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A globally convergent method for nonlinear least-squares problems based on the Gauss-Newton model with spectral correction

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In Honor of the 60th Birthday of Professor Marcos Raydan

Abstract

This work addresses a spectral correction for the Gauss-Newton model in the solution of nonlinear least-squares problems within a globally convergent algorithmic framework. The nonmonotone line search of Zhang and Hager is the chosen globalization tool. We show that the search directions obtained from the corrected Gauss-Newton model satisfy the conditions that ensure the global convergence under such a line search scheme. A numerical study assesses the impact of using the spectral correction for solving two sets of test problems from the literature.

Keywords: Nonlinear least squares, spectral parameter, Gauss-Newton method, global convergence, numerical tests.

1 Introduction

Nonlinear least-squares (NLS) problems are a class of structured unconstrained minimization problems that has a practical importance in several

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scenarios. From data fitting [1], parameter identification [2], and data assimilation [3] to regularization of ill-posed problems [4], to name a few, many applications may be addressed within the NLS framework.

Concerning the iterative numerical techniques employed to solve NLS problems, the Gauss-Newton (GN) is very popular. The associated linear system that must be solved at each iteration may not be safely positive definite, so a scalar and positive correction is adopted, giving rise to the Levenberg-Morrison-Marquardt approach [5–7]. Recent works have proposed adaptive strategies to update the regularizing parameter. See [8–11] and references therein. Newton's method is also a possibility, as long as the second order derivatives are available [12, 13].

The aforementioned scalar correction, however, might be sign-free in case it plays the role of the second-order derivative matrix. This is precisely the room where the spectral correction fits in. Such a correction was exploited for NLS with quadratic residues, and upon the local perspective [14]. The spectral correction for the Gauss-Newton method was motivated by the spectral step size to the gradient method, proposed by Barzilai and Borwein [15] and Raydan [16]. In the former work, the authors presented a convergence analysis to bidimensional quadratics, whereas in the latter, the convergence was extended to n-dimensional strictly convex quadratic problems. General unconstrained minimization problems were addressed by means of the spectral perspective by Raydan in [17]. Adding upon these ideas, Spectral Projected Gradient (SPG) methods were proposed by Birgin, Martínez and Raydan [18], applicable to large-scale convex constrained problems in which the projection onto the feasible set can be inexpensively computed. The surveys [19, 20] provide a broad perspective of the spectral projected gradient methods. Concerning the solution of nonlinear systems of equations, La Cruz and Raydan [21] used the spectral approach for such a goal, further analyzed by La Cruz, Martínez and Raydan [22] in a gradient-free scenario.

This work addresses the general NLS problem by means of the GN method with the spectral correction. Notation and basic definitions are given in Section 2, including the spectral correction. Section 3 presents the algorithmic framework, discussing some implementation details and the global convergence analysis. The numerical performance is investigated along with two distinct globalization strategies, based on monotone and nonmonotone line searches, as well as with a benchmark. The numerical results for two sets of test problems from the literature are shown and analyzed in Section 4. Final remarks are stated in Section 5.

2 Preliminaries and the spectral correction

Given the residual function $F : \mathbb{R}^n \to \mathbb{R}^m$, $m \geq n$, with F_i twice continuously differentiable functions for $i = 1, \ldots, m$, the NLS problem is stated as

$$\min_{x \in \mathbb{R}^n} f(x) \tag{1}$$

where $f(x) := \frac{1}{2}\|F(x)\|^2$ and $\|\cdot\|$ is the Euclidean vector norm and the induced matrix operator norm. Denoting the Jacobian of the residual function F computed at x as the matrix $J(x) \in \mathbb{R}^{m \times n}$, the derivatives of the objective function f computed at x are given by $\nabla f(x) = J(x)^T F(x)$ and $\nabla^2 f(x) = J(x)^T J(x) + S(x)$, where $S(x) = \sum_{i=1}^m F_i(x) \nabla^2 F_i(x)$. We also adopt the reduced notation $F_k \equiv F(x_k)$, $J_k \equiv J(x_k)$ and $S_k \equiv S(x_k)$.

The iterative scheme of Newton's method applied to the nonlinear equations $\nabla f(x) = J(x)^T F(x) = 0$ in its pure local form is written as

$$x_{k+1} = x_k - (J_k^T J_k + S_k)^{-1} J_k^T F_k. \tag{2}$$

The Gauss-Newton and the Levenberg-Morrison-Marquardt are popular alternatives to circumvent the need of computing the matrix S_k. In the former, this matrix is just dropped from (2), whereas in the latter a scalar matrix (i.e. diagonal with identical elements) of the form $\mu_k I$ is added to $J_k^T J_k$, leading to the globalized iteration

$$x_{k+1} = x_k - t_k (J_k^T J_k + \mu_k I)^{-1} J_k^T F_k, \tag{3}$$

where $\mu_k \geq 0$ is interpreted as a regularization parameter and $t_k \in (0, 1]$ is the step size, computed to accomplish a sufficient decrease condition upon f.

In this work we address the usage of a spectral choice for the parameter μ_k, which leads to a simple second order correction for the Gauss-Newton (GN) model based on the curvature information contained in approximations for the residual Hessians at the current iterate. Notice that μ_k may be negative in certain iterations, according with the residual values and Hessians. Thus, the second term of the matrix $\nabla^2 f(x_k)$ is approximated by

$$S_k \approx \sum_{i=1}^m F_i(x_k) \sigma_{i,k} I.$$

The scalar $\sigma_{i,k}$ is a spectral parameter (cf. [15–17]), updated by

$$\sigma_{i,k} = \frac{y_{i,k-1}^T s_{k-1}}{s_{k-1}^T s_{k-1}}, \quad i = 1, \ldots, m$$

where $y_{i,k-1} = \nabla F_i(x_k) - \nabla F_i(x_{k-1})$ and $s_{k-1} = x_k - x_{k-1}$.

Therefore, $S_k \approx \mu_k I$, and the spectral parameter μ_k is defined by

$$\mu_k := \sum_{i=1}^{m} F_i(x_k) \frac{(\nabla F_i(x_k) - \nabla F_i(x_{k-1}))^T s_{k-1}}{s_{k-1}^T s_{k-1}}, \tag{4}$$

which may be alternatively stated in matrix form as

$$\mu_k = \frac{F_k^T (J_k - J_{k-1}) s_{k-1}}{s_{k-1}^T s_{k-1}}. \tag{5}$$

By applying the Taylor expansion with integral remainder to (4), we obtain

$$\mu_k = \sum_{i=1}^{m} F_i(x_k) \frac{s_{k-1}^T \left(\int_0^1 \nabla^2 F_i(x_{k-1} + t s_{k-1}) dt \right) s_{k-1}}{s_{k-1}^T s_{k-1}}, \tag{6}$$

so that the parameter μ_k may be interpreted as well as a weighted sum of the Rayleigh quotients of average residual Hessians, for which the weights are the corresponding components of the residual functions computed at the current iterate.

From a somewhat different perspective, due to the relationship $S_k(x_k - x_{k-1}) \approx (J_k - J_{k-1})^T F_k$, under the assumption that the effect a *quasi-Newton* approximation B_k on the vector s_{k-1} should be similar to the one of the matrix S_k (cf. [23]), one must impose that $B_k s_{k-1} = (J_k - J_{k-1})^T F_k$. Relaxing such a condition we have $s_{k-1}^T B_k s_{k-1} = s_{k-1}^T (J_k - J_{k-1})^T F_k$, so that, with the scalar approximation $B_k = \mu_k I$, the expression μ_k as defined in (5) is also obtained. Hence, a *weak secant condition* is verified [12], which means that the matrix $\mu_k I$ carries some information on how the matrix S_k contributes to the curvature of the model along the segment that joins x_{k-1} and $x_{k-1} + s_{k-1}$.

3 A globally convergent algorithmic framework

Next we present the main algorithm of this work. We call the iteration scheme (3) with the spectral choice for the parameter μ_k as the Gauss-Newton iteration with spectral correction (GN+SC).

Algorithm 1. Global framework for the GN+SC method

Input : $x_0 \in \mathbb{R}^n$, $\mu_0 \in \mathbb{R}$, $\mu_{\max} > 0$, $\beta > 1$, $\Delta_{\max} > 0$, $\gamma \in (0,1)$, $Q_0 = 1$, $0 \leq \eta_{\min} \leq \eta_{\max} \leq 1$

1. Set $k = 0$, evaluate F_k, J_k and set $C_k = \frac{1}{2}\|F_k\|^2$
2. **while** the stopping criteria are not satisfied **do**
3.   **if** $\mu_k \geq 0$ **then**
4.   Solve $(J_k^T J_k + \mu_k I)d = -J_k^T F_k$, and set $d_k = d$, $\alpha_k = 0$
5.   **else**
6.   Choose $\Delta_k \in \left[\frac{1}{\beta}\|J_k^T F_k\|, \min\left\{\beta\|J_k^T F_k\|, \Delta_{\max}\right\}\right]$.
7.   Compute (d_k, α_k) as a primal-dual solution of

$$\begin{array}{ll} \min & \frac{1}{2}\|J_k d + F_k\|^2 + \frac{\mu_k}{2}\|d\|^2 \\ \text{s.t.} & \|d\| \leq \Delta_k. \end{array}$$

8.   **end if**
9.   Set $t = 1$
10.   **while** $\frac{1}{2}\|F(x_k + td_k)\|^2 > C_k + \gamma t d_k^T J_k^T F_k$ **do**
11. $t = t/2$
12.   **end while**
13. $t_k = t$
14. $x_{k+1} = x_k + t_k d_k$, $s_k = x_{k+1} - x_k$
15.   Evaluate F_{k+1}, J_{k+1} and compute
$$\mu_{k+1} = \max\left\{\min\left\{\frac{s_k^T (J_{k+1} - J_k)^T F_{k+1}}{s_k^T s_k}, \mu_{\max}\right\}, -\mu_{\max}\right\}$$
16.   Choose $\eta_k \in [\eta_{\min}, \eta_{\max}]$ and set $Q_{k+1} = \eta_k Q_k + 1$,
$C_{k+1} = \left(\eta_k Q_k C_k + \frac{1}{2}\|F_{k+1}\|^2\right)/Q_{k+1}$
17.   Set $k = k + 1$
18. **end while**

Remarks about the Algorithm 1.

1. The algorithm may start with the pure Gauss-Newton step, i.e. $\mu_0 = 0$.
2. The verification at line **3** immediately implies in the positive definiteness of $J_k^T J_k + \mu_k I$ whenever $\mu_k > 0$, and in such a case, the linear system of the normal equations at line **4** might be solved by the Cholesky factorization. We have adopted the more stable alternative proposed by Moré in [24], despite its higher computational cost, which constitutes in solving the linear least-squares problem

$$\min_{d \in \mathbb{R}^n} \frac{1}{2} \left\| \begin{bmatrix} J_k \\ \sqrt{\mu_k} I \end{bmatrix} d + \begin{bmatrix} F_k \\ 0 \end{bmatrix} \right\|^2$$

by a QR factorization of the augmented matrix.

Besides, as the current Jacobian might not have full rank, whenever $\mu_k = 0$, first we compute a QR factorization of J_k, to verify if the GN step is an option, i.e. if the factor R is safely full-rank. In case it is not, or if the sign-free spectral parameter is negative, then the trust-region subproblem of line **7** is solved to produce a descent direction.

3. The quadratic norm constrained subproblem of line **7** is solved by the Moré-Sorensen strategy [25], so that the pair $(d_k, \alpha_k) \in \mathbb{R}^n \times \mathbb{R}_+$ verifies

$$\left(J_k^T J_k + (\mu_k + \alpha_k) I\right) d_k = -J_k^T F_k \tag{7}$$

with

$$\alpha_k \geq \max\left\{0, -\lambda_{\min}(J_k^T J_k + \mu_k I)\right\} \tag{8}$$

($\lambda_{\min}(A)$ denotes the smallest eigenvalue of the symmetric matrix A), $\|d_k\|^2 \leq \Delta_k^2$, $\alpha_k(\|d_k\|^2 - \Delta_k^2) = 0$, and the matrix $J_k^T J_k + (\mu_k + \alpha_k) I$ is positive semidefinite.

The safeguarding scheme that defines the radius Δ_k takes into account the stationarity measure at the current iterate. It aims to allow the Newton's step for the subproblem, namely $d_k = -(J_k^T J_k + \mu_k I)^{-1}(J_k^T F_k)$, to be feasible in case it is a descent direction.

4. The line search procedure of lines **9** – **13** is based on the work of Zhang and Hager [26], with the updating scheme of line **16**. The choice $\eta_k = 0$ provides a monotone linesearch, whereas any choice $\eta_k \in (0, 1]$ generates a nonmonotone line search. Concerning the sequences Q_k and C_k, from the updating expressions at line **16**, it is easy to see that C_{k+1} is a convex combination of C_k and $\frac{1}{2}\|F_{k+1}\|^2$. Since $C_0 = \frac{1}{2}\|F_0\|^2$, it follows that C_k is a convex combination of the function values $\frac{1}{2}\|F_0\|^2, \frac{1}{2}\|F_1\|^2, \ldots, \frac{1}{2}\|F_k\|^2$. For further details and properties of the (non)monotone line search we refer the reader to [26].

5. From the previous reasoning about the computation of the (descent) step s_k, we stress that the Algorithm 1 is well defined, that is, it always computes a descent direction d_k and the line search (lines **9** – **13**) finishes after a finite number of steps.

The global convergence of Algorithm 1 is analyzed in the following, based upon the development of Zhang and Hager [26]. In a preliminary result we prove that their fundamental assumptions upon the directions are satisfied.

Lemma 1. *If $\|J(x)\| \leq \zeta$, $\zeta > 0$, for any $x \in \mathbb{R}^n$, then the directions generated by the Algorithm 1 satisfy the conditions*

a) $g_k^T d_k \leq -c_1 \|g_k\|^2$,

b) $\|d_k\| \leq c_2 \|g_k\|$,

for all k, where $g_k := J_k^T F_k$, and c_1 and c_2 are positive constants.

Proof. For a given threshold $\mu_+ > 0$, and a fixed iteration k, let us split the analysis in two cases.

Case 1. The spectral parameter is safely positive, that is, μ_k is such that $\mu_+ \leq \mu_k \leq \mu_{\max}$.

It is clear that
$$\lambda_{\min}(J_k^T J_k + \mu_k I) \geq \mu_+.$$
Thus
$$\|d_k\| = \|(J_k^T J_k + \mu_k I)^{-1} g_k\| \leq \|(J_k^T J_k + \mu_k I)^{-1}\| \|g_k\| \leq \frac{1}{\mu_+} \|g_k\|.$$
Additionally
$$g_k^T d_k = -g_k^T (J_k^T J_k + \mu_k I)^{-1} g_k \leq \frac{-1}{\zeta^2 + \mu_{\max}} \|g_k\|^2,$$
where the last inequality follows from
$$\lambda_{\max}(J_k^T J_k) + \mu_k = \|J_k^T J_k\| + \mu_k \leq \|J_k\|^2 + \mu_{\max} \leq \zeta^2 + \mu_{\max},$$
where $\lambda_{\max}(A)$ denotes the largest eigenvalue of the symmetric matrix A. Therefore (a) and (b) hold with $c_1 = 1/(\zeta^2 + \mu_{\max})$ and $c_2 = 1/\mu_+$.

Case 2. The spectral parameter is below the threshold, i.e., $-\mu_{\max} \leq \mu_k < \mu_+$

In this second case, the following trust-region subproblem is solved
$$\begin{array}{ll} \min\limits_{d} & \|J_k d + F_k\|^2 + \frac{\mu_k}{2}\|d\|^2 \\ \text{s.t.} & \|d\| \leq \Delta_k. \end{array} \tag{9}$$

Let (d_k, α_k) be a primal-dual solution of (9), and consider the SVD decomposition

$$(J_k^T J_k + \mu_k I + \alpha_k I) = Q_k \Sigma_k Q_k^T,$$

where $Q_k = [q_k^1 \cdots q_k^n] \in \mathbb{R}^{n\times n}$ is orthogonal, $\Sigma_k := |\Lambda_k + \mu_k I + \alpha_k I|$ with $\Lambda_k = \mathrm{diag}(\lambda_k^1, \ldots, \lambda_k^n)$, $\lambda_k^1 \geq \ldots \geq \lambda_k^n \geq 0$, so that $\sigma_k^i := |\lambda_k^i + \mu_k + \alpha_k|$, and $\sigma_k^1 \geq \cdots \geq \sigma_k^r > 0 = \sigma_k^{r+1} = \cdots = \sigma_k^n$. Notice that (d_k, α_k) is a solution of (9), and due to (8),

$$\lambda_k^i + \mu_k + \alpha_k \geq 0, \quad \forall i.$$

Hence, for all i it holds $|\lambda_k^i + \mu_k + \alpha_k| = \lambda_k^i + \mu_k + \alpha_k$.

The direction d_k may be expressed as

$$d_k = -(J_k^T J_k + \mu_k I + \alpha_k I)^+ g_k + v_k = -\sum_{\sigma_k^i \neq 0} \frac{(q_k^i)^T g_k}{\lambda_k^i + \mu_k + \alpha_k} q_k^i + v_k,$$

where A^+ denotes the generalized inverse of the matrix A and v_k is a vector in the null space of

$$B_k := (J_k^T J_k + \mu_k I + \alpha_k I),$$

so that $v_k \in \mathrm{span}\{q_k^{r+1} \cdots q_k^n\}$, whereas, due to (7), $g_k \in \mathrm{span}\{q_k^1 \cdots q_k^r\}$. Therefore $v_k^T g_k = 0$ and we obtain

$$g_k^T d_k = -\sum_{\sigma_k^i \neq 0} \frac{((q_k^i)^T g_k)^2}{\lambda_k^i + \mu_k + \alpha_k}.$$

If $\|d_k\| < \Delta_k$, then $\alpha_k = 0$ and since $\lambda_k^i \leq \lambda_{\max}(J_k^T J_k) = \|J_k^T J_k\| \leq \zeta^2$, we have

$$g_k^T d_k = -\sum_{\sigma_k^i \neq 0} \frac{((q_k^i)^T g_k)^2}{\lambda_k^i + \mu_k} \leq \frac{-1}{\zeta^2 + \mu_+} \sum_{\sigma_k^i \neq 0} ((q_k^i)^T g_k)^2 = \frac{-1}{\zeta^2 + \mu_+} \|g_k\|^2.$$

Now, if $\|d_k\| = \Delta_k$, from (7), reasoning as in the proof of Lemma 2.3 of Nocedal and Yuan [27], and due to the conditions $\frac{1}{\beta}\|g_k\| \leq \Delta_k$ and $-\mu_{\max} \leq \mu_k$ it follows that

$$\begin{aligned}
\|B_k d_k\| = \|g_k\| \quad &\Rightarrow \quad \lambda_{\min}(B_k)\|d_k\| \leq \|g_k\| \quad \Rightarrow \quad \lambda_{\min}(B_k) \leq \frac{\|g_k\|}{\Delta_k} \\
&\Rightarrow \quad \min_i \left(\lambda_k^i + \mu_k + \alpha_k\right) = \min_i \left(\lambda_k^i + \mu_k\right) + \alpha_k \leq \frac{\|g_k\|}{\Delta_k} \\
&\Rightarrow \quad \alpha_k \leq \frac{\|g_k\|}{\Delta_k} - \min_i \left(\lambda_k^i + \mu_k\right) \leq \beta + \mu_{\max}.
\end{aligned}$$

Consequently,

$$\lambda_k^i + \mu_k + \alpha_k \quad \leq \quad \zeta^2 + \mu_+ + \beta + \mu_{\max}.$$

Therefore

$$g_k^T d_k = -\sum_{\sigma_k^i \neq 0} \frac{(q_i^T g_k)^2}{\lambda_k^i + \mu_k + \alpha_k} \leq \frac{-\|g_k\|^2}{\zeta^2 + \mu_+ + \beta + \mu_{\max}}.$$

Moreover, because $\Delta_k \leq \beta\|g_k\|$, we have

$$\|d_k\| = \Delta_k \leq \beta\|g_k\|,$$

and thus the conditions (a) and (b) hold in this case for $c_1 = 1/(\zeta^2 + \mu_+ + \beta + \mu_{\max})$ and $c_2 = \beta$.

Finally, observing that

$$\max\left\{\frac{1}{\zeta^2 + \mu_+}, \frac{1}{\zeta^2 + \mu_{\max}}, \frac{1}{\zeta^2 + \mu_+ + \beta + \mu_{\max}}\right\} = \frac{1}{\zeta^2 + \mu_+},$$

setting

$$c_1 = \frac{1}{\zeta^2 + \mu_+} \quad \text{and} \quad c_2 = \min\left\{\frac{1}{\mu_+}, \beta\right\}$$

completes the proof. □

As in [26], when the conditions (a) and (b) of Lemma 1 are satisfied by a set of search directions, we say that the *Direction Assumption* holds. Next, for the reader's convenience, we restate the result of Zhang and Hager [26, Theorem 2.2] that assures the global convergence of Algorithm 1.

Theorem 1. *Suppose $f(x)$ is bounded from below and the Direction Assumption holds. Assume that the gradient of the objective function is Lipschitz continuous on an open convex set Ω that contains the level set $\mathcal{L}(x_0) = \{x \in \mathbb{R}^n \mid f(x) \leq f(x_0)\}$, being $x_0 \in \mathbb{R}^n$ a given initial iterate. Then the iterates x_k generated by the nonmonotone line search of Algorithm 1 have the property that*

$$\liminf_{k\to\infty} \|\nabla f(x_k)\| = 0.$$

Moreover, if $\eta_{\max} < 1$ *then*

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

Hence, every convergent subsequence of the iterates approaches a point x_*, *where* $\nabla f(x_*) = 0$.

Proof. We remark that the boundedness from below for the objective function clearly holds for problem (1) and, by Lemma 1, the search directions generated by Algorithm 1 satisfy the Direction Assumption. The remainder of the proof follows as in Theorem 2.2 of [26]. □

It is worthwhile noticing that the previous analysis is valid for any choice of a bounded sequence $\{\mu_k\}$. Nevertheless, the spectral correction provided at line **15** of the Algorithm 1 is a legitimate choice, whose practical performance is enlightened next.

4 Numerical results

To investigate the efficiency and the robustness of the Algorithm 1, we have implemented it in Fortran and solved two collections of problems from the literature: (i) the first 18 nonlinear least squares problems listed in Table 1 were presented by Moré, Garbow and Hillstrom [28]; (ii) the last 22 problems were proposed by Lukšan [29]. Table 1 also brings the number of variables n, number of residual functions (equations) m and a classification according with the residual size at the solution.

Although the test set is composed by small-scale problems ($n \leq 100$ and $m \leq 500$), it is important to stress the wide variety of such problems: zero (47.5%), small (22.5%) and large (30%) residual problems; bad scaled problems and problems with rank deficient Jacobian.

The tests were performed using the GNU-Fortran compiler (64-bits), version 5.3.0, in an Intel MacBook Pro, with 2.4 GHz, RAM of 8 Gb and Cache L2: 256Kb (per core) and Cache L3: 6Mb.

The parametric and algorithmic choices were

$$\beta = \begin{cases} 100, & \text{if} \quad \|J_0^T F_0\|\|F_0\| \leq 10^3 \\ 10, & \text{if} \quad 10^3 < \|J_0^T F_0\|\|F_0\| \leq 10^6 \\ 4, & \text{otherwise,} \end{cases}$$

Tab. 1: Nonlinear least squares test problems

#	Problem	n	m	Residual-size
1	Rosenbrock	2	2	zero
2	Powel singular	4	4	zero
3	Bard	3	15	small
4	Chebyquad	9	9	zero
5	Brown and Dennis	4	20	large
6	Watson	12	31	zero
7	Jenrich and Sampson	2	10	large
8	Kowalik and Osborne	4	11	small
9	Freudenstein and Roth	2	2	large
10	Box 3D	3	10	zero
11	Helical valley	3	3	zero
12	Brown almost linear	10	10	zero
13	Osborne 1	5	33	small
14	Osborne 2	11	65	small
15	Meyer	3	16	large
16	Linear full rank	10	10	zero
17	Linear rank one	10	10	small
18	Linear rank one with zeros	3	3	small
19	Chained Rosenbrock	100	198	zero
20	Chained Wood	100	294	zero
21	Chained Powell	100	196	zero
22	Chained Cragg and Levy	100	245	small
23	Generalized Broyden tridiagonal	100	100	zero
24	Chained Broyden Banded	100	100	zero
25	Extended Freudensein and Roth	100	198	large
26	Wright and Holt zero residual	100	500	zero
27	Toint quadractic merging	100	294	large
28	Chained exponential	100	199	large
29	Chained serpentine	100	198	zero
30	Chained and modified HS-47	98	192	large
31	Chained and modified HS-48	98	224	large
32	Chained and modified HS-53	98	224	large
33	Sparse sigmoidal	100	196	small
34	Sparse exponential	100	196	small
35	Sparse trigonometric	100	196	zero
36	Countercurrent reactors problem 1	100	100	zero
37	Tridiagonal system	100	100	zero
38	Structured Jacobian problem	100	100	zero
39	Modified discrete boundary-value problem	100	100	large
40	Attracting-repelling problem	100	198	large

$\gamma = 10^{-4}$, $\mu_0 = 0$, $\mu_{\max} = 10^6$, $\Delta_{\max} = \min\left\{100, 2\|J_0^T F_0\|\right\}$, $\Delta_0 = \beta\|J_0^T F_0\|$, $\Delta_k = \max\{(1/\beta)\|J_k^T F_k\|, \min\{\beta\|J_k^T F_k\|, \beta\|s_{k-1}\|, \Delta_{\max}\}\}$ and $\eta_k \in \{0, 1\}$.

The starting points were selected as in the references [28, 29] and the trust-region subproblems were solved by the routine `GQTPAR` of `MINPACK-2` (see http://ftp.mcs.anl.gov/pub/MINPACK-2/).

Setting $\varepsilon_{\text{mach}}$ as the machine precision, the implemented stopping criteria were as follows.

- Convergence to a stationary point was reached
  `flag 2:` $\|J_k^T F_k\| \le$ `gtol` $(= 10^{-8})$;

- The computed search direction is too small
  `flag 3:` $\|d_k\| \le$ `xtol` $(= 10^{-14})$;

- The variation between two consecutive iterates is too small
  `flag 4:` $\|s_k\| = \|t_k d_k\| \le$ `xtol`$\left[\sqrt{\varepsilon_{\text{mach}}} + \|x_k\|\right]$;

- The line search failed
  `flag 5:` $t_k \le$ `tolstep` $(= 10^{-15})$;

- The variation of the objective function is too small
  `flag 6:` $|\|F_{k+1}\|^2 - \|F_k\|^2| \le$ `tolres` $\|F_k\|^2$, (i) `tolres`$=10^{-12}$ for the first set of problems; (ii) `tolres`$=10^{-8}$ for the second set, due to problems with very large residual;

- The maximum allowed number of iterations was reached
  `flag 99: itmax` $= 400$.

Table 2 presents a comparison between the monotone and nonmonotone line-search strategies for Algorithm 1 when applied to the 40 problems listed in Table 1. It contains the number of iterations (IT) and function evaluations (FE) required for each variant of Algorithm 1 to reach one of the coded stopping criteria, indicated in the column *flag*. The squared residual norm $\|F_k\|^2$ and the gradient norm $\|J_k^T F_k\|$ at the last iterate are also presented.

As we can see from the figures of Table 2, Algorithm 1 integrated with both line-search strategies could solve almost all of problems, stopping by the tolerance in the gradient norm, which happens for most part of the zero and small residual problems, whereas the flag 6 (too small variation in the objective function) predominates among the large residual problems. Algorithm 1 with the monotone line search fails to solve only one problem: problem 36

Tab. 2: Numerical results for the monotone and nonmonotone strategies

	monotone					nonmonotone				
#	IT	FE	$\|F_k\|^2$	$\|J_k^T F_k\|$	flag	IT	FE	$\|F_k\|^2$	$\|J_k^T F_k\|$	flag
1	22	32	0.00000E+00	0.00E+00	2	18	25	1.34353E–30	2.45E–14	2
2	19	20	2.60254E–12	4.11E–09	2	19	20	2.60254E–12	4.11E–09	2
3	9	10	8.21488E–03	2.55E–10	2	9	10	8.21488E–03	2.55E–10	2
4	12	25	1.92146E–22	5.50E–11	2	16	33	7.32440E–23	2.29E–11	2
5	24	30	8.58222E+04	3.13E–03	6	21	24	8.58222E+04	1.25E–02	6
6	15	16	4.72527E–10	1.70E–10	2	15	16	4.72527E–10	1.70E–10	2
7	8	11	1.24362E+02	6.30E–08	6	8	11	1.24362E+02	6.30E–08	6
8	14	16	3.07506E–04	7.09E–10	2	14	16	3.07506E–04	7.09E–10	2
9	25	27	4.89843E+01	2.22E–05	6	26	27	4.89843E+01	1.35E–05	6
10	8	9	2.25414E–19	1.10E–10	2	8	9	2.25414E–19	1.10E–10	2
11	13	19	2.39151E–19	3.29E–09	2	15	22	6.91772E–33	3.66E–16	2
12	9	19	4.11690E–21	6.92E–11	2	9	19	4.11690E–21	6.92E–11	2
13	31	42	5.46489E–05	1.12E–10	2	23	24	5.46489E–05	2.39E–10	2
14	14	17	4.01377E–02	3.15E–09	2	18	22	4.01377E–02	4.10E–09	2
15	158	261	8.79459E+01	1.28E–04	6	35	53	8.79459E+01	5.46E–04	6
16	1	2	7.14905E–30	2.67E–15	2	1	2	7.14905E–30	2.67E–15	2
17	2	3	2.14286E+00	1.01E–06	6	2	3	2.14286E+00	1.01E–06	6
18	1	2	2.00000E+00	0.00E+00	2	1	2	2.00000E+00	0.00E+00	2
19	180	207	9.23929E–19	2.19E–09	2	169	170	4.80886E–20	1.36E–09	2
20	45	60	4.44440E–19	4.60E–09	2	39	40	4.38771E–20	1.17E–09	2
21	18	19	4.40338E–12	8.60E–09	2	18	19	4.40338E–12	8.60E–09	2
22	20	21	2.52061E+01	5.91E–04	6	20	21	2.52061E+01	5.91E–04	6
23	5	6	1.08621E–22	3.13E–11	2	5	6	1.08621E–22	3.13E–11	2
24	6	7	7.39953E–20	1.27E–09	2	6	7	7.39953E–20	1.27E–09	2
25	18	23	1.19646E+04	2.25E–02	6	25	26	1.19646E+04	1.59E–02	6
26	23	31	1.21017E–09	9.77E–09	2	23	31	1.21017E–09	9.77E–09	2
27	58	75	4.41616E+02	5.04E–03	6	63	65	4.41616E+02	1.11E–02	6
28	10	12	3.87395E+01	1.71E–05	6	10	12	3.87395E+01	1.71E–05	6
29	381	477	4.93038E–32	2.22E–16	2	323	343	2.95274E–20	1.67E–09	2
30	13	31	4.29220E+03	7.64E–03	6	17	26	4.29220E+03	8.51E–03	6
31	24	39	2.51889E+04	7.41E–02	6	23	30	2.51889E+04	6.81E–02	6
32	7	13	2.13121E+01	2.21E–05	6	9	11	2.13121E+01	1.26E–03	6
33	6	7	3.56970E+00	7.36E–07	6	6	7	3.56970E+00	7.36E–07	6
34	11	12	4.93161E–01	1.14E–06	6	11	12	4.93161E–01	1.14E–06	6
35	15	16	1.64116E–21	2.40E–11	2	15	16	1.64116E–21	2.40E–11	2
36	401	569	8.70870E–01	3.27E+00	99	53	54	1.10351E–25	3.64E–12	2
37	13	14	3.82880E–19	2.80E–09	2	13	14	3.82880E–19	2.80E–09	2
38	11	18	8.30418E–19	9.93E–11	2	7	13	7.87067E–16	3.06E–09	2
39	17	48	1.23924E+02	1.94E–02	6	18	20	1.23924E+02	1.05E–03	6
40	110	289	8.73951E+02	2.10E–01	6	131	134	8.73915E+02	3.17E–02	6

(Counter current reactors problem 1), for which the maximum number of iterations was reached. Besides the fact that the nonmonotone strategy increases a bit (less than 8) the number of iterations in 9 out of 40 problems, it reduces considerably the number of iterations in the harder problems when compared with the monotone line search (especially problems 15 and 36).

To contextualize our results, we have also solved both sets of test problems using the routine `LMDER` of `MINPACK`, with the aforementioned stopping criteria and the scaling option inhibited. `LMDER` is an implementation of the Levenberg-Marquardt algorithm due to Moré [24], within the trust-region philosophy, based on the model

$$\begin{array}{ll} \min & \frac{1}{2}\|J_k d + F_k\|^2 \\ \text{s.t.} & \|d\| \leq \Delta_k. \end{array}$$

The results are shown in Table 3, which has the same structure of presentation of the Table 2.

Both robustness and efficiency may be better appreciated from the performance profiles [30] of Figure 1. We have considered the number of iterations (left) and the number of function evaluations (right) demanded by the algorithm GN+SC with each variant of the line search, together with `LMDER`. Concerning the first performance measure, both variants of the line search are comparable in terms of efficiency: 37% and 40% of the problems were solved with the fewest number of iterations by GN+SC with the monotone and the nonmonotone line search, respectively. `LMDER` is the most efficient one, solving 62.5% of the problems with the fewest number of iterations. When it comes to robustness, however, only the nonmonotone variant of GN+SC managed to solve the whole set of test problems. Both the monotone GN+SC and `LMDER` did not manage to solve just one problem within the 400 iterations budget, reaching 97.5% of success. With respect to the efficiency of the second performance measure, the difference between the three analyzed strategies is more significant: 30%, 45% and 62.5% of the problems were solved with the fewest number of function evaluations by the monotone GN+SC, the nonmonotone GN+SC and `LMDER`, respectively. In terms of robustness, the outcome is similar to the one of the first performance measure.

Concerning the ratio FE/IT, which assesses the efectiveness of the computed step, the box plots of Figure 2 depicts a comparative overview of the strategies under analysis. Considering the two variants of GN+SC, the more concentrated and thus more favourable data distribution associated with the

Tab. 3: Numerical results for the `LMDER` routine

#	LMDER (MINPACK)				
	IT	FE	$\|F_k\|^2$	$\|J_k^T F_k\|$	flag
1	16	21	0.00000E+00	0.00E+00	2
2	13	13	5.71987E–13	3.29E–09	2
3	6	6	8.21488E–03	3.04E–09	2
4	9	12	6.63760E–26	6.31E–13	2
5	23	35	8.58222E+04	1.87E–02	6
6	6	6	1.70822E–09	1.07E–10	2
7	13	22	1.24362E+02	3.82E–04	6
8	25	28	3.07506E–04	6.95E–09	2
9	20	32	4.89843E+01	8.49E–05	6
10	6	6	1.13586E–19	4.88E–10	2
11	11	15	9.54175E–29	1.84E–13	2
12	7	8	2.28724E–25	1.42E–12	2
13	18	21	5.46489E–05	3.23E–08	6
14	11	15	4.01377E–02	1.15E–07	6
15	114	128	8.79459E+01	3.59E–05	6
16	2	2	1.14385E–29	3.38E–15	2
17	2	2	2.14286E+00	1.10E–09	2
18	2	2	2.00000E+00	0.00E+00	2
19	133	136	6.51223E–22	3.72E–10	2
20	102	122	9.52118E–29	3.00E–13	2
21	13	13	1.27500E–12	4.49E–09	2
22	29	32	2.52061E+01	2.36E–03	6
23	6	6	1.67941E–30	6.92E–15	2
24	7	7	9.08124E–31	3.30E–15	2
25	18	25	1.19646E+04	5.33E–02	6
26	13	15	3.05290E–11	1.39E–09	2
27	26	27	4.34919E+02	4.49E–03	6
28	9	19	3.87395E+01	3.94E–04	6
29	265	276	0.00000E+00	0.00E+00	2
30	13	22	4.29220E+03	5.58E–01	6
31	19	31	2.51889E+04	4.82E–02	6
32	6	13	2.13121E+01	1.93E–02	6
33	6	6	3.56970E+00	5.33E–04	6
34	11	20	4.93161E–01	8.38E–04	6
35	12	15	1.60010E–22	1.45E–11	2
36	401	412	8.99843E–01	1.06E+01	99
37	15	15	4.48088E–19	3.02E–09	2
38	10	12	4.68425E–22	3.27E–12	2
39	20	22	1.23924E+02	1.90E–03	6
40	117	127	8.73941E+02	2.20E–02	6

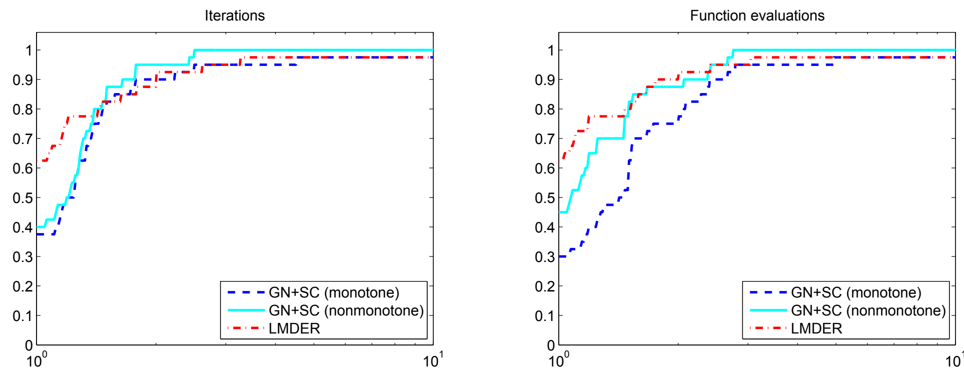

Fig. 1: Performance profiles (log scaled) of the number of iterations (left) and the number of function evaluations (right).

nonmonotone line search suggests that this variant is preferable to the monotone one. Furthermore, one can see that GN+SC nonmonotone and `LMDER` behave quite similarly for this measure.

5 Final remarks

We have proposed a spectral correction for the Gauss-Newton method as an option for solving general nonlinear least-squares for which the residual Hessians are not easily available. We have adopted the nonmonotone line-search framework of Zhang and Hager [26] as the globalization tool. The directions computed by our algorithm were proved to satisfy the descent condition assumed by Zhang and Hager, so that their global convergence result applies. A numerical study with problems from the literature corroborates the reliability of adopting the spectral correction for the Gauss-Newton model within a nonmonotone line-search framework. This approach turned out to be robust and competitive with the benchmark `LMDER`.

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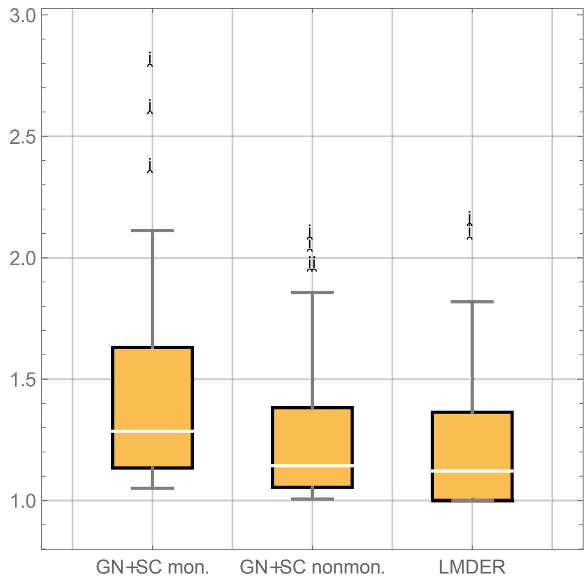

Fig. 2: Box plots of the ratios FE/IT for the results of GN+SC with the monotone and the nonmonotone line-search strategies (Table 2) as well as the results of `LMDER` (Table 3). The corresponding medians are 1.285, 1.143 and 1.121.

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