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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 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.

1 Introduction

Consider a given, sufficiently smooth, vector-valued function $r : \mathbb{R}^n \longrightarrow \mathbb{R}^m$. A ubiquitous problem is to find the value of $x \in \mathbb{R}^n$ so that $\|r(x)\|$ is a small as possible, where here and elsewhere $\|\cdot\|$ is the Euclidean norm. A common approach is to consider instead the equivalent problem of minimizing

$$\Phi(x) := \tfrac{1}{2}\|r(x)\|^2. \tag{1.1}$$

The resulting problem is thereafter tackled using a generic method for unconstrained optimization, or one that exploits the special structure of Φ.

A question of interest in general smooth unconstrained optimization is how many evaluations of an objective function $f(x)$ and its derivatives are necessary to reduce some measure of optimality below a specified (small) $\epsilon > 0$ from some arbitrary 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 [5], while this may be improved to $\Theta(\epsilon^{-3/2})$ evaluations for second-order methods with cubic regularization or using specialised trust-region tools [7,12,22]. 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.

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

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

However, it has been argued [8] 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

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

where $\epsilon_p > 0$ and $\epsilon_d > 0$ are required accuracy tolerances and

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

Note that the scaled gradient $g_r(x)$ 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 subdifferential of $r(x)$. It has been shown that a second-order method based on cubic regularization will satisfy (1.3) after $O\left(\max(\epsilon_d^{-3/2}, \epsilon_p^{-1/2})\right)$ evaluations [8, Theorem 3.2]. Our aim here is to show, amongst other things, a similar bound for the tensor-Newton method we are advocating.

To put our proposal into context, arguably the most 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 $x_{k+1} = x_k+s_k$ [17,18,20]. The iteration is usually stabilized either by imposing a trust-region constraint on the permitted s, or by including a quadratic regularization term [2,19]. 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 [6,13,14]. 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 [16] 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 [3,4] 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 [24,25], 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 [26,27], 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.

We propose a regularized tensor-Newton method in §2, and analyse both its global convergence and its evaluation complexity in §3. The regularization order, r, permitted by the algorithm proposed in §2 is restricted to be no larger than 3, and so in §4 we introduce a modified algorithm for which $r > 3$ is possible.

2 The tensor-Newton method

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

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

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

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

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

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

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

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

We consider the following algorithm (Algorithm 2.1 on the following page) 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 $k = 0, 1, \ldots$, 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 $m^{\mathrm{R}}(x_k, s, \sigma_k)$ so that

$$m^{\mathrm{R}}(x_k, s_k, \sigma_k) < m^{\mathrm{R}}(x_k, 0, \sigma_k) \tag{2.5}$$

and

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

hold.

3. Compute $\Phi(x_k + s_k)$ and

$$\rho_k = \frac{\Phi(x_k) - \Phi(x_k + s_k)}{m(x_k, 0) - m(x_k, s_k)}. \tag{2.7}$$

If $\rho_k \geq \eta_1$, set $x_{k+1} = x_k + s_k$. Otherwise set $x_{k+1} = x_k$.

4. Set

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

and go to Step 2 if $\rho_k < \eta_1$.

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 value s_k that both reduces $m^{\mathrm{R}}(x_k, s, \sigma_k)$ and satisfies $\|\nabla_s m^{\mathrm{R}}(x_k, s_k, \sigma_k)\| \leq \theta \|s_k\|^{r-1}$. Since $m^{\mathrm{R}}(x_k, s, \sigma_k)$ 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 $m^{\mathrm{R}}(x_k, s, \sigma_k)$, 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 $m^{\mathrm{R}}(x_k, s, \sigma_k)$, not the true objective, and thus costs 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 as $\mathcal{S}_k := \{0 \leq l \leq k \mid \rho_l \geq \eta_1\}$ and let $\mathcal{S} := \{k \geq 0 \mid \rho_k \geq \eta_1\}$ be the set of all successful iterations.

3 Convergence analysis

We shall 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 [9, 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 ith component is

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

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

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

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

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

and

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

for some $L_{\mathrm{f}}, L_{\mathrm{g}} > 0$ and all $k \geq 0$ for which $\|s_k\| \leq 1$ (see Appendix A).

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

$$\|J^T(x_k) r(x_k)\| \leq \|J^T(x_k)\| \|r(x_k)\| \leq L_{\mathrm{J}} \|r(x_0)\| \tag{3.3}$$

and

$$\|H(x_k, r(x_k))\| \leq L_{\mathrm{H}} \|r(x_k)\| \leq L_{\mathrm{H}} \|r(x_0)\| \tag{3.4}$$

for some $L_{\mathrm{J}}, L_{\mathrm{H}} > 0$ 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

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

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

$$\sigma_k < 2\|H(x_k, r(x_k))\| \tag{3.6}$$

or

$$\sigma_k\|s_k\| < 4\|J^T(x_k)r(x_k)\| \tag{3.7}$$

holds, while if $r>2$, it follows that

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

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

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

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

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

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

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

and this implies that

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

(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

$$\sigma_k \geq \sqrt{\frac{8L_{\rm f}L_{\rm J}\|r(x_0)\|}{1-\eta_2}}. \tag{3.11}$$

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

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

and hence

$$|\,\rho_k - 1| \leq \frac{8L_{\rm f}\|J^T(x_k)r(x_k)\|}{\sigma_k^2} \leq \frac{8L_{\rm f}L_{\rm J}\|r(x_0)\|}{\sigma_k^2} \leq 1-\eta_2$$

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

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

$$\sigma_k \leq \sigma_{\max} := \gamma_3 \max\left(\sqrt{\frac{8L_{\rm f}L_{\rm J}\|r(x_0)\|}{1-\eta_2}}, \sigma_0, 2\max(L_{\rm H}, 2L_{\rm J})\|r(x_0)\|\right) \tag{3.12}$$

for all $k \geq 0$.

Proof. Let

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

Suppose that $k+1 \in \mathcal{B}_{\gamma_3}$ is the first iteration for which $\sigma_{k+1} \geq \sigma_{\max}^{\rm B}$. 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,

$$\gamma_3 \sigma_k \geq \sigma_{k+1} \geq \sigma_{\max}^{\rm B} \geq \gamma_3 \sqrt{\frac{8 L_{\rm f} L_{\rm J} \|r(x_0)\|}{1-\eta_2}}$$

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

$$\sigma_k < \sigma_{\max}^{\rm B} \tag{3.13}$$

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 $\mathcal{B}_{\gamma_3}$, and the bounds (3.3) and (3.4) give

$$\sigma_k < 2\gamma_3 \max(\|H(x_k, r(x_k))\|, 2\|J^T(x_k) r(x_k))\|) \leq 2\gamma_3 \max(L_{\rm H}, 2L_{\rm J}) \|r(x_0)\|. \tag{3.14}$$

Combining (3.13) and (3.14) gives (3.12). □

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

$$\sigma_k \geq \max\left(\left(\frac{r L_{\rm f} \left(r L_{\rm H} \|r(x_0)\|\right)^{\frac{3-r}{r-1}}}{1-\eta_2} \right)^{\frac{r-1}{2}}, \left(\frac{r L_{\rm f} \left(2 r L_{\rm J} \|r(x_0)\|\right)^{\frac{3-r}{r-2}}}{1-\eta_2} \right)^{r-2} \right) \tag{3.15}$$

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

$$\begin{aligned} |\,\rho_k - 1| = \;& \frac{|\Phi(x_k+s_k) - m(x_k,s_k)|}{m(x_k,0) - m(x_k,s_k)} \leq \frac{r L_{\rm f} \|s_k\|^{3-r}}{\sigma_k} \\ <\;& r L_{\rm f} \max\Big((r\|H(x_k, r(x_k))\|)^{(3-r)/(r-1)} \sigma_k^{-2/(r-1)}, \\ & \qquad (2r\|J^T(x_k) r(x_k)\|)^{(3-r)/(r-2)} \sigma_k^{-1/(r-2)} \Big) \\ \leq\;& r L_{\rm f} \max\Big((r L_{\rm H} \|r(x_0)\|)^{(3-r)/(r-1)} \sigma_k^{-2/(r-1)}, \\ & \qquad (2 r L_{\rm J} \|r(x_0)\|)^{(3-r)/(r-2)} \sigma_k^{-1/(r-2)} \Big) \\ \leq\;& 1-\eta_2. \end{aligned}$$

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

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

$$\sigma_k \le \sigma_{\max} := \gamma_3 \max\left(\left(\frac{rL_{\mathrm{f}}\,(pL_{\mathrm{H}}\|r(x_0)\|)^{\frac{3-r}{r-1}}}{1-\eta_2}\right)^{\frac{r-1}{2}}, \left(\frac{rL_{\mathrm{f}}\,(2rL_{\mathrm{J}}\|r(x_0)\|)^{\frac{3-r}{r-2}}}{1-\eta_2}\right)^{r-2}, \sigma_0, r\max(L_{\mathrm{H}}, 2L_{\mathrm{J}})\|r(x_0)\|\right) \tag{3.16}$$

for all $k \ge 0$.

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

$$\sigma_{k+1} \ge \sigma_{\max}^{\mathrm{B}} := \gamma_3 \max\left(\left(\frac{rL_{\mathrm{f}}\,(rL_{\mathrm{H}}\|r(x_0)\|)^{\frac{3-r}{r-1}}}{1-\eta_2}\right)^{\frac{r-1}{2}}, \left(\frac{rL_{\mathrm{f}}\,(2rL_{\mathrm{J}}\|r(x_0)\|)^{\frac{3-r}{r-2}}}{1-\eta_2}\right)^{r-2}, \sigma_0\right).$$

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

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

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 (3.16), while the others arise as for the proof of Lemma 3.3 when $k \notin \mathcal{B}_{\gamma_3}$. □

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

Lemma 3.6. [7, Theorem 2.1]. Algorithm 2.1 ensures that

$$k \le \kappa_u|\mathcal{S}_k| + \kappa_s, \quad \text{where } \kappa_u := \left(1 - \frac{\log\gamma_1}{\log\gamma_2}\right), \kappa_s := \frac{1}{\log\gamma_2}\log\left(\frac{\sigma_{\max}}{\sigma_0}\right), \tag{3.17}$$

and $\sigma_{\max}$ 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 $\mathcal{L} := \{k \mid \|s_k\| \le 1\}$, and let $\mathcal{G} := \{k \mid \|s_k\| > 1\}$ be its compliment. We then have the following crucial bounds.

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

$$m(x_k, 0) - m(x_k, s_k) \ge \begin{cases} \sigma_{\min}\left(\dfrac{\|\nabla_x\Phi(x_k+s_k)\|}{L_{\mathrm{g}} + \theta + \sigma_{\max}}\right)^{\frac{r}{r-1}} & \text{if } k \in \mathcal{L} \\ \frac{1}{r}\sigma_{\min} & \text{if } k \in \mathcal{G}. \end{cases} \tag{3.18}$$

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

$$\begin{aligned}\|\nabla_x \Phi(x_k+s_k)\| &= \big\|(\nabla_x \Phi(x_k+s_k) - \nabla_s m(x_k,s_k)) + \big(\nabla_s m(x_k,s_k) + \sigma_k \|s_k\|^{r-2} s_k\big) \\ &\quad -\sigma_k \|s_k\|^{r-2} s_k\big\| \\ &\leq \|\nabla_x \Phi(x_k+s_k) - \nabla_s m(x_k,s_k)\| + \|\nabla_s m^{\mathrm{R}}(x_k,s_k,\sigma_k)\| + \sigma_k \|s_k\|^{r-1}.\end{aligned} \tag{3.19}$$

Combining (3.19) with (3.2), (2.6), (3.12), (3.16) and $\|s_k\| \leq 1$ we have

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

and thus that

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

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

$$\sigma_k \geq \sigma_{\min} \tag{3.20}$$

imposed by Algorithm 2.1 and (3.5) provides the first possibility in (3.18).

By contrast, if $k \in \mathcal{G}$, (3.5), $\|s_k\| > 1$ and (3.20) ensure the second possibility in (3.18). □

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

$$\Phi(x_k) - \Phi(x_{k+1}) \geq \begin{cases} \eta_1 \sigma_{\min} \left(\frac{\|\nabla_x \Phi(x_k+s_k)\|}{L_{\mathrm{g}} + \theta + \sigma_{\max}}\right)^{\frac{r}{r-1}} & \text{if } k \in \mathcal{L} \cap \mathcal{S} \\ \frac{1}{r} \eta_1 \sigma_{\min} & \text{if } k \in \mathcal{G} \cap \mathcal{S}. \end{cases} \tag{3.21}$$

Proof. The result follows directly from and (2.7) and (3.18). □

We now provide our three main convergence results. Firstly, we establish the global convergence of our algorithm to a first-order critical point 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

$$\liminf_{k \to \infty} \|\nabla_x \Phi(x_k)\| = 0 \tag{3.22}$$

if no non-trivial termination test is provided.

Proof. Suppose that

$$\|\nabla_x \Phi(x_k)\| \geq \epsilon > 0 \tag{3.23}$$

for all $k > 0$. Then for each successful iteration, we have from (3.21) that

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

Thus summing 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

$$\tfrac{1}{2}\|r(x_0)\|^2 \geq \Phi(x_0) - \Phi(x_{k+1}) \geq |\mathcal{S}_k|\delta, \tag{3.24}$$

and hence 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, since (2.8) imposes $\sigma_{k+1} \geq \gamma_2\sigma_k$ when $k \notin \mathcal{S}$. But as this contradicts Lemmas 3.3 & 3.5, (3.23) cannot be true, and therefore (3.22) holds. □

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

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

$$\left\lceil \frac{\kappa_u\|r(x_0)\|^2\left(L_{\rm g} + \theta + \sigma_{\max}\right)^{\frac{r}{r-1}}}{2\eta_1\sigma_{\min}}\epsilon^{-\frac{r}{r-1}} \right\rceil + \kappa_s + 1 \tag{3.25}$$

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 (3.17).

Proof. If the algorithm has not terminated, (3.23) holds, and then (3.24) ensures that

$$\tfrac{1}{2}\|r(x_0)\|^2 \geq |\mathcal{S}_k|\eta_1\sigma_{\min}\left(\frac{\epsilon}{L_{\rm g} + \theta + \sigma_{\max}}\right)^{\frac{r}{r-1}}$$

since $\epsilon < 1$, and thus that

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

Combining this with (3.17) and remembering that we need to evaluate the function and gradient at the final x_{k+1} yields the bound (3.25). □

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 [8, §3.2; 10, §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 $j \leq i$. □

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

$$i \geq i_0 := \left\lceil \log_2 \left(\frac{r-1}{r-2} \right) \right\rceil \tag{3.26}$$

is given. Then Algorithm 2.1 requires at most

$$\left\lceil \kappa_u \max \left(\kappa_c^{-1}, \kappa_g^{-1} \epsilon_d^{-r/(r-1)}, \kappa_r^{-1} \epsilon_p^{-1/2^i} \right) \right\rceil + \kappa_s + 1 \tag{3.27}$$

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

$$\|r(x_k)\| \leq \epsilon_p \quad \text{or} \quad \|g_r(x_k)\| \leq \epsilon_d, \tag{3.28}$$

is satisfied for given $\epsilon_p > 0$ and $\epsilon_d > 0$, where κ_u and κ_s are defined in (3.17), κ_c, κ_g and κ_r are given by (3.37) 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

$$\frac{2^{i+1}-1}{2^i} \geq \frac{r}{r-1}, \tag{3.29}$$

that is i satisfies (3.26).

First, consider $l \in \mathcal{G} \cap \mathcal{S}$. Then (3.21) gives that $\|r(x_l)\|^2 - \|r(x_{l+1})\|^2 \geq \eta_1 \sigma_{\min}$ and, since

$$\|r(x_{l+1})\| < \|r(x_l)\| \leq \|r(x_0)\| \tag{3.30}$$

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

$$\begin{aligned} \|r(x_l)\|^{1/2^i} - \|r(x_{l+1})\|^{1/2^i} &\geq \tfrac{1}{2}^{i+1} \eta_1 \sigma_{\min} \|r(x_l)\|^{-(2^{i+1}-1)/2^i} \\ &\geq \tfrac{1}{2}^{i+1} \eta_1 \sigma_{\min} \|r(x_0)\|^{-(2^{i+1}-1)/2^i}. \end{aligned} \tag{3.31}$$

By contrast, for $l \in \mathcal{L} \cap \mathcal{S}$, (3.21) gives that

$$\|r(x_l)\|^2 - \|r(x_{l+1})\|^2 \geq \kappa \|J^T(x_{l+1}) r(x_{l+1})\|^{r/(r-1)}, \;\text{ where }\; \kappa = \frac{2\eta_1 \sigma_{\min}}{(L + \theta + \sigma_{\max})^{r/(r-1)}}. \tag{3.32}$$

If additionally $l \in \mathcal{S}_\beta$, (3.32) may be refined as

$$\begin{aligned} \|r(x_l)\|^2 - \|r(x_{l+1})\|^2 &\geq \kappa \left(\frac{\|J^T(x_{l+1})r(x_{l+1})\|}{\|r(x_{l+1})\|}\right)^{r/(r-1)} \|r(x_{l+1})\|^{r/(r-1)} \\ &\geq \kappa \left(\frac{\|J^T(x_{l+1})r(x_{l+1})\|}{\|r(x_{l+1})\|}\right)^{r/(r-1)} \|r(x_{l+1})\|^{r/(r-1)} \\ &\geq \kappa \beta^{r/(r-1)} \|g_r(x_{l+1})\|^{r/(r-1)} \|r(x_l)\|^{r/(r-1)} \end{aligned} \tag{3.33}$$

from (1.4) and the requirement that $\|r(x_{l+1})\| > \beta\|r(x_l)\|$. Using (3.33), (3.30), Lemma 3.11 and (3.29), we then obtain the bound

$$\begin{aligned} \|r(x_l)\|^{1/2^i} - \|r(x_{l+1})\|^{1/2^i} &\geq \tfrac{1}{2}^{i+1} \kappa \beta^{r/(r-1)} \|g_r(x_{l+1})\|^{r/(r-1)} \|r(x_l)\|^{\left(r/(r-1)-(2^{i+1}-1)/2^i\right)} \\ &\geq \tfrac{1}{2}^{i+1} \kappa \beta^{r/(r-1)} \|r(x_0)\|^{\left(r/(r-1)-(2^{i+1}-1)/2^i\right)} \|g_r(x_{l+1})\|^{r/(r-1)} \end{aligned} \tag{3.34}$$

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

$$\begin{aligned} \|r(x_l)\|^{1/2^i} - \|r(x_{l+1})\|^{1/2^i} &\geq (1 - \beta^{1/2^i})\|r(x_l)\|^{1/2^i} \\ &\geq \tfrac{1-\beta^{1/2^i}}{\beta^{1/2^i}} \|r(x_{l+1})\|^{1/2^i} \end{aligned} \tag{3.35}$$

for all $l \in \mathcal{L} \cap (\mathcal{S} \setminus \mathcal{S}_\beta)$. Thus, combining (3.31), (3.34) and (3.35), we have that

$$\|r(x_l)\|^{1/2^i} - \|r(x_{l+1})\|^{1/2^i} \geq \min\left(\kappa_c, \kappa_g \|g_r(x_{l+1})\|^{r/(r-1)}, \kappa_r \|r(x_{l+1})\|^{1/2^i}\right), \tag{3.36}$$

where

$$\begin{aligned} \kappa_c &:= \tfrac{1}{2}^{i+1} \eta_1 \sigma_{\min} \|r(x_0)\|^{-(2^{i+1}-1)/2^i}, \\ \kappa_g &:= \frac{\tfrac{1}{2}^i \eta_1 \sigma_{\min} \beta^{r/(r-1)}}{(L+\theta+\sigma_{\max})^{r/(r-1)}} \|r(x_0)\|^{\left(r/(r-1)-(2^{i+1}-1)/2^i\right)} \\ \text{and} \quad \kappa_r &:= \frac{1-\beta^{1/2^i}}{\beta^{1/2^i}}, \end{aligned} \tag{3.37}$$

for all $l \in \mathcal{S}$.

Now suppose that the stopping rule (3.28) has not been satisfied up until the start of iteration $k+1$, and thus that

$$\|r(x_{l+1})\| > \epsilon_p \quad \text{and} \quad \|g_r(x_{l+1})\| > \epsilon_d \tag{3.38}$$

for all $l \in \mathcal{S}_k$. Combining this with (3.36), 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 (3.30),

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

As before, combining this with (3.17) and remembering that we need to evaluate the function and gradient at the final x_{k+1} yields the bound (3.27). □

If $i < i_0$, a weaker bound that includes $r = 2$ is possible. The key is to note that the purpose of (3.29) is to guarantee the second inequality in (3.34). Without this, we have instead

$$\|r(x_l)\|^{1/2^i} - \|r(x_{l+1})\|^{1/2^i} \geq \tfrac{1}{2}^{i+1}\kappa\beta^{r/(r-1)}\|g_r(x_{l+1})\|^{r/(r-1)}\|r(x_{l+1})\|^{\left(r/(r-1)-(2^{i+1}-1)/2^i\right)} \quad (3.39)$$

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

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

where

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

if (3.38) holds. This results in a bound of $O\left(\max(1, \epsilon_d^{r/(r-1)} \cdot \epsilon_p^{\left(r/(r-1)-(2^{i+1}-1)/2^i\right)}, \epsilon_p^{1/2^i})\right)$ function evaluations, which approaches that in (3.27) as i increases to infinity when $r = 2$.

4 A modified algorithm for higher-than-cubic 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 [11].

Algorithm 4.1: Adaptive Tensor-Newton Regularization when $r > 3$.

A starting point x_0, an initial and a minimal regularization parameter $\sigma_0 \geq \sigma_{\min} > 0$ 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 $k = 0, 1, \ldots$, until **termination**, do:

1. Compute derivatives of $r(x)$ at x_k.

2. Compute a step s_k by approximately minimizing $m^{\mathrm{R}}(x_k, s, \sigma_k)$ so that

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

and

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

hold.

3. Test for termination at $x_k + s_k$.
4. Compute $\Phi(x_k + s_k)$ and
$$\rho_k = \frac{\Phi(x_k) - \Phi(x_k + s_k)}{m(x_k, 0) - m(x_k, s_k)}.$$
If $\rho_k \geq \eta_1$ and
$$\sigma_k \|s_k\|^{r-1} \geq \alpha \|\nabla_x \Phi(x_k + s_k)\|, \tag{4.2}$$
set $x_{k+1} = x_k + s_k$. Otherwise set $x_{k+1} = x_k$.
5. Set
$$\sigma_{k+1} \in \begin{cases} [\max(\sigma_{\min}, \gamma_1 \sigma_k), \sigma_k] & \text{if } \rho_k \geq \eta_2 \text{ and (4.2) holds} \\ [\sigma_k, \gamma_2 \sigma_k] & \text{if } \eta_1 \leq \rho_k < \eta_2 \text{ and (4.2) holds} \\ [\gamma_2 \sigma_k, \gamma_3 \sigma_k] & \text{if } \rho_k < \eta_2 \text{ or (4.2) fails,} \end{cases} \tag{4.3}$$
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. Likewise, a very successful iteration is now one for which $\rho_k \geq \eta_2$ and (4.2) holds.

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

Lemma 4.1. Suppose that AS.1 holds, $r > 3$, $k \in \mathcal{B}$ and
$$\sigma_k \| \|s_k\|^{r-3} \geq \kappa_2, \quad \text{where } \kappa_2 := \frac{rL}{1 - \eta_2} \text{ and } L = \max(L_{\rm f}, L_{\rm g}, \theta). \tag{4.4}$$
Then iteration k of Algorithm 4.1 is very successful.

Proof. It follows immediately from (2.7), (3.10), (3.1), (3.5) and (4.4) that
$$|\rho_k - 1| = \frac{|\Phi(x_k + s_k) - m(x_k, s_k)|}{m(x_k, 0) - m(x_k, s_k)} \leq \frac{rL_{\rm f}\|s_k\|^{3-r}}{\sigma_k} \leq \frac{rL\|s_k\|^{3-r}}{\sigma_k} \leq 1 - \eta_2,$$
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 (3.19), (3.2) and (4.1) that
$$\|\nabla_x \Phi(x_k + s_k) \leq L_{\rm g}\|s_k\|^2 + \theta\|s_k\|^2 + \sigma_k\|s_k\|^{r-1} = (L_{\rm g} + \theta + \sigma_k\| \|s_k\|^{r-3})\|s_k\|^2 \tag{4.6}$$
and thus from (4.4), (4.5) and the algorithmic restriction $3 \leq 1/\alpha$ that
$$\|\nabla_x \Phi(x_k + s_k)\| \leq (2L + \sigma_k\| \|s_k\|^{r-3})\|s_k\|^2 \leq (3\sigma_k\| \|s_k\|^{r-3})\|s_k\|^2 = 3\sigma_k\|s_k\|^{r-1} \leq \frac{\sigma_k}{\alpha}\|s_k\|^{r-1}.$$

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

Lemma 4.2. Suppose that AS.1 holds, $r > 3$, $k \in \mathcal{B}$ and

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

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). Suppose 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 for $r \leq 3$, 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

$$\sigma_k \|s_k\|^{r-1} \geq \alpha \epsilon \tag{4.10}$$

for $k \in \mathcal{S}_l$. In this case, we can show that σ_k is bounded from above.

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

$$\sigma_k \leq \sigma_{\max} := \gamma_3 \max\left(\kappa_1 \epsilon^{(3-r)/2}, \kappa_\sigma\right), \quad \text{where} \quad \kappa_\sigma := \max\left(\sigma_0, r \max(L_{\text{H}}, 2L_{\text{J}})\|r(x_0)\|\right). \tag{4.11}$$

Proof. The proof is similar to that of Lemma 3.5. Suppose that iteration $k+1 \in \mathcal{B}_{\gamma_3}$ (with $k \leq l$) is the first for which

$$\sigma_{k+1} \geq \sigma_{\max}^{\text{B}} := \sigma_{\max} := \gamma_3 \max\left(\kappa_1 \epsilon^{(3-r)/2}, \sigma_0\right).$$

Then, since $\sigma_k < \sigma_{k+1}$, iteration k must have been unsuccessful and (4.3) gives that

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

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). In addition, as $k + 1 \in \mathcal{B}_{\gamma_3}$ and iteration k was unsuccessful, it follows that $k \in \mathcal{B}$. But then Lemma 4.2 implies that iteration k must be very successful. This contradiction provides the first two terms in (4.11). The other terms result directly as in the proof of Lemma 3.3 when $k \notin \mathcal{B}_{\gamma_3}$. □

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

Theorem 4.4. Suppose that AS.1 holds and $r > 3$. Then the iterates $\{x_k\}$ generated by Algorithm 4.1 satisfy

$$\lim_{k\to\infty} \inf \|\nabla_x \Phi(x_k)\| = 0 \tag{4.12}$$

if no non-trivial termination test is provided.

Proof. Suppose that (4.12) does not hold, in which case (4.9) holds for some $0 < \epsilon \leq 1$ and all $k \geq 0$. If $k \in \mathcal{S}$, it follows from (3.5), (4.10) and (4.11) that

$$\begin{aligned}\Phi(x_k) - \Phi(x_{k+1}) &\geq \eta_1(m(x_k, 0) - m(x_k, s_k)) > \frac{\eta_1}{r}\sigma_k \|s_k\|^r \\ &= \frac{\eta_1}{r}(\sigma_k \|s_k\|^{r-1})\|s_k\| \geq \frac{\eta_1}{r}\alpha\epsilon \frac{(\alpha\epsilon)^{1/(r-1)}}{\sigma_k^{1/(r-1)}} \geq \frac{\eta(\alpha\epsilon)^{r/(r-1)}}{r\sigma_{\max}^{1/(r-1)}} \\ &\geq \frac{\eta\alpha^{r/(r-1)}}{r\kappa_3^{1/(r-1)}} \frac{\epsilon^{r/(r-1)}}{(\epsilon^{(3-r)/2})^{1/(r-1)}} = \kappa_4 \epsilon^{3/2} > 0,\end{aligned} \tag{4.13}$$

where

$$\kappa_3 = \gamma_3 \max(\kappa_\sigma, \kappa_1) \;\text{ and }\; \kappa_4 := \frac{\eta\alpha^{r/(r-1)}}{r\kappa_3^{1/(r-1)}}.$$

Just as in the proof of Theorem 3.10, we then deduce (3.24) which shows 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 (4.12) holds. □

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

Theorem 4.5. Suppose that AS.1 holds and $r > 3$. Then Algorithm 2.1 requires at most

$$\begin{array}{ll} \left\lceil \kappa_u \dfrac{\|r(x_0)\|^2}{2\kappa_4}\epsilon^{-3/2} + \kappa_i + \kappa_e \log \epsilon^{-1} \right\rceil + 1 & \text{if } \epsilon < \left(\dfrac{\kappa_1}{\kappa_\sigma}\right)^{2/(r-3)} \text{ or} \\ \left\lceil \kappa_u \dfrac{\|r(x_0)\|^2}{2\kappa_4}\epsilon^{-3/2} + \kappa_a \right\rceil + 1 & \text{otherwise} \end{array} \tag{4.14}$$

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

$$\kappa_i := \frac{\log(\gamma_3 \kappa_1/\kappa_\sigma)}{\log \gamma_2}, \quad \kappa_e := \frac{r-3}{2\log \gamma_2} \quad \text{and} \quad \kappa_a := \frac{\log \gamma_3}{\log \gamma_2}, \tag{4.15}$$

κ_u is defined in (3.17), κ_1 in (4.7) and κ_σ in (4.11).

Proof. If the algorithm has not terminated on or before iteration k, (4.9) holds, and so summing (4.13) 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

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

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 (4.14). □

We note in passing that in order to derive Theorem 4.5, 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 (3.28).

Theorem 4.6. Suppose that AS.1 holds, $r > 3$ and an $i \geq 1$ is given. Then Algorithm 2.1 requires at most

$$\begin{array}{l} \left\lceil \kappa_u \|r(x_0)\|^{1/2^i} \max\left(\kappa_g^{-1} \epsilon_d^{-3/2}, \kappa_r^{-1} \epsilon_p^{-1/2^i}\right) + \kappa_i + \kappa_e(\log \epsilon_d^{-1} + \log \epsilon_p^{-1}) \right\rceil + 1 \\ \text{if } \epsilon_p \epsilon_d < \left(\dfrac{\kappa_1}{\kappa_\sigma}\right)^{2/(r-3)}, \quad \text{or otherwise} \\ \left\lceil \kappa_u \|r(x_0)\|^{1/2^i} \max\left(\kappa_g^{-1} \epsilon_d^{-3/2}, \kappa_r^{-1} \epsilon_p^{-1/2^i}\right) + \kappa_a \right\rceil + 1, \end{array} \tag{4.16}$$

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_c, κ_g and κ_r are given by (3.37), κ_u is defined in (3.17), κ_1 in (4.7), κ_σ in (4.11), and $\beta \in (0, 1)$ is a fixed problem-independent constant.

Proof. As in the proof of Theorem 3.12, let $\mathcal{S}_\beta := \{l \in \mathcal{S} \mid \|r(x_{l+1})\| > \beta\|r(x_l)\|\}$ for a given $\beta \in (0,1)$. For $l \in \mathcal{S}_\beta$, it follows from (3.5), (4.2) and the definition (1.4) that

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

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

$$\begin{aligned}\|r(x_l)\|^{1/2^i} - \|r(x_{l+1})\|^{1/2^i} &\geq \frac{\eta_1\alpha^{r/(r-1)}}{2^i r}\sigma_l^{-1/(r-1)}\|g_r(x_{l+1})\|^{r/(r-1)}\|r(x_l)\|^{(r/(r-1)-(2^{i+1}-1)/2^i)} \\ &= \frac{\eta_1\alpha^{r/(r-1)}}{2^i r}\sigma_l^{-1/(r-1)}\|g_r(x_{l+1})\|^{r/(r-1)}\|r(x_l)\|^{(r/(r-1)-3/2)}\|r(x_l)\|^{(3/2-(2^{i+1}-1)/2^i)} \\ &\geq \kappa_d\sigma_l^{-1/(r-1)}\|g_r(x_{l+1})\|^{r/(r-1)}\|r(x_l)\|^{(r/(r-1)-3/2)}, \\ \text{where } \kappa_d &:= \frac{\eta_1\alpha^{r/(r-1)}}{2^i r}\|r(x_0)\|^{(3/2-(2^{i+1}-1)/2^i)},\end{aligned} \tag{4.17}$$

as $3/2 \leq (2^{i+1}-1)/2^i$ and (3.30) holds. But since the algorithm has not yet terminated,

$$\|r(x_k)\| > \epsilon_p \quad \text{and} \quad \|g_r(x_k)\| > \epsilon_d \tag{4.18}$$

for all $k \leq l+1$ and in particular (4.17) becomes

$$\|r(x_l)\|^{1/2^i} - \|r(x_{l+1})\|^{1/2^i} \geq \kappa_d\sigma_l^{-1/(r-1)}\epsilon_p^{(3-r)/2(r-1)}\epsilon_d^{r/(r-1)} \tag{4.19}$$

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

$$\sigma_l \leq \sigma_{\max} := \gamma_3 \max\left(\kappa_1\epsilon_p^{(3-r)/2}\epsilon_d^{(3-r)/2}, \kappa_\sigma\right) \tag{4.20}$$

from Lemma 3.3. Consider the possibility

$$\kappa_1\epsilon_p^{(3-r)/2}\epsilon_d^{(3-r)/2} \geq \kappa_\sigma. \tag{4.21}$$

In this case, (4.20) 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 (4.19), we find that

$$\|r(x_l)\|^{1/2^i} - \|r(x_{l+1})\|^{1/2^i} \geq \frac{\kappa_d}{(\gamma_3\kappa_1)^{1/(r-1)}}\epsilon_d^{3/2} \tag{4.22}$$

If (4.21) does not hold,

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

and thus (4.19) implies that

$$\|r(x_l)\|^{1/2^i} - \|r(x_{l+1})\|^{1/2^i} \geq \frac{\kappa_d}{(\gamma_3\kappa_\sigma)^{1/(r-1)}}\epsilon_p^{(3-r)/2(r-1)}\epsilon_d^{r/(r-1)} \geq \frac{\kappa_d}{(\gamma_3\kappa_\sigma)^{1/(r-1)}}\epsilon_d^{3/2} \tag{4.23}$$

since ϵ_p and $\epsilon_d \leq 1$ and $r > 3$. Hence (4.22) and (4.23) 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 (4.18), we have that

$$\|r(x_l)\|^{1/2^i} - \|r(x_{l+1})\|^{1/2^i} \geq (1 - \beta^{1/2^i}) \|r(x_l)\|^{1/2^i} \geq (1 - \beta^{1/2^i}) \epsilon_p^{1/2^i} \tag{4.24}$$

for all $l \in \mathcal{S} \setminus \mathcal{S}_\beta$. Thus, combining (4.22),(4.23) and (4.24), 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

$$\kappa_g := \frac{\eta_1 \alpha^{r/(r-1)}}{2^i r \gamma_3^{1/(r-1)}} \min\left(\frac{1}{\kappa_1}, \frac{1}{\kappa_\sigma}\right)^{1/(r-1)} \|r(x_0)\|^{(3/2-(2^{i+1}-1)/2^i)} \text{ and } \kappa_r := (1 - \beta^{1/2^i}). \tag{4.25}$$

Summing over $l \in \mathcal{S}_k$ and using (3.30),

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

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, 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 (4.16). □

Comparing (3.27) with (4.16), there seems little theoretical advantage (aside from constants) in using regularization of order more than three.

5 Conclusions

We have proposed and analysed a related pair of tensor-Newton algorithms for solving non-linear 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 $O\left(\epsilon^{-\min(r/(r-1),3/2)}\right)$ 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 $O\left(\max(\epsilon_d^{-\min(r/(r-1),3/2)}, \epsilon_p^{-1/2^i}\right)$ 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 [1] 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 [8, 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 [10,11]. The limiting applicability will likely be the cost of computing higher-order derivative tensors.

Our interest in these algorithms has been prompted by observed good behaviour when applied to practical problems [16]. The resulting software is available as part of the `RALFit` [23] and GALAHAD [15] software libraries.

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

We assume that $r_i(x)$, $i = 1, \ldots, m$ 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

$$\|r(x) - r(y)\| \leq L_{\text{r}}\|x - y\|, \ \ \|J(x) - J(y)\| \leq L_{\text{j}}\|x - y\| \ \text{ and } \ \|\nabla_{xx} r_i(x) - \nabla_{xx} r_i(y)\| \leq L_{\text{h}}\|x - y\| \tag{A.1}$$

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

$$\|\nabla_x r_i(x)\| \leq L_{\text{r}}, \ \ \|J(x)\| \leq L_{\text{r}} \ \text{ and } \ \|\nabla_{xx} r_i(x)\| \leq L_{\text{j}} \tag{A.2}$$

for $x \in \mathcal{F}_k$ [21, Lemma 1.2.2]. It follows from Taylor's theorem and (A.1) that

$$|r_i(x_k + s_k) - t_i(x_k, s_k)| \leq \tfrac{1}{6} L_{\text{h}} \|s_k\|^3, \tag{A.3}$$

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

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

But, using (A.3)–(A.5),

$$\begin{aligned} |r_i^2(x_k + s_k) - t_i^2(x_k, s_k)| &= |r_i(x_k + s_k) - t_i(x_k, s_k)||r_i(x_k + s_k) + t_i(x_k, s_k)| \\ &\leq \tfrac{1}{6} L_{\text{h}}\|s_k\|^3(|2t_i(x_k, s_k)| + L_{\text{h}}\|s_k\|^3) \\ &\leq \tfrac{1}{6} L_{\text{h}}\|s_k\|^3(2\|r(x_0)\| + 2L_{\text{r}}\|s_k\| + L_{\text{j}}\|s_k\|^2 + L_{\text{h}}\|s_k\|^3). \end{aligned}$$

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

$$|\tfrac{1}{2}\|r(x_k + s_k)\|^2 - \tfrac{1}{2}\|t(x_k, s_k)\|^2| \leq \tfrac{1}{12} m L_{\text{h}}(2\|r(x_0)\| + 2L_{\text{r}} + L_{\text{j}} + L_{\text{h}})$$

which provides the bound (3.1) with $L_{\text{f}} := \frac{1}{12} m L_{\text{h}}(2\|r(x_0)\| + 2L_{\text{r}} + L_{\text{j}} + L_{\text{h}})$.

Taylor's theorem once again gives that

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

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

$$\begin{aligned}
&\|r_i(x_k+s_k)\nabla_x r_i(x_k+s_k) - t_i(x_k,s_k)\nabla_s t_i(x_k,s_k)\| \\
&= \|(r_i(x_k+s_k) - t_i(x_k,s_k))\nabla_x r_i(x_k+s_k) + t_i(x_k,s_k)(\nabla_x r_i(x_k+s_k) - \nabla_s t_i(x_k,s_k))\| \\
&\le |r_i(x_k+s_k) - t_i(x_k,s_k)|\|\nabla_x r_i(x_k+s_k)\| + |t_i(x_k,s_k)|\|\nabla_x r_i(x_k+s_k) - \nabla_s t_i(x_k,s_k)\| \\
&\le \tfrac{1}{6}L_{\rm h}L_{\rm j}\|s_k\|^3 + \tfrac{1}{2}L_{\rm j}(\|r(x_0)\| + L_{\rm r}\|s_k\| + \tfrac{1}{2}L_{\rm j}\|s_k\|^2)\|s_k\|^2.
\end{aligned}$$

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

$$|\Phi(x_k+s_k) - m(x_k,s_k)| \le m\left(\tfrac{1}{6}L_{\rm h}L_{\rm j} + \tfrac{1}{2}L_{\rm j}(\|r(x_0)\| + L_{\rm r} + \tfrac{1}{2}L_{\rm j})\right),$$

which is (3.2) with $L_{\rm g} := m(\frac{1}{6}L_{\rm h}L_{\rm j} + \frac{1}{2}L_{\rm j}(\|r(x_0)\| + L_{\rm r} + \frac{1}{2}L_{\rm j})$.

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

$$\|H(x_k,r(x_k))\| = \left\|\sum_{i=1}^m r_i(x_k)\nabla_{xx}r_i(x_k)\right\| \le \sum_{i=1}^m |r_i(x_k)|\|\nabla_{xx}r_i(x_k)\| \le \|r(x_k)\|_1 L_{\rm j} \le \sqrt{m}L_{\rm j}\|r(x_0)\|,$$

which is (3.4) with $L_{\rm H} := \sqrt{m}L_{\rm j}$.