\kappa_g^{-1} \epsilon_d^{-3/2}, \kappa_r^{-1} \epsilon_p^{-1/2^i}\right).$$

successful iterations. As before, combining this with Lemma 3.6 for $\epsilon = \epsilon_p \epsilon_d$, accounting for the max in (4.11) and remembering that we need to evaluate the function and gradient at the final x_{k+1} yields the bound (4.17). \square

Comparing (3.30) with (4.17), there seems little theoretical advantage (aside from constants) in using regularization of order more than three. We note, however, that the constants in the complexity bounds in Sect. 3 depend (inversely) on σ_{\min} , while those in Sect. 4 do not; whether this is important in practice for small chosen σ_{\min} depends on quite how tight our bounds actually are when $r = 3$.

5 Numerical experiments

We compare the performance of the newly proposed algorithm with a Gauss–Newton method, with regularization of order two, and a Newton method, with regularization of order three. We use implementations of these algorithms found in our RALFit software [28], which is an open-source Fortran package for solving nonlinear least-squares problems. We apply tensor-Newton methods with regularization powers $r = 2$ and 3, and we solve the subproblem (Step 2 of Algorithm 2.1) by calling the RALFit code recursively; see [19] for details.

Table 1 reports the number of iterations, function evaluations, and Jacobian evaluations needed to solve the 26 problems in the NIST nonlinear regression test set [27]. We also include the median numbers over all tests.

Table 1 reports that, for most problems in the test set, the tensor-Newton methods required fewer iterations, function evaluations, and Jacobian evaluations. We can learn more about the performance of individual problems by looking at convergence curves that plot the gradient, $\|J^T r\|$, at each iteration; we give these for a number of the problems, chosen to represent different behaviours, in Fig. 1. As should be expected, the asymptotic convergence rate of the Newton approximation is better than that of Gauss–Newton. We also see that, despite the inferior asymptotic convergence rate of Gauss–Newton, it often converges in fewer iterations than Newton due to the fact that it takes longer for Newton to enter this asymptotic regime (see, e.g., [13]). This is the case in Fig. 1a–c (see also Table 1). Our newly proposed tensor-Newton algorithm seems to converge at the same asymptotic rate as Newton, but with this regime being entered into much earlier, as is typical of Gauss–Newton. We credit this behaviour to the fact that, unlike Newton, the Gauss–Newton and tensor-Newton models are themselves sums-of-squares. We note that, although we observe something close to

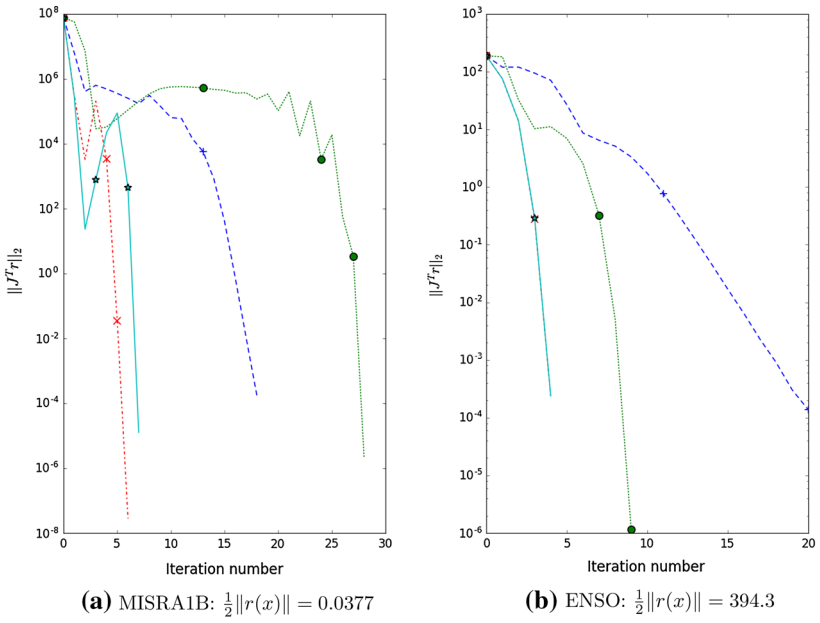
Table 1 Results for the NIST test set

Problem	Gauss-Newton			Newton			Tensor Newton ($r = 2$)			Tensor Newton ($r = 3$)		
	it	fe	je	it	fe	je	it	fe	je	it	fe	je
BENNETT5	429	436	430	597	880	598	4	5	5	4	5	5
BOXBOD	36	64	37	6	8	7	3	4	4	4	5	5
CHWIRUT1	14	20	15	13	16	14	4	5	5	4	5	5
CHWIRUT2	13	19	14	11	14	12	4	5	5	4	5	5
DANWOOD	7	8	8	10	11	11	4	5	5	4	5	5
ECKERLE4	21	40	22	1	2	2	3	4	4	3	4	4
ENSO	20	26	21	9	12	10	4	5	5	4	5	5
GAUSS1	5	6	6	7	8	8	3	4	4	3	4	4
GAUSS2	6	7	7	7	8	8	3	4	4	3	4	4
GAUSS3	7	8	8	9	10	10	3	4	4	3	4	4
HAHNI	19	20	20	50	86	51	17	29	18	16	26	17
LANCZOS1	67	68	68	35	48	36	38	63	39	28	45	29
LANCZOS2	68	69	69	35	49	36	38	63	39	28	45	29
LANCZOS3	121	122	122	36	51	37	41	66	42	30	47	31
MGH09	141	156	142	-5000	-7296	-5001	54	101	55	32	50	33
MGH10	-5000	-5016	-5001	481	840	482	86	168	87	55	96	56
MGH17	37	67	38	3113	3340	3114	3	4	4	7	9	8
MISRA1A	22	24	23	34	49	35	6	7	7	8	9	9
MISRA1B	18	20	19	28	40	29	6	7	7	7	8	8
MISRA1C	10	11	11	29	40	30	6	7	7	7	8	8

Table 1 continued

Problem	Gauss-Newton			Newton			Tensor Newton ($r = 2$)			Tensor Newton ($r = 3$)		
	it	fe	je	it	fe	je	it	fe	je	it	fe	je
MISRAID	13	14	14	34	47	35	6	7	7	7	8	8
NELSON	71	81	72	81	124	82	167	310	168	341	462	342
RAT42	9	10	10	31	50	32	4	5	5	4	5	5
RAT43	18	19	19	25	32	26	7	11	8	5	6	6
ROZMAN1	21	30	22	17	142	18	24	25	25	146	147	147
THURBER	33	34	34	26	27	27	5	6	6	9	11	10
Median	20.5	25.0	21.5	28.5	43.5	29.5	5.5	6.5	6.5	7.0	8.0	8.0

A negative value indicates that the method did not converge within 5000 iterations. it: iterations, fe: function evaluations, je: Jacobian evaluations. The best performer in each category is boldface



+ + Gauss-Newton ●●● Newton ×× tensor-Newton ($p=2$) ★★ tensor-Newton ($p=8$)

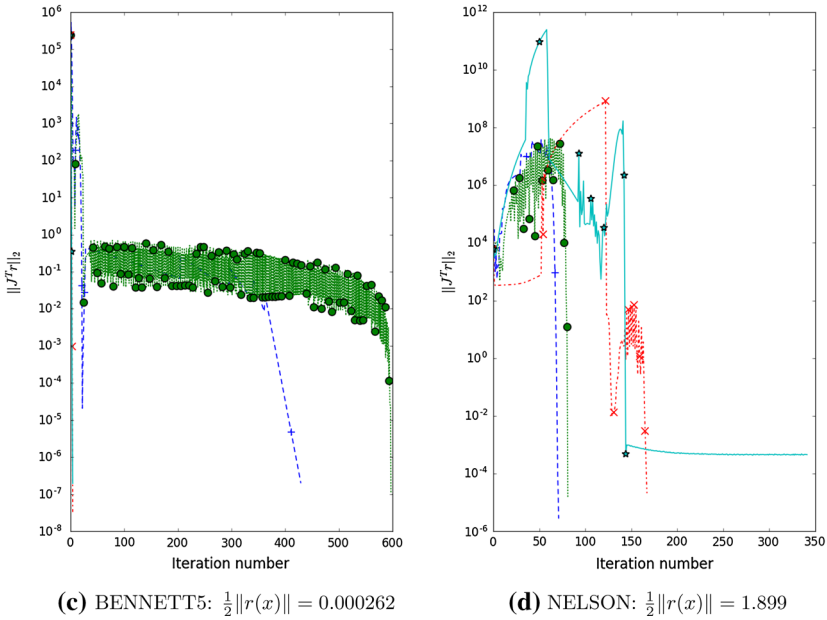


Fig. 1 Convergence curves for examples from the NIST test set

Table 2 Wallclock timings (seconds), with the number of iterations in brackets, for NIST problems where at least one solver took over 0.5 s

Problem	GaussNewton	Newton	Tensor Newton ($r = 2$)	Tensor Newton ($r = 3$)
BENNETT5	0.40 (429)	0.59 (597)	0.03 (4)	0.08 (4)
HAHN1	0.01 (19)	0.04 (50)	0.56 (17)	0.58 (16)
LANCZOS1	0.01 (67)	0.02 (35)	0.55 (38)	0.28 (28)
LANCZOS2	< 0.01 (68)	0.02 (35)	0.14 (38)	0.52 (28)
LANCZOS3	0.02 (121)	0.03 (36)	0.56 (41)	0.18 (30)
MGH09	0.01 (141)	0.62 (− 5000)	0.23 (54)	0.03 (32)
MGH10	0.31 (− 5000)	0.36 (481)	0.18 (86)	0.59 (55)
MGH17	0.01 (37)	0.74 (3113)	< 0.01 (3)	< 0.01 (7)
NELSON	0.01 (71)	0.05 (81)	0.51 (167)	0.90 (341)
ROSZMAN1	< 0.01 (21)	< 0.01 (17)	0.01 (24)	0.55 (146)

A negative number of iterations means the method did not converge

quadratic convergence in practice, whether this is always the asymptotic convergence rate is an open question (but see “Appendix B”).

Figure 1d shows convergence curves for one of the few tests where the performance of tensor-Newton is worse than that of the alternatives. All four methods struggle with this problem initially, but Gauss–Newton and Newton fall into the asymptotic regime first. Figure 1c, by contrast, shows an example where both variants of tensor-Newton perform much better than Gauss–Newton/Newton, which both suffer from a long period of stagnation.

The NIST examples are generally too small to make useful time comparisons. In Table 2 we report timings for those where at least one of the solvers took over 0.5s. These computations were performed on a desktop machine running Linux Mint 18.2, with an Intel Core i7-7700 and 16GB RAM, and we used the `gfortran` compiler.

We see that the cost of carrying out an iteration of the tensor-Newton method is significantly higher than that of Gauss–Newton/Newton, but there are examples (e.g., BENNETT5, MGH17) where it is the fastest.

In order to demonstrate the behaviour of the algorithms with an expensive function evaluation, we performed an experiment where we read in the data at each function/derivative evaluation from a directory stored on a remote computer. We performed this test for the example closest to the median behaviour in Table 1: MISRA1B. Here, Gauss–Newton took 0.108 s, Newton 0.148 s, and tensor-Newton 0.004 s. This highlights that, while more work needs to be done per iteration in the tensor-Newton method, once the function has been evaluated and the derivatives calculated, it makes greater use of the information, which can lead to a faster solution time.

6 Conclusions

We have proposed and analysed a related pair of tensor-Newton algorithms for solving nonlinear least-squares problems. Under reasonable assumptions, the algorithms have

been shown to converge globally to a first-order critical point. Moreover, their function-evaluation complexity is as good as the best-known algorithms for such problems. In particular, convergence to an ϵ -first-order critical point of the sum-of-squares objective (1.1) requires at most $O(\epsilon^{-\min(r/(r-1), 3/2)})$ function evaluations with r -th-order regularization with $r \geq 2$. Moreover, convergence to a point that satisfies the more natural convergence criteria (1.3) takes at most $O(\max(\epsilon_d^{-\min(r/(r-1), 3/2)}, \epsilon_p^{-1/2^i}))$ evaluations for any chosen $i \geq \lceil \log_2((r-1)/(r-2)) \rceil$. Whether such bounds may be achieved is an open question.

Although quadratic ($r = 2$) regularization produces the poorest theoretical worst-case bound in the above, in practice it often performs well. Moreover, although quadratic regularization is rarely mentioned for general optimization in the literature (but see [2] for a recent example), it is perhaps more natural in the least-squares setting since the Gauss- and tensor-Newton approximations (2.2) are naturally bounded from below and thus it might be argued that regularization need not be so severe. The rather weak dependence of the second bound above on ϵ_p is worth noting. Indeed, increasing i reduces the influence, but of course the constant hidden by the $O(\cdot)$ notation grows with i . A similar improvement on the related bound in [9, Theorem 3.2] is possible using the same arguments.

It is also possible to imagine generalizations of the methods here in which the quadratic tensor-Newton model in (2.1) is replaced by a p -th-order Taylor approximation ($p > 2$). One might then anticipate evaluation-complexity bounds in which the exponents $\min(r/(r-1), 3/2)$ mentioned above are replaced by $\min(r/(r-1), (p+1)/p)$, along the lines considered elsewhere [11, 12]. The limiting applicability will likely be the cost of computing higher-order derivative tensors.

An open question relates to the asymptotic rates of convergence of our methods. It is well known that Gauss–Newton methods converge quadratically for rank-deficient problems under reasonable assumptions, but that a Newton-like method is needed to achieve this rate when the optimal residuals are nonzero. It is not clear what the rate is for our tensor-Newton method. The main obstacle to a convincing analysis is that, unlike its quadratic counterpart, a quartic model such as used by the tensor-Newton may have multiple minimizers. Our inner-iteration stopping criteria make no attempt to distinguish, indeed to do so would require global optimality conditions. In practice, however, we generally observe at least quadratic convergence, sometimes even faster when the optimal residuals are zero. In “Appendix B”, we indicate that a reasonable choice of the step s_k in Algorithm 2.1 does indeed converge with an asymptotic Q rate of $r - 1$ for $2 < r < 3$ under standard assumptions. Extending this to Algorithm 4.1 is less obvious as it is unclear that the additional required acceptance test (4.2) might not deny an otherwise rapidly-converging natural choice of the step.

Our interest in these algorithms has been prompted by observed good behaviour when applied to practical problems [19]. The resulting software is available as part of the RALFit [28] and GALAHAD [18] software libraries.

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Appendix A: Proofs of function bounds (3.1)–(3.4)

We assume that $r_i(x)$, $i = 1, \dots, m$ are twice-continuously differentiable, and that they and their first two derivatives are Lipschitz on the intervals $\mathcal{F}_k = \{x : x = x_k + \alpha s_k \text{ for some } \alpha \in [0, 1]\}$. Therefore

$$\begin{aligned} \|r(x) - r(y)\| &\leq L_r \|x - y\|, \quad \|J(x) - J(y)\| \leq L_j \|x - y\| \\ \text{and } \|\nabla_{xx} r_i(x) - \nabla_{xx} r_i(y)\| &\leq L_h \|x - y\| \end{aligned} \tag{A.1}$$

for $x, y \in \mathcal{F}_k$. Moreover, these Lipschitz bounds imply that

$$\|\nabla_x r_i(x)\| \leq L_r, \quad \|J(x)\| \leq L_r \text{ and } \|\nabla_{xx} r_i(x)\| \leq L_j \tag{A.2}$$

for $x \in \mathcal{F}_k$ [25, Lemma 1.2.2]. It follows from Taylor’s theorem and (A.1) that

$$|r_i(x_k + s_k) - t_i(x_k, s_k)| \leq \frac{1}{6} L_h \|s_k\|^3, \tag{A.3}$$

and from the definition (2.1) of $t_i(x, s)$, the Cauchy-Schwarz inequality, (A.2) and the monotonicity bound

$$|r_i(x_k)| \leq \|r(x_k)\| \leq \|r(x_0)\| \tag{A.4}$$

that

$$\begin{aligned} |t_i(x_k, s_k)| &\leq |r_i(x_k)| + \|\nabla_x r_i(x_k)\| \|s_k\| + \frac{1}{2} \|\nabla_{xx} r_i(x_k)\| \|s_k\|^2 \\ &\leq \|r(x_0)\| + L_r \|s_k\| + \frac{1}{2} L_j \|s_k\|^2. \end{aligned} \tag{A.5}$$

But, using (A.3)–(A.5),

$$\begin{aligned} |r_i^2(x_k + s_k) - t_i^2(x_k, s_k)| &= |r_i(x_k + s_k) - t_i(x_k, s_k)| |r_i(x_k + s_k) + t_i(x_k, s_k)| \\ &\leq \frac{1}{6} L_h \|s_k\|^3 (|2t_i(x_k, s_k)| + L_h \|s_k\|^3) \\ &\leq \frac{1}{6} L_h \|s_k\|^3 (2\|r(x_0)\| + 2L_r \|s_k\| + L_j \|s_k\|^2 + L_h \|s_k\|^3). \end{aligned}$$

Thus if $\|s_k\| \leq 1$, it follows from the triangle inequality that

$$\left| \frac{1}{2} \|r(x_k + s_k)\|^2 - \frac{1}{2} \|t(x_k, s_k)\|^2 \right| \leq \frac{1}{12} m L_h (2\|r(x_0)\| + 2L_r + L_j + L_h)$$

which provides the bound (3.1) with $L_r := \frac{1}{12} m L_h (2\|r(x_0)\| + 2L_r + L_j + L_h)$.

Taylor’s theorem once again gives that

$$\|\nabla_x r_i(x_k + s_k) - \nabla_s t_i(x_k, s_k)\| \leq \frac{1}{2} L_j \|s\|^2. \tag{A.6}$$

But then the triangle inequality together with (A.3), (A.5) and (A.6) give

$$\begin{aligned} & \|r_i(x_k + s_k)\nabla_x r_i(x_k + s_k) - t_i(x_k, s_k)\nabla_s t_i(x_k, s_k)\| \\ &= \|(r_i(x_k + s_k) - t_i(x_k, s_k))\nabla_x r_i(x_k + s_k) \\ &\quad + t_i(x_k, s_k)(\nabla_x r_i(x_k + s_k) - \nabla_s t_i(x_k, s_k))\| \\ &\leq |r_i(x_k + s_k) - t_i(x_k, s_k)|\|\nabla_x r_i(x_k + s_k)\| \\ &\quad + |t_i(x_k, s_k)|\|\nabla_x r_i(x_k + s_k) - \nabla_s t_i(x_k, s_k)\| \\ &\leq \frac{1}{6}L_h L_j \|s_k\|^3 + \frac{1}{2}L_j(\|r(x_0)\| + L_r\|s_k\| + \frac{1}{2}L_j\|s_k\|^2)\|s_k\|^2. \end{aligned}$$

Hence, if $\|s_k\| \leq 1$, we have that

$$|\Phi(x_k + s_k) - m(x_k, s_k)| \leq m \left(\frac{1}{6}L_h L_j + \frac{1}{2}L_j(\|r(x_0)\| + L_r + \frac{1}{2}L_j) \right),$$

which is (3.2) with $L_g := m(\frac{1}{6}L_h L_j + \frac{1}{2}L_j(\|r(x_0)\| + L_r + \frac{1}{2}L_j))$.

The bound (3.3) follows immediately from Cauchy-Schwarz and (A.2) with $L_j := L_r$. Finally (A.2), (A.4) and the well-known relationship $\|\cdot\|_1 \leq \sqrt{m}\|\cdot\|$ between the ℓ_1 and Euclidean norms give

$$\begin{aligned} \|H(x_k, r(x_k))\| &= \left\| \sum_{i=1}^m r_i(x_k)\nabla_{xx} r_i(x_k) \right\| \leq \sum_{i=1}^m |r_i(x_k)|\|\nabla_{xx} r_i(x_k)\| \\ &\leq \|r(x_k)\|_1 L_j \leq \sqrt{m}L_j\|r(x_0)\|, \end{aligned}$$

which is (3.4) with $L_H := \sqrt{m}L_j$.

Appendix B: Superlinear convergence

We focus on Algorithm 2.1 and² the case $2 < r < 3$. Denote the leftmost eigenvalue of a generic real symmetric matrix H by $\lambda_{\min}[H]$. Consider the gradient $\nabla_s m^R(x, s, \sigma)$ of the regularized model given by (2.4). It follows from (2.1) and (2.2) that

$$\begin{aligned} & \nabla_s m^R(x_k, s, \sigma_k) \\ &= \sum_{i=1}^m \left(r_i(x_k) + s^T \nabla_x r_i(x_k) + \frac{1}{2}s^T \nabla_{xx} r_i(x_k)s \right) (\nabla_x r_i(x_k) + \nabla_{xx} r_i(x_k)s) + \sigma_k \|s\|^{r-2}s \\ &= g_k + (H_k + \sigma_k \|s\|^{r-2}I)s + \sum_{i=1}^m \left(s^T \nabla_x r_i(x_k) \right) \nabla_{xx} r_i(x_k)s \\ &\quad + \frac{1}{2} \sum_{i=1}^m \left(s^T \nabla_{xx} r_i(x_k)s \right) \nabla_x r_i(x_k) + \frac{1}{2} \sum_{i=1}^m \left(s^T \nabla_{xx} r_i(x_k)s \right) \nabla_{xx} r_i(x_k)s, \end{aligned} \tag{B.1}$$

² It is unclear what happens when $r = 2$ or 3 .

where for brevity we have written

$$g_k := \nabla_x \Phi(x_k) \equiv J^T(x_k)r(x_k) \text{ and } H_k := \nabla_{xx} \Phi(x_k) \equiv H(x_k, r(x_k)) + J^T(x_k)J(x_k).$$

Ideally one might hope to choose s in (B.1) to make $\nabla_s m^R(x_k, s, \sigma_k) = 0$, but this is generally unrealistic as $\nabla_s m^R(x, s, \sigma)$ is a combination of a cubic function and the derivative of the regularization term. A tractable compromise is to pick $s = s_k^N$, so that

$$(H_k + \lambda_k I)s_k^N = -g_k, \tag{B.2}$$

where

$$\lambda_k := \sigma_k \|s_k^N\|^{r-2} \geq 0. \tag{B.3}$$

since this provides a zero of the lower-order terms in (B.1).

We will try $s_k = s_k^N$ if H_k is positive definite, with leftmost eigenvalue $\lambda_{\min,k} := \lambda_{\min}[H_k] > 0$, and three essential properties hold, namely that

$$m^R(x_k, s_k^N, \sigma_k) < m^R(x_k, 0, \sigma_k), \tag{B.4}$$

$$\|\nabla_s m^R(x_k, s_k^N, \sigma_k)\| \leq \theta \|s_k^N\|^{r-1} \text{ and} \tag{B.5}$$

$$\frac{\Phi(x_k) - \Phi(x_k + s_k^N)}{m(x_k, 0) - m(x_k, s_k^N)} \geq \eta_1 \tag{B.6}$$

If so, s_k^N provides a successful step in Algorithm 2.1, since (B.4)–(B.6) are then that (2.5)–(2.6) and $\rho_k \geq \eta_1$ hold. We are not specific about how s_k is chosen when H_k is not positive definite, nor how s_k might be chosen if s_k^N does not provide a successful step.

Consider the sub-sequence of iterates $\{x_k\}$, $k \in \mathcal{K}$, whose limit is x_* (and thus for which $g_* := \nabla_x \Phi(x_*) = 0$ because of Theorem 3.9), suppose that $\nabla_x \Phi(x)$ is Lipschitz continuous in an open neighbourhood of x_* and that $\lambda_{\min,*} := \lambda_{\min}[\nabla_{xx} \Phi(x_*)] > 0$. Then, for all $k \in \mathcal{K}$ sufficiently large, $\lambda_{\min,k} \geq \frac{1}{2} \lambda_{\min,*}$. This ensures that

$$\|(H_k + \lambda_k I)^{-1}\| \leq \frac{1}{\lambda_{\min,k} + \lambda_k} \leq \frac{1}{\lambda_{\min,k}} \leq \frac{2}{\lambda_{\min,*}}, \tag{B.7}$$

and hence (B.2) and (B.7) provides the bound

$$\|s_k^N\| \leq \|(H_k + \lambda_k I)^{-1}\| \|g_k\| \leq \frac{2\|g_k\|}{\lambda_{\min,*}}. \tag{B.8}$$

But Lipschitz continuity and Taylor’s theorem applied to $\nabla_x \Phi(x)$ yields

$$\|g_k\| = \|g_* - g_k\| \leq L_1 \|x_* - x_k\|$$

and

$$\|g_* - g_k - H_k(x_* - x_k)\|_2 \leq L_2 \|x_* - x_k\|_2^2 \tag{B.9}$$

for some constants $L_1, L_2 > 0$, and thus

$$\|s_k^N\| \leq \frac{2L_1}{\lambda_{\min,*}} \|x_* - x_k\| \tag{B.10}$$

because of (B.8).

Define

$$\kappa_s := \frac{2L_2}{\lambda_{\min,*}} \left(L_2 + \sigma_{\max} \left(\frac{2L_1}{\lambda_{\min,*}} \right)^{r-2} \right), \tag{B.11}$$

where σ_{\max} is given by (3.17), and suppose that $x_k \in \mathcal{X}$, where

$$\mathcal{X} = \left\{ x \left| \begin{array}{l} x \in \mathcal{B}_\delta \text{ and } \|x - x_*\| \leq \min \left(\left(\frac{1}{2\kappa_s} \right)^{1/(r-2)}, \right. \right. \\ \left. \left. \frac{\lambda_{\min,*}}{2L_1} \min \left[1, \min \left(\frac{(r-2)\sigma_{\min}}{mrL_j(L_r + L_j)}, \frac{2\theta}{mL_j(3L_r + L_j)}, \frac{\sigma_{\min}(1-\eta_2)}{rL_r} \right)^{1/(3-r)} \right] \right) \right. \right\}. \tag{B.12}$$

and $\mathcal{B}_\delta = \{x \mid \|x - x_*\| \leq \delta\}$ is any ball around x_* of fixed radius $\delta > 0$ for which $\lambda_{\min}[\nabla_{xx} \Phi(x)] \geq \frac{1}{2} \lambda_{\min,*}$ for all $x \in \mathcal{B}_\delta$. In this case (B.10) guarantees that

$$\|s_k^N\| \leq \min \left[1, \left(\frac{(r-2)\sigma_{\min}}{mrL_j(L_r + L_j)} \right)^{1/(3-r)} \left(\frac{2\theta}{mL_j(3L_r + L_j)} \right)^{1/(3-r)} \left(\frac{\sigma_{\min}(1-\eta_2)}{rL_r} \right)^{1/(3-r)} \right], \tag{B.13}$$

and hence, trivially,

$$\|s_k^N\|^3 \leq \|s_k^N\|^2 \leq \|s_k^N\|^{r-1} \leq \|s_k^N\|. \tag{B.14}$$

We now establish the required bounds (B.4)–(B.6). Firstly, expanding the definition (2.2) of $m(x, s)$ gives

$$\begin{aligned} m(x_k, s_k^N) - m(x_k, 0) &= g_k^T s_k^N + \frac{1}{2} s_k^N T H_k s_k^N + e(x_k, s_k^N), \\ \text{where } e(x_k, s_k^N) &:= \frac{1}{2} \sum_{i=1}^m s_k^N T \nabla_x r_i(x_k) s_k^N T \nabla_{xx} r_i(x_k) s_k^N + \frac{1}{8} \sum_{i=1}^m \left(s_k^N T \nabla_{xx} r_i(x_k) s_k^N \right)^2, \end{aligned} \tag{B.15}$$

and it follows directly from the Cauchy-Schwarz inequality, (A.2) and (B.14) that

$$e(x_k, s_k^N) \leq \frac{1}{2}m \|s_k^N\|^3 L_r L_j + \frac{1}{8}m L_j^2 \|s_k^N\|^4 < \frac{1}{2}m L_j (L_r + L_j) \|s_k^N\|^3. \tag{B.16}$$

Substituting (B.15) into the definition (2.3) of the regularized model $m^R(x, s, \sigma)$ gives

$$\begin{aligned} m^R(x_k, s_k^N, \sigma_k) - m^R(x_k, 0, \sigma_k) &= m(x_k, s_k^N) - m(x_k, 0) + \frac{\sigma_k}{r} \|s_k^N\|^r \\ &= g_k^T s_k^N + \frac{1}{2} s_k^N T H_k s_k^N + \frac{\sigma_k}{r} \|s_k^N\|^r + e(x_k, s_k^N) \\ &= -\frac{1}{2} s_k^N T (H_k + \lambda_k I) s_k^N - \frac{r-2}{2r} \sigma_k \|s_k^N\|^r + e(x_k, s_k^N) \\ &< -\frac{1}{2} \frac{r-2}{r} \sigma_{\min} \|s_k^N\|^r + \frac{1}{2} m L_j (L_r + L_j) \|s_k^N\|^3 < 0 \end{aligned}$$

because of the positive semi-definiteness of $H_k + \lambda_k I$, the requirement that $\sigma_k \geq \sigma_{\min} > 0$, and the bounds (A.2) and (B.16) and the second term in (B.13). This provides the required bound (B.4).

It also follows immediately from (B.1) and (B.2) that

$$\|\nabla_s m^R(x_k, s_k^N, \sigma_k)\| \leq \frac{3}{2}m L_r L_j \|s_k^N\|^2 + \frac{1}{2}m L_j^2 \|s_k^N\|^3 \leq \theta \|s_k^N\|^{r-1}$$

using the triangle inequality, (A.2) and the third term in (B.13), which establishes (B.5).

Finally, it follows precisely as in (3.16) that

$$|\rho_k - 1| = \frac{|\Phi(x_k + s_k^N) - m(x_k, s_k^N)|}{m(x_k, 0) - m(x_k, s_k^N)} \leq \frac{r L_r}{\sigma_k} \|s_k^N\|^{3-r} \leq \frac{r L_r}{\sigma_{\min}} \|s_k^N\|^{3-r}$$

since $\sigma_k \geq \sigma_{\min} > 0$. Combining this with the fourth term in (B.13) immediately gives that $|\rho_k - 1| \leq 1 - \eta_2$ and hence that (B.6) holds. Thus we have shown that s_k^N is allowed by Step 2 of Algorithm 2.1, and leads to a successful iteration for which $x_{k+1} = x_k + s_k^N$.

Our intention is to show that

$$\|x_{k+1} - x_*\| \leq \kappa \|x_k - x_*\|^{r-1} \tag{B.17}$$

for some $\kappa > 0$, and hence the resulting iteration ultimately converges at a (Q-order $r - 1$) superlinear rate. The iterate $x_{k+1} = x_k + s_k^N$ satisfies

$$\begin{aligned} x_{k+1} - x_* &= x_k + s_k^N - x_* \\ &= x_k - x_* - (H_k + \lambda_k I)^{-1} g_k \\ &= x_k - x_* - (H_k + \lambda_k I)^{-1} (g_k - g_*) \\ &= (H_k + \lambda_k I)^{-1} (g_* - g_k - (H_k + \lambda_k I)(x_* - x_k)) \\ &= (H_k + \lambda_k I)^{-1} (g_* - g_k - H_k(x_* - x_k) - \lambda_k(x_* - x_k)). \end{aligned} \tag{B.18}$$

Taking norms and combining this with (B.9) gives

$$\begin{aligned} \|x_{k+1} - x_*\| &\leq L_2 \|(H_k + \lambda_k I)^{-1}\| \left(L_2 \|x_* - x_k\|^2 + \lambda_k \|x_* - x_k\| \right) \\ &\leq \frac{2L_2}{\lambda_{\min,*}} \left(L_2 \|x_* - x_k\|^2 + \sigma_{\max} \left(\frac{2L_1}{\lambda_{\min,*}} \right)^{r-2} \|x_* - x_k\|^{r-1} \right) \\ &\leq \kappa_s \|x_* - x_k\|^{r-1} \end{aligned} \quad (\text{B.19})$$

using (B.18), (B.7), (B.3), (B.10) and (B.11) and the appropriate bound $\sigma_k \leq \sigma_{\max}$ from (3.17). Thus (B.17) holds. Moreover, it also follows from (B.19) and the first term in (B.12) that

$$\|x_{k+1} - x_*\| \leq \frac{1}{2} \|x_k - x_*\|,$$

in which case $x_{k+1} \in \mathcal{X}$ and thus (B.12) continues to hold at iteration $k + 1$. Hence once an iterate enters \mathcal{X} , it will remain there, and the remaining sequence will converge superlinearly to x_* .

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