

INSEAN

National Research Center for Ships
and Marine Systems



INSEAN Technical Report 2008-035/rt

**A nonmonotone truncated Newton-Krylov method
exploiting negative curvature directions, for large scale
unconstrained optimization: complete results**

Giovanni Fasano & Stefano Lucidi

A nonmonotone truncated Newton-Krylov method exploiting negative curvature directions, for large scale unconstrained optimization: complete results

G. Fasano*

S. Lucidi†

Abstract

We propose a new truncated Newton method for large scale unconstrained optimization, where a Conjugate Gradient (CG)-based technique is adopted to solve Newton's equation. In the current iteration, the Krylov method computes a pair of search directions: the first approximates the Newton step of the quadratic convex model, while the second is a suitable negative curvature direction. A test based on the quadratic model of the objective function is used to select the most promising between the two search directions. Both the latter selection rule and the CG stopping criterion for approximately solving Newton's equation, strongly rely on conjugacy conditions. An appropriate linesearch technique is adopted for each search direction: a nonmonotone stabilization is used with the approximate Newton step, while an Armijo type linesearch is used for the negative curvature direction. We prove both the global and the super-linear convergence to stationary points satisfying second order necessary conditions. We carry out a significant numerical experience in order to test our proposal.

Keywords: Truncated Newton methods, Conjugate directions, negative curvatures, nonmonotone stabilization technique, second order necessary conditions.

1 Introduction

We consider the solution of the unconstrained minimization problem

$$\min_{x \in \mathbb{R}^n} f(x), \quad (1.1)$$

where $f(x)$ is twice continuously differentiable on \mathbb{R}^n and n is large. Several appealing algorithms have already been proposed in the literature to solve (1.1) [1, 4, 6, 10, 11, 13, 17, 19, 7], however the definition of both robust and efficient methods for large scale unconstrained problems is still a challenging task. In particular, we observe that the state-of-the-art Newton-type methods are based on the idea of exploiting the local information on the function $f(x)$, obtained by investigating the second order derivatives. In the context of large scale problems, the latter task is pursued by computing at the outer iteration k the pair (d_k, s_k) of promising search directions [4, 6, 13, 16, 7],

*Dipartimento di Matematica Applicata. Università Ca'Foscari di Venezia, Dorsoduro 3825/e, 30123 Venezia, Italy. E-mail: fasano@unive.it. This author wishes to thank the 'Programma di Ricerca INSEAN 2007-2009' for the support received.

†Dipartimento di Informatica e Sistemistica, 'Sapienza' Università di Roma, via Ariosto 25 - 00185 Roma, Italy. E-mail: lucidi@dis.uniroma1.it

by means of efficient iterative techniques. Roughly speaking, d_k summarizes the local convexity of $f(x)$ at the current iterate, while s_k takes into account the local non-convexity of the objective function.

In several earlier papers [4, 6, 13, 17] the latter directions were suitably combined in a curvilinear framework, so that the new iterate is laid on the two dimensional manifold identified by the search directions. On the other hand, in [7] a couple of search directions is computed, too. Then, a suitable test attempts to determine if either the first or the second direction is more promising. Furthermore, according with the chosen direction, a proper monotone linesearch technique is applied in order to provide the new iterate. The rationale behind using a different linesearch technique for each direction, is the possibility of capturing possible differences between the two directions.

In this paper we draw our inspiration from [7], whose results are suitably extended and partially generalized. In particular, we extend the approach in [7] by introducing the following effective ingredients.

- (a) We propose an effective use of conjugate directions computed via a CG-based method, for both the computation and the comparison between the search directions d_k and s_k .
- (b) We use a nonmonotone scheme to improve the stabilization technique. Our stabilization includes a nonmonotone linesearch technique along the direction d_k , and a monotone one along the negative curvature direction s_k .

As regards (a), the use of CG-based methods has a twofold importance. On one hand, they are often the methods of choice to inexpensively and reliably compute a satisfactory approximation of Newton's direction. On the other hand they provide, as a by product, a set of conjugate directions, containing relevant local information of the objective function on an independent set [5]. As a consequence, the conjugate directions can be suitably combined into the pair of search directions d_k and s_k , in order to separately summarize the local information on the convexity and non-convexity of $f(x)$. Moreover, the conjugate directions are "similarly scaled" and so are d_k , s_k . The latter property may be considerably helpful to select the most promising direction in the pair. As regards (b), the role of nonmonotonicity within Newton-type methods was largely investigated in [4, 11, 12, 13]. The significant numerical experience reported in [13, 14] suggests that over highly nonlinear and ill-conditioned problems, a nonmonotone stabilization can be very effective when combined with a Newton-type direction.

This paper is organized as follows. In Section 2 we describe the use of the CG method to both generate the search directions and satisfy specific conditions for the convergence. In Section 3 we describe our Adaptive Linesearch Algorithm (ALA) for the solution of problem (1.1), along with the convergence properties. We provide sufficient conditions so that the algorithm ALA is globally and superlinearly convergent to stationary points, which satisfy both the first and the second order necessary optimality conditions. Finally, Section 4 reports a detailed numerical experience of algorithm ALA, over a significant set of large scale problems of CUTEr [8], selected from [10]. An Appendix completes the paper.

We use the symbol $A \succeq 0$ to denote the positive semidefinite matrix A , and $\|\cdot\|$ represents the Euclidean norm of either a vector or a matrix. With H_k and g_k we respectively indicate the Hessian $\nabla^2 f(x_k)$ and the gradient $\nabla f(x_k)$ at the current iterate x_k .

2 The generation of search directions d_k and s_k

Our truncated Newton method generates the sequence $\{x_k\}$ according with the iterative scheme $x_{k+1} = x_k + \alpha_k z_k$, where $z_k \in \{d_k, s_k\}$ and α_k is a suitable stepsize. Throughout this paper we consider that the following assumption holds.

Assumption 1

- The function $f(x)$ is twice continuously differentiable on \mathbb{R}^n ;
- Given $x_0 \in \mathbb{R}^n$, the level set $\mathcal{L}_0 = \{x \in \mathbb{R}^n : f(x) \leq f(x_0)\}$ is compact.

Let us assume that at the current iterate x_k we apply the following iterative scheme CG_gen to solve the Newton equation¹.

CG_gen: Conjugate directions generation

Data. $x_k, g_k, H_k, \varepsilon \in (0, 2)$.

Initialization. $r_0 = -g_k, p_0 = -g_k$. Set $i = 0$.

Do

If $|p_i^T H_k p_i| < \varepsilon \|p_i\|^2$ Stop.

Compute $r_{i+1} = r_i - \rho_i H_k p_i$, with $\rho_i = p_i^T r_i / p_i^T H_k p_i$.

If a stopping criterion is satisfied Stop (see Section 4).

Compute $p_{i+1} = r_{i+1} + \beta_i p_i$, with $\beta_i = \|r_{i+1}\|^2 / \|r_i\|^2$.

Set $i = i + 1$.

End do

After $m + 1$ steps the $m + 1$ directions p_0, \dots, p_m have been generated. In particular, when $m > 0$ we introduce the disjoint sets of indices

$$I_k^P = \{i \in [0, m] : p_i^T H_k p_i \geq \varepsilon \|p_i\|^2\}, \quad I_k^N = \{i \in [0, m] : p_i^T H_k p_i \leq -\varepsilon \|p_i\|^2\}. \quad (2.1)$$

Now, we can use the set $\{p_0, \dots, p_m\}$ to generate at step k both a *negative curvature direction* s_k and a *positive curvature direction* d_k (search directions). Furthermore, we can select the most promising direction between s_k and d_k , according with the decrease of the local quadratic model $q(x_k, z)$ at iterate x_k , defined as

$$q(x_k, z) = \frac{1}{2} z^T H_k z + g_k^T z. \quad (2.2)$$

We obtain the following resulting scheme (we recall that $p_i^T r_i = -p_i^T g_k$):

¹For the sake of simplicity we omit the dependency of p_i from the index k .

Scheme 1

If $|p_0^T H_k p_0| < \varepsilon \|p_0\|^2$ **then**

$$\begin{cases} d_k = p_0 = -g_k, \\ s_k = 0. \end{cases} \quad (2.3)$$

Else

$$d_k = \begin{cases} \sum_{i \in I_k^P} \rho_i p_i = - \sum_{i \in I_k^P} \frac{g_k^T p_i}{p_i^T H_k p_i} p_i, & \text{if } I_k^P \neq \emptyset \\ 0 & \text{if } I_k^P = \emptyset, \end{cases} \quad (2.4)$$

$$s_k = \begin{cases} - \sum_{i \in I_k^N} \rho_i p_i = - \sum_{i \in I_k^N} \frac{g_k^T p_i}{|p_i^T H_k p_i|} p_i, & \text{if } I_k^N \neq \emptyset \\ 0 & \text{if } I_k^N = \emptyset. \end{cases} \quad (2.5)$$

End if

If $q(x_k, d_k) \leq q(x_k, s_k)$ choose the direction d_k
 If $q(x_k, d_k) > q(x_k, s_k)$ choose the direction s_k

The next proposition proves that the search direction z corresponding to the largest decrease of $q(x_k, z)$ satisfies a *suitable angle condition* for an optimization framework.

Proposition 2.1 *Assume that the directions d_k and s_k are computed by **Scheme 1**. Then, there exist positive constants c_1 and c_2 such that*

$$\max\{\|d_k\|, \|s_k\|\} \leq c_1 \|g_k\|, \quad (2.6)$$

and

$$\text{if } d_k \text{ is chosen then } g_k^T d_k \leq -c_2 \|g_k\|^2; \quad (2.7)$$

$$\text{if } s_k \text{ is chosen then } g_k^T s_k \leq -c_2 \|g_k\|^2. \quad (2.8)$$

Proof. First we study the case $|p_0^T H_k p_0| < \varepsilon \|p_0\|^2$ in **Scheme 1**. Observe that in the latter case $d_k = -g_k$ and $s_k = 0$, so that $q(x_k, s_k) = 0$; furthermore, $q(x_k, -g_k) \leq -\|g_k\|^2 + \varepsilon/2 \|g_k\|^2 = -(1 - \varepsilon/2) \|g_k\|^2$. Thus, (2.6) and (2.7) hold with $c_1 = c_2 = 1$.

On the other hand, for the cases in which $|p_0^T H_k p_0| \geq \varepsilon \|p_0\|^2$, from [11] (see formulae (11)-(12)) the positive constants \tilde{c}_1 and \tilde{c}_2 exist such that

$$\max\{\|d_k\|, \|s_k\|\} \leq \tilde{c}_1 \|g_k\| \quad (2.9)$$

and

$$g_k^T (d_k + s_k) \leq -\tilde{c}_2 \|g_k\|^2. \quad (2.10)$$

Thus, relation (2.6) follows straightforwardly from (2.9) by setting $c_1 = \tilde{c}_1$.

Now we prove (2.7)-(2.8). Since the directions $\{p_i\}$ are computed by `CG_gen`, the following relations hold:

$$g_k^T d_k + \frac{1}{2} d_k^T H_k d_k = g_k^T d_k + \frac{1}{2} \left(- \sum_{i \in I_k^P} \frac{g_k^T p_i}{p_i^T H_k p_i} p_i \right)^T H_k \left(- \sum_{i \in I_k^P} \frac{g_k^T p_i}{p_i^T H_k p_i} p_i \right) = \frac{1}{2} g_k^T d_k, \quad (2.11)$$

$$g_k^T s_k + \frac{1}{2} s_k^T H_k s_k = g_k^T s_k + \frac{1}{2} \left(\sum_{i \in I_k^N} \frac{g_k^T p_i}{p_i^T H_k p_i} p_i \right)^T H_k \left(\sum_{i \in I_k^N} \frac{g_k^T p_i}{p_i^T H_k p_i} p_i \right) = \frac{3}{2} g_k^T s_k. \quad (2.12)$$

If $q(x_k, d_k) \leq q(x_k, s_k)$, from (2.11) and (2.12)

$$g_k^T d_k \leq 3g_k^T s_k;$$

then, (2.10) yields

$$4g_k^T d_k \leq 3g_k^T (d_k + s_k) \leq -3\tilde{c}_2 \|g_k\|^2. \quad (2.13)$$

On the other hand if $q(x_k, d_k) > q(x_k, s_k)$, we have similarly from (2.11) and (2.12)

$$3g_k^T s_k < g_k^T d_k;$$

then, again (2.10) yields

$$4g_k^T s_k < g_k^T (d_k + s_k) \leq -\tilde{c}_2 \|g_k\|^2. \quad (2.14)$$

Finally, relations (2.13)-(2.14) yield (2.7)-(2.8) with respectively $c_2 = 3/4\tilde{c}_2$ and $c_2 = \tilde{c}_2/4$. \square

In order to ensure the convergence results to critical points satisfying second order necessary conditions, we need a negative curvature direction which conveys more information on the local non-convexity of the objective function. This can be done by adding, when needed, to the negative curvature direction produced by **Scheme 1**, an additional negative curvature direction \hat{s}_k which satisfies the following assumption.

Assumption 2 For any outer iteration $k \geq 0$ a bounded direction \hat{s}_k exists such that

(a) $g_k^T \hat{s}_k \leq 0$;

(b) $\hat{s}_k^T H_k \hat{s}_k \leq 0$;

(c) for every $x^* \in \mathbb{R}^n$, with $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*) \not\leq 0$, there exist $\sigma > 0$ and $\tilde{\epsilon} > 0$ such that if $\|x_k - x^*\| \leq \sigma$, then $\hat{s}_k^T H_k \hat{s}_k \leq -\tilde{\epsilon}$.

Assumption 2 generalizes the properties of the negative curvature directions proposed in literature, for defining minimization algorithms globally converging towards second order stationary points (see, for example [16, 4, 3, 13]). Now we can consider the following **Scheme 2** including \hat{s}_k .

Scheme 2

Data: let \bar{d}_k and \bar{s}_k be directions given by (2.3)-(2.5) of **Scheme 1**,
let \hat{s}_k be a direction satisfying Assumption 2.

Compute:

$$d_k = \bar{d}_k$$

$$s_k = \begin{cases} \bar{s}_k + \hat{s}_k, & \text{if } (\bar{s}_k + \hat{s}_k)^T H_k (\bar{s}_k + \hat{s}_k) < 0, \\ \bar{s}_k & \text{otherwise.} \end{cases} \quad (2.15)$$

If $q(x_k, d_k) \leq q(x_k, s_k)$ choose the direction d_k

If $q(x_k, d_k) > q(x_k, s_k)$ choose the direction s_k

The following proposition describes the properties of the directions computed by **Scheme 2**.

Proposition 2.2 *Let us assume that the directions d_k and s_k are computed by **Scheme 2**. Then,*

i) there exist positive constants \hat{c}_1 and \hat{c}_2 such that

$$\max\{\|d_k\|, \|\bar{s}_k\|\} \leq c_1 \|g_k\|, \quad (2.16)$$

$$\max\{\|d_k\|, \|s_k\|\} \leq \hat{c}_1,$$

where c_1 is defined in (2.6), and

$$\text{if } d_k \text{ is chosen then } g_k^T d_k \leq -\hat{c}_2 \|g_k\|^2, \quad (2.17)$$

$$\text{if } s_k \text{ is chosen then } g_k^T s_k + \frac{1}{2} s_k^T H_k s_k \leq -\hat{c}_2 \|g_k\|^2; \quad (2.18)$$

ii) for every $x^ \in \mathbb{R}^n$, with $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*) \not\prec 0$, there exists $\sigma > 0$ such that if $\|x_k - x^*\| \leq \sigma$, then*

$$g_k^T s_k + \frac{1}{2} s_k^T H_k s_k < -\frac{\tilde{\epsilon}}{4}.$$

Proof. As regards *i)*, relation (2.16) follows directly from Proposition 2.1 and Assumption 2.

Now, to prove (2.17) and (2.18) we first consider the case $|p_0^T H_k p_0| < \varepsilon \|p_0\|^2$ in **Scheme 1**. In this case $d_k = -g_k$ and $\bar{s}_k = 0$, and two subcases must be considered. If $q(x_k, -g_k) \leq q(x_k, s_k) \equiv q(x_k, \hat{s}_k)$ then (2.17) follows from the proof of Proposition 2.1. On the other hand if $q(x_k, -g_k) > q(x_k, \hat{s}_k)$ then we have

$$g_k^T s_k + \frac{1}{2} s_k^T H_k s_k = g_k^T \hat{s}_k + \frac{1}{2} \hat{s}_k^T H_k \hat{s}_k < -\|g_k\|^2 + \frac{1}{2} g_k^T H_k g_k \leq -\left(1 - \frac{1}{2}\varepsilon\right) \|g_k\|^2,$$

so that (2.18) holds with $\hat{c}_2 = 1 - \varepsilon/2$.

Let us consider now the case $|p_0^T H_k p_0| \geq \varepsilon \|p_0\|^2$ in **Scheme 1**. If $q(x_k, d_k) \leq q(x_k, s_k)$ then the **Scheme 2** and the Assumption 2 yield:

$$g_k^T d_k + \frac{1}{2} d_k^T H_k d_k \leq g_k^T s_k + \frac{1}{2} s_k^T H_k s_k \leq g_k^T \bar{s}_k. \quad (2.19)$$

Moreover, since the directions \bar{d}_k and \bar{s}_k are computed in **Scheme 1**, it is possible to repeat the arguments of Proposition 2.1. In particular, recalling (2.11), relation (2.19) yields

$$g_k^T d_k + \frac{1}{2} d_k^T H_k d_k = g_k^T \bar{d}_k + \frac{1}{2} \bar{d}_k^T H_k \bar{d}_k = \frac{1}{2} g_k^T \bar{d}_k \leq g_k^T \bar{s}_k,$$

from which, using (2.10)

$$\frac{3}{2} g_k^T \bar{d}_k \leq g_k^T (\bar{d}_k + \bar{s}_k) \leq -\hat{c}_2 \|g_k\|^2, \quad (2.20)$$

so that (2.17) holds with $\hat{c}_2 = \tilde{c}_2$.

If $q(x_k, s_k) < q(x_k, d_k)$, since $d_k = \bar{d}_k$ and the direction \bar{d}_k is given by (2.4), we can use again (2.11) to obtain

$$g_k^T s_k + \frac{1}{2} s_k^T H_k s_k < \frac{1}{2} g_k^T \bar{d}_k; \quad (2.21)$$

then, by the definition of s_k

$$\frac{1}{2} \left[g_k^T s_k + \frac{1}{2} s_k^T H_k s_k \right] < \frac{1}{2} g_k^T \bar{s}_k. \quad (2.22)$$

Adding term to term (2.21) and (2.22) we obtain:

$$\frac{3}{2} \left[g_k^T s_k + \frac{1}{2} s_k^T H_k s_k \right] < \frac{1}{2} g_k^T (\bar{d}_k + \bar{s}_k),$$

so that, recalling again (2.10), we obtain

$$\frac{3}{2} (g_k^T s_k + \frac{1}{2} s_k^T H_k s_k) < -\frac{1}{2} \tilde{c}_2 \|g_k\|^2, \quad (2.23)$$

which yields (2.18) with $\hat{c}_2 = \tilde{c}_2/2$.

The proof of *ii*) easily follows from (2.16) and Assumption 2. In fact, (2.6) ensures that for every stationary point x^* of $f(x)$, there are neighborhoods where the norm of \bar{s}_k is sufficiently small. On the other hand, Assumption 2 implies that the negative scalar $\hat{s}_k^T H_k \hat{s}_k$ is bounded away from zero in a sufficiently small neighborhood of the stationary point x^* , which does not satisfy the second order necessary conditions. Therefore we can conclude that for such stationary points there exists sufficiently small $\sigma > 0$, such that if $\|x_k - x^*\| \leq \sigma$, then from Assumption 2

$$g_k^T s_k + \frac{1}{2} s_k^T H_k s_k < -\frac{\tilde{\epsilon}}{4}.$$

□

3 The Adaptive Linesearch Algorithm

In this section we describe our new algorithmic framework, which uses the search directions d_k and s_k computed in Section 2. We propose at the outer iteration k an **Adaptive Linesearch Algorithm (ALA)**, in which the globalization strategy is tailored on the local curvatures of $f(x)$. The relevant steps of algorithm ALA are summarized in the following points:

Computation and choice of the search direction: We compute at the current iterate x_k the pair of search directions d_k and s_k , according with either **Scheme 1** or **Scheme 2**. The first direction d_k is given by a linear combination of conjugate vectors, which are positive curvature directions for $f(x)$ at x_k . It can be regarded as a Newton-type direction. On the other hand, the vector s_k is a negative curvature direction for $f(x)$ at x_k , which contains relevant information on the subspace of non-convexity of $f(x)$ at x_k . Then, a test based on a quadratic model of $f(x)$ is used to select either d_k or s_k .

Computation of the new point along the positive curvature direction: When the Newton-type direction d_k is selected by the test, we investigate whether x_k is in a region where the super-linear convergence rate holds for d_k (i.e. $\|d_k\|$ decreases at a suitable rate). In this case, the unit stepsize is desirable for d_k [1]. Thus, we adopt a non-monotone strategy to allow the acceptance of the unit stepsize along d_k , as frequently as possible [12].

Computation of the new point along the negative curvature direction: In case the negative curvature direction s_k is selected by the test, a stepsize is computed by a monotone linesearch, which includes the negative term $s_k^T H_k s_k$ (see also [15]). In order to compute stepsizes which take advantage of the *second order descent property* of negative curvature directions, we also include extrapolation along s_k .

For the sake of simplicity we prefer to give here an informal description of some quantities used in Algorithm ALA.

Similarly to [12], in algorithm ALA the objective function is not evaluated at any iterate x_k ; anyway, it is computed at least once on any N iterations. In addition, when linesearch is performed at iteration k along the search direction d_k , then the objective function values on the trial points are not compared with $f(x_k)$. Indeed, they are compared with the largest value of the objective function, over the last M iterates before k in which it was computed.

On this guideline, at iteration k we denote by ℓ the largest iteration index, not exceeding k , where f is evaluated. Moreover, we use f_ℓ^M to indicate the largest value of the objective function, over the last M iterates before k in which it was computed (see also [12]).

According with the latter notation we propose the algorithm ALA in Table 3.1. Now we complete this section by reporting the main convergence results relative to the algorithm ALA. For the sake of clarity, both the proof of the following theorem and some intermediate lemmas are detailed in Section 5.

Theorem 3.1 *Suppose the algorithm ALA generates the sequence $\{x_k\}$.*

- (a) *If the search directions are computed by **Scheme 1** then, either an integer $h \geq 0$ exists such that $\nabla f(x_h) = 0$, or the sequence $\{x_k\}$ is infinite, every limit point x^* belongs to \mathcal{L}_0 and satisfies the relation $\nabla f(x^*) = 0$.*
- (b) *If the search directions are computed by **Scheme 2** then, either an integer $h \geq 0$ exists such that $\nabla f(x_h) = 0$ and $\nabla^2 f(x_h) \succeq 0$, or the sequence $\{x_k\}$ is infinite and every limit point x^* satisfies the relations $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*) \succeq 0$.*

Proof. See Section 5. □

4 Implementation issues and Numerical results

We report here a numerical experience with our algorithm **ALA** on a set of standard test problems from the literature. We applied the algorithm **ALA** in Table 3.1 in order to generate the sequence $\{x_k\}$. In the practical implementation of **ALA** x_0 is the starting point proposed in the literature. Moreover, in **ALA** we set the parameters $\beta = 0.5$, $\Delta_0 = 10^3$, $\delta = 0.9$, $N = 20$, $M = 100$, $\mu = 10^{-3}$, and in the procedure **CG-gen** we set $\varepsilon = 10^{-8}$. We considered the test set from **CUTEr** collection [8] proposed in [10], discarding the test problems with too few unknowns (< 49). The list of our test problems and the relative number of unknowns is reported in Table 4.1.

We coded **ALA** in Fortran 90 (Compaq Visual Fortran) and we used a Pentium 4, 2.53 Ghz, 1Gb RAM, to perform the computation. For each test problem we set the following limits: 500s CPU-time, 100000 outer iterations or function evaluations, 300000 inner iterations. The stopping criterion in the iterative scheme **CG-gen** is the Nash-Sofer rule in [18]. However, based on our experience, we reformulated the latter rule and considered:

- the possible nonconvexity of the objective function;
- the possible conjugacy loss.

On this purpose, in order to cope with the nonconvexity of $f(x)$, the Nash-Sofer stopping criterion is modified as

$$\left| \frac{q(x_k, d_i) - q(x_k, d_{i-1})}{q(x_k, d_i)/i} \right| \leq \gamma, \quad \gamma \in (0, 1). \quad (4.1)$$

In addition, observe from (2.11) that $d_i^T H_k d_i + g_k^T d_i = 0$ and $g_k^T d_i = 2q(x_k, d_i)$, so that

$$2q(x_k, d_i) = g_k^T d_i = g_k^T d_i - 2(d_i^T H_k d_i + g_k^T d_i) = -2d_i^T H_k d_i - g_k^T d_i = -\tilde{q}(x_k, d_i).$$

Thus, the criterion (4.1) can be replaced by

$$\left| \frac{\tilde{q}(x_k, d_i) - \tilde{q}(x_k, d_{i-1})}{\tilde{q}(x_k, d_i)/i} \right| \leq \gamma, \quad \gamma \in (0, 1), \quad (4.2)$$

and since $\tilde{q}(x_k, d_i) = 2d_i^T H_k d_i + g_k^T d_i = 3/2 d_i^T H_k d_i + q(x_k, d_i)$, from (4.1) and (4.2) we have

$$\left| \frac{[q(x_k, d_i) - q(x_k, d_{i-1})] - \frac{3}{2}[g_k^T d_i - g_k^T d_{i-1}]}{q(x_k, d_i) - \frac{3}{2}g_k^T d_i} \right| \leq \gamma, \quad \gamma \in (0, 1), \quad (4.3)$$

which is the criterion we used. We remark that (4.3) is theoretically equivalent to (4.1) in exact arithmetic. However, on our test set when conjugacy loss is experienced in practice, (4.3) performs much better. The latter result may be interpreted as follows. When i increases, the conjugacy loss may seriously affect the quadratic model used in the test (4.1). In (4.3) (see Proposition 2.2) we monitor the decrease of *both* the quadratic model and the directional derivative of the current Newton-type direction d_i , in order to deflate the conjugacy loss.

Finally, the direction \hat{s}_k in **Scheme 2** may be computed as in [3] so that the theoretical assumptions on \hat{s}_k are satisfied (in addition, the latter choice of \hat{s}_k always satisfies the condition $(\bar{s}_k + \hat{s}_k)^T H_k (\bar{s}_k + \hat{s}_k) < 0$). However, for practical efficiency (see Figure 4.1 for comparative results), we preferred to set directly $s_k = \alpha_N p_N$, where p_N is the first conjugate direction computed by **CG-gen**, such that $p_N^T H_k p_N < 0$. As remarked in [5], the latter choice is partially motivated by the fact that in the early inner iterations the CG exploits the eigenspaces associated with the largest (in absolute value) eigenvalues of H_k . Thus, the first conjugate directions collect significant information on the

local curvatures of the objective function.
The algorithm ALA stops (as in [9]) when

$$\|\nabla f(x_k)\|_\infty \leq 10^{-5}.$$

Figures 4.1 and 4.2 report the performance profiles [2] of a comparison among LANCELOT B, the curvilinear truncated Newton method in [13] and ALA. The profiles compare the number of inner iterations. The legends in the figures also report the failures of each algorithm on the test set.

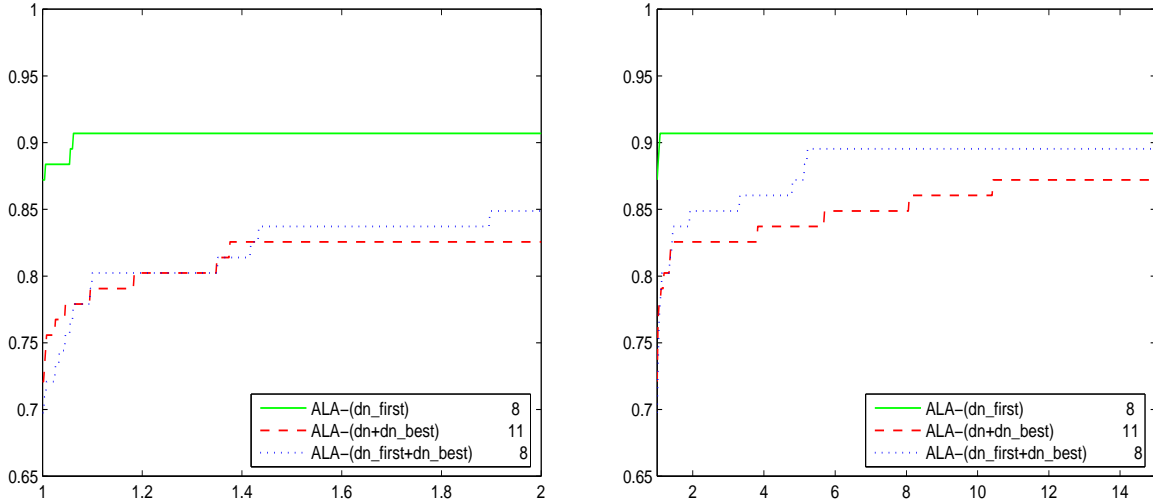


Figure 4.1: (*left*) Detail of the performance profile and (*right*) complete performance profile, on the comparison among three implementations of ALA. The negative curvature direction s_k in the three implementations is given by: (dn_first) $s_k = \alpha_N p_N$, where p_N is the first conjugate direction computed by CG_gen, such that $p_N^T H_k p_N < 0$; (dn + dn_best) $s_k = \bar{s}_k + \hat{s}_k$ as in Scheme 2, where \hat{s}_k is computed according with [3]; (dn_first + dn_best) $s_k = \alpha_N p_N + \hat{s}_k$, where again \hat{s}_k is computed as in [3]. The comparison refers to inner iterations.

5 Appendix

In this section we include the proof of Theorem 3.1, along with the lemmas which provide intermediate results to Theorem 3.1.

Lemma 5.1 *Suppose the algorithm ALA produces an infinite sequence $\{x_k\}$; then*

- (1) $\{f_j^M\}$ is nonincreasing and converges to the value \hat{f}^M ;
- (2) for any fixed $j > 0$ we have:

$$f_h^M < f_j^M \quad \forall h > j + M;$$

- (3) the sequence $\{x_k\}$ is such that $x_k \in \bar{\mathcal{L}}$, for all k , where $\bar{\mathcal{L}}$ is a compact set.

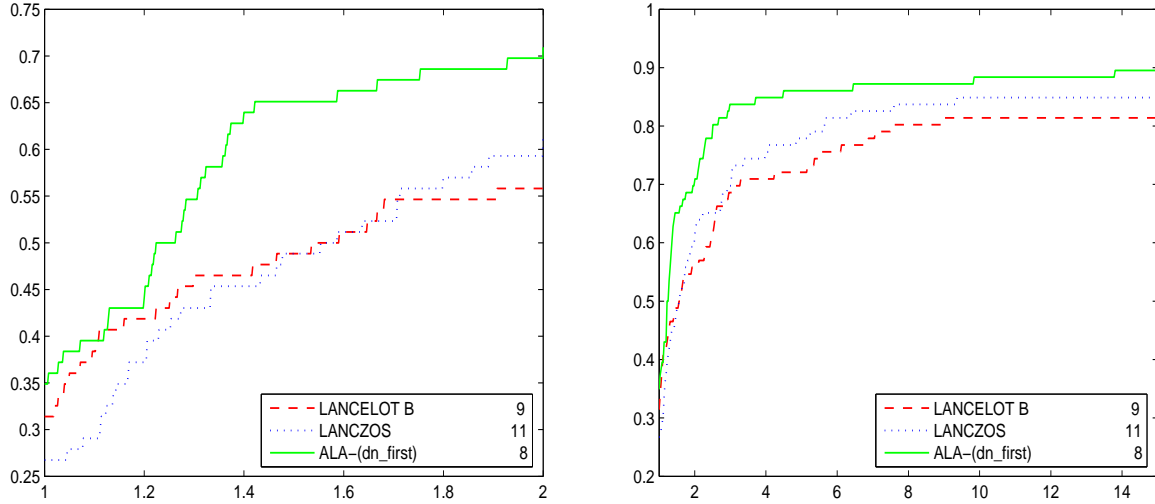


Figure 4.2: (*left*) Detail of the performance profile and (*right*) complete performance profile, on the comparison among LANCELOT B, the curvilinear Lanczos-based code in [13] and ALA. Here, the negative curvature direction s_k used in ALA is given by $s_k = \alpha_N p_N$, where p_N is simply the first conjugate direction computed by CG_gen, such that $p_N^T H_k p_N < 0$. The comparison refers to inner iterations.

Proof. By definition $\{x_k\} \supseteq \{x_{\ell(j)}\}$ and for every $j \geq 0$ we have $f(x_{\ell(j)}) = f_j$; consequently by (3.1) we have $f_j^M = \max_{0 \leq i \leq m(j)} f_{j-i}$, where $m(j) = \min[m(j-1) + 1, M]$, $m(0) = 0$. Therefore,

$$m(j+1) \leq m(j) + 1$$

and

$$\begin{aligned} f_{j+1}^M &= \max_{0 \leq i \leq m(j+1)} f(x_{\ell(j+1-i)}) \leq \max_{0 \leq i \leq m(j)+1} f(x_{\ell(j+1-i)}) = \\ &= \max \left\{ f(x_{\ell(j+1)}), \max_{0 \leq i \leq m(j)} f_{j-i} \right\} = \max \left\{ f(x_{\ell(j+1)}), f_j^M \right\}. \end{aligned}$$

Furthermore, since by the instructions of ALA $f(x_{\ell(j+1)}) < f_j^M$, the **Step 3.1** (b) and the previous relation yield

$$f_{j+1}^M \leq f_j^M \leq f_0^M = f(x_0), \quad (5.1)$$

which proves that $\{f_j^M\}$ is nonincreasing. Now observe that from (5.1) it is

$$x_{\ell(j)} \in \mathcal{L}_0, \quad (5.2)$$

therefore the nonincreasing sequence $\{f_j^M\}$ is bounded from below, hence

$$\lim_{j \rightarrow \infty} f_j^M = \hat{f}^M,$$

i.e. the point (1) is proved.

The point (2) follows from the relation $f(x_{\ell(h+1)}) < f_h^M$, and the fact that in relation (3.1) f_h^M is calculated considering at most M values of the objective function.

As regards the point (3), at first observe that (5.2) and the compactness assumption on \mathcal{L}_0 implies that a scalar $\gamma > 0$ exists, such that

$$\gamma = \sup_{x \in \mathcal{L}_0} \|x\|. \quad (5.3)$$

Now consider the points x_k such that $k \neq \ell(j)$, $\forall j$, i.e. those points where the objective function is not evaluated and which can be generated only at **Step 3.2** of ALA. Let \hat{j} be the largest index such that $\ell(\hat{j}) < k$. Then, since $\ell(j+1) - \ell(j) \leq N$, for all j , from the instructions of algorithm ALA an integer $\nu_k < N$ exists such that

$$x_k = x_{\ell(\hat{j})} + \sum_{h=0}^{\nu_k} d_{\ell(\hat{j})+h}. \quad (5.4)$$

Finally, since

$$f(x_{\ell(\hat{j})}) \leq f(x_{\ell(0)}) = f(x_0), \quad (5.5)$$

we have $x_{\ell(\hat{j})} \in \mathcal{L}_0$. Now, from (5.4), (5.5) and (5.3), and recalling that $\|d_{\ell(\hat{j})+h}\| \leq \Delta_0$

$$\|x_k\| \leq \gamma + N\Delta_0.$$

This proves the point (3), where

$$\bar{\mathcal{L}} = \left\{ y \in \mathbb{R}^n : \|y\| \leq \sup_{x \in \mathcal{L}_0} \{\|x\|\} + N\Delta_0 \right\},$$

which is a compact set by the assumptions. □

Let us consider now the following technical Lemma whose proof can be found in [12].

Lemma 5.2 *Suppose that the algorithm ALA determines the infinite sequence $\{x_k\}$ and let $\{x_{\ell(j)}\}$ be the sequence where the objective function $f(x)$ is evaluated. Let $q(k)$ be the index such that*

$$q(k) = \max \{j : \ell(j) \leq k\}. \quad (5.6)$$

Then a subsequence $\{x_{t(j)}\} \subseteq \{x_{\ell(j)}\}$ exists such that:

1. $f_j^M = f(x_{t(j)})$, $j=0,1, \dots$;
2. for any integer k the pair of indices h_k and j_k exists such that:

$$0 < h_k - k \leq N(M+1), \quad h_k = t(j_k), \quad (5.7)$$

$$f_{j_k}^M = f(x_{h_k}) < f_{q(k)}^M. \quad (5.8)$$

Lemma 5.3 *Suppose the algorithm ALA produces the infinite sequence $\{x_k\}$. Then, we have*

$$\lim_{k \rightarrow \infty} f(x_k) = \lim_{j \rightarrow \infty} f_j^M = \hat{f}^M. \quad (5.9)$$

Proof. For the proof we define the following three disjoint subsets of iteration indices $\mathcal{K}_i \subseteq \{1, 2, \dots\}$, $i = 1, 2, 3$:

$$\mathcal{K}_1 = \{k : \text{the iterate } x_{k+1} \text{ is calculated at **Step 3.2**}\}$$

$$\mathcal{K}_2 = \{k : \text{the iterate } x_{k+1} \text{ is calculated at **Step 3.3**}\}$$

$$\mathcal{K}_3 = \{k : \text{the iterate } x_{k+1} \text{ is calculated at **Step 2.2**}\}.$$

Suppose \mathcal{K}_1 is an infinite subset; by the test at **Step 3.2** we have

$$\|d_k\| \leq \delta^{p_k} \Delta_0 \quad k \in \mathcal{K}_1, \quad (5.10)$$

where

$$\lim_{k \rightarrow \infty, k \in \mathcal{K}_1} p_k = +\infty. \quad (5.11)$$

By defining $\alpha_k = 1$, $k \in \mathcal{K}_1$, from (5.10) and (5.11), considering that $\delta \in (0, 1)$ we obtain

$$\lim_{k \rightarrow \infty, k \in \mathcal{K}_1} \alpha_k \|d_k\| = 0. \quad (5.12)$$

Now, consider the indices $t(j)$ in the set $\{\ell(j), \ell(j) - 1, \dots, \ell(j) - m(j)\}$ and $q(k)$, which were defined in Lemma 5.2; we prove by induction that for any fixed integer $i \geq 1$ we have:

$$\lim_{j \rightarrow \infty} f(x_{t(j)-i}) = \lim_{j \rightarrow \infty} f(x_{t(j)}) = \lim_{j \rightarrow \infty} f_j^M = \hat{f}^M. \quad (5.13)$$

(Without loss of generality we assume that the index j is large enough to avoid the occurrence of negative subscripts.)

Suppose at first $i = 1$. If $t(j) - 1 \in \mathcal{K}_1$ then (5.12) yields

$$\lim_{j \rightarrow \infty, t(j)-1 \in \mathcal{K}_1} \|x_{t(j)} - x_{t(j)-1}\| = 0, \quad (5.14)$$

so that (5.13) holds from the uniform continuity of $f(x)$ over the compact set $\bar{\mathcal{L}}$.

If $t(j) - 1 \in \mathcal{K}_2$, the relation (3.5) becomes:

$$\begin{aligned} f_j^M &= f(x_{t(j)}) = f(x_{t(j)-1} + \alpha_{t(j)-1} d_{t(j)-1}) \leq \\ &\leq f_{q(t(j)-1)}^M + \mu \alpha_{t(j)-1} g(x_{t(j)-1})^T d_{t(j)-1} \end{aligned} \quad (5.15)$$

which yields

$$f_{q(t(j)-1)}^M - f_j^M \geq \mu \alpha_{t(j)-1} \left| g(x_{t(j)-1})^T d_{t(j)-1} \right|. \quad (5.16)$$

Thus, recalling the point (1) of Lemma 5.1 we obtain

$$\lim_{j \rightarrow \infty, t(j)-1 \in \mathcal{K}_2} \alpha_{t(j)-1} g(x_{t(j)-1})^T d_{t(j)-1} = 0,$$

so that from Proposition 2.1 along with relation $\alpha_{t(j)-1} \leq 1$, we obtain

$$\lim_{j \rightarrow \infty, t(j)-1 \in \mathcal{K}_2} \alpha_{t(j)-1} \|d_{t(j)-1}\| = 0. \quad (5.17)$$

Again, the uniform continuity of $f(x)$ over $\bar{\mathcal{L}}$ and relation (5.17) yield (5.13).

If $t(j) - 1 \in \mathcal{K}_3$, then

$$f_j^M = f(x_{t(j)}) \leq f(x_{t(j)-1}) + \mu \left(\alpha_{t(j)-1} g_{t(j)-1}^T s_{t(j)-1} + \frac{1}{2} \alpha_{t(j)-1}^2 s_{t(j)-1}^T H_{t(j)-1} s_{t(j)-1} \right), \quad (5.18)$$

therefore from Proposition 2.1 and considering that $s_k^T H_k s_k < 0$, (5.8) yields

$$f_j^M \leq f(x_{t(j)-1}) \leq f_{q(t(j)-1)}^M$$

so that taking the limit $j \rightarrow \infty$, $t(j) - 1 \in \mathcal{K}_3$, we obtain (5.13).

Suppose now that the relation (5.13) holds for the index i , i.e.

$$\lim_{j \rightarrow \infty} f(x_{t(j)-i}) = \hat{f}^M = \lim_{j \rightarrow \infty} f_j^M, \quad (5.19)$$

then we prove relation (5.13) for index $i + 1$. We consider again three cases.

If $t(j) - i - 1 \in \mathcal{K}_1$ then (5.12) yields

$$\lim_{j \rightarrow \infty, t(j)-i-1 \in \mathcal{K}_1} \|x_{t(j)-i} - x_{t(j)-i-1}\| = 0, \quad (5.20)$$

so that (5.13) holds for index $i + 1$ from the uniform continuity of $f(x)$ over the compact set $\bar{\mathcal{L}}$.

If $t(j) - i - 1 \in \mathcal{K}_2$, the relation (3.5) becomes:

$$f(x_{t(j)-i}) \leq f_{q(t(j)-i-1)}^M + \mu \alpha_{t(j)-i-1} g(x_{t(j)-i-1})^T d_{t(j)-i-1} \quad (5.21)$$

which yields

$$f_{q(t(j)-i-1)}^M - f(x_{t(j)-i}) \geq \mu \alpha_{t(j)-i-1} \left| g(x_{t(j)-i-1})^T d_{t(j)-i-1} \right|. \quad (5.22)$$

Thus, from (5.19) we obtain

$$\lim_{j \rightarrow \infty, t(j)-i-1 \in \mathcal{K}_2} \alpha_{t(j)-i-1} g(x_{t(j)-i-1})^T d_{t(j)-i-1} = 0,$$

so that from Proposition 2.1 along with relation $\alpha_{t(j)-i-1} \leq 1$, we have

$$\lim_{j \rightarrow \infty, t(j)-i-1 \in \mathcal{K}_2} \alpha_{t(j)-i-1} \|d_{t(j)-i-1}\| = 0. \quad (5.23)$$

Again, the uniform continuity of $f(x)$ over $\bar{\mathcal{L}}$ and relation (5.23) yield (5.13) for index $i + 1$.

If $t(j) - i - 1 \in \mathcal{K}_3$, then

$$f(x_{t(j)-i}) \leq f(x_{t(j)-i-1}) + \mu \left(\alpha_{t(j)-i-1} g_{t(j)-i-1}^T s_{t(j)-i-1} + \frac{1}{2} \alpha_{t(j)-i-1}^2 s_{t(j)-i-1}^T H_{t(j)-i-1} s_{t(j)-i-1} \right), \quad (5.24)$$

therefore from Proposition 2.1 and considering that $s_k^T H_k s_k < 0$, (5.8) yields

$$f(x_{t(j)-i}) \leq f(x_{t(j)-i-1}) \leq f_{q(t(j)-i-1)}^M$$

so that taking the limit $j \rightarrow \infty$, $t(j) - i - 1 \in \mathcal{K}_3$, from (5.19) we obtain (5.13) for index $i + 1$.

Finally, recalling relations (5.7) and (5.8) we can write for any index k

$$f(x_k) = f(x_{h_k}) - \sum_{i=0}^{h_k-k-1} [f(x_{h_k-i}) - f(x_{h_k-i-1})], \quad (5.25)$$

and from (5.13), taking the limit $k \rightarrow \infty$ we obtain

$$\lim_{k \rightarrow \infty} f(x_k) = \lim_{k \rightarrow \infty} f(x_{h_k}) = \hat{f}^M,$$

which is the final statement (5.9). □

Proof of Theorem 3.1

Proof. From the point (3) of Lemma 5.1 $x_k \in \bar{\mathcal{L}}$, for any $k \geq 0$, where $\bar{\mathcal{L}}$ is a compact set. Therefore, from Lemma 5.3 and relation (5.1) the sequence $\{x_k\}$ admits limit points in \mathcal{L}_0 . Now, let x^* be any limit point of $\{x_k\}$, and let $\{x_k\}_{\mathcal{K}}$ be a subsequence such that $\{x_k\}_{\mathcal{K}} \rightarrow x^*$. Consider the subsets \mathcal{K}_1 , \mathcal{K}_2 and \mathcal{K}_3 introduced in Lemma 5.3.

If the subsequence $\{x_k\}_{\mathcal{K} \cap \mathcal{K}_1}$ is infinite, from (5.12) and since $\alpha_k = 1$, we have

$$\lim_{k \rightarrow \infty, k \in \mathcal{K} \cap \mathcal{K}_1} \|d_k\| = 0. \quad (5.26)$$

Therefore relation (2.7) of Proposition 2.1 and the latter relation yield (a).

Suppose now that the subsequence $\{x_k\}_{\mathcal{K} \cap \mathcal{K}_2}$ is infinite. From (3.5)

$$\left| f_j^M - f(x_k + \alpha_k d_k) \right| \geq \mu \alpha_k g_k^T d_k,$$

so that from Lemma 5.1 and Lemma 5.3 $\left| f_j^M - f(x_k + \alpha_k d_k) \right| \rightarrow 0$; thus, two cases must be considered: either

$$\lim_{k \rightarrow \infty, k \in \mathcal{K} \cap \mathcal{K}_2} \alpha_k = 0 \quad (5.27)$$

or

$$\lim_{k \rightarrow \infty, k \in \mathcal{K} \cap \mathcal{K}_2} g_k^T d_k = 0. \quad (5.28)$$

In the first case an index \bar{k} exists such that $\alpha_k < 1$, $k > \bar{k}$, $k \in \mathcal{K} \cap \mathcal{K}_2$, and from (3.5) we have

$$f\left(x_k + \frac{\alpha_k}{\beta} d_k\right) > f_j^M + \frac{\alpha_k}{\beta} \mu g_k^T d_k \geq f(x_k) + \frac{\alpha_k}{\beta} \mu g_k^T d_k, \quad k \in \mathcal{K} \cap \mathcal{K}_2. \quad (5.29)$$

From the Mean Value Theorem $f[x_k + (\alpha_k/\beta)d_k] = f(x_k) + (\alpha_k/\beta)g(u_k)^T d_k$, for any $k > \bar{k}$, $u_k = x_k + \xi_k \alpha_k / \beta d_k$, $\xi_k \in [0, 1]$. Thus, since $\alpha_k > 0$, $\beta > 0$ we obtain from (5.29)

$$g(u_k)^T d_k > \mu g_k^T d_k, \quad k \in \mathcal{K} \cap \mathcal{K}_2, k > \bar{k}; \quad (5.30)$$

moreover as $k \rightarrow \infty$, $k \in \mathcal{K} \cap \mathcal{K}_2$, $x_k \rightarrow x^*$, $u_k \rightarrow x^*$. Recalling that $\mu \in (0, 1/2)$ the latter relation and (2.7) of Proposition 2.1 imply $g_k^T d_k \rightarrow 0$, $k \in \mathcal{K} \cap \mathcal{K}_2$, so that (5.27) implies (5.28).

In the second case if (5.28) holds, again (2.7) of Proposition 2.1 ensures that $g_k \rightarrow 0$, $k \in \mathcal{K} \cap \mathcal{K}_2$, which yields (a).

Finally suppose that the subsequence $\{x_k\}_{\mathcal{K} \cap \mathcal{K}_3}$ is infinite. From (3.3)

$$|f(x_{k+1}) - f(x_k)| \geq \mu \left| \alpha_k g_k^T s_k + \frac{1}{2} \alpha_k^2 s_k^T H_k s_k \right|, \quad k \in \mathcal{K} \cap \mathcal{K}_3,$$

so that Lemma 5.3 yields

$$\lim_{k \rightarrow \infty, k \in \mathcal{K} \cap \mathcal{K}_3} \left| \alpha_k g_k^T s_k + \frac{1}{2} \alpha_k^2 s_k^T H_k s_k \right| = 0;$$

therefore either

$$\lim_{k \rightarrow \infty, k \in \mathcal{K} \cap \mathcal{K}_3} \alpha_k = 0 \quad (5.31)$$

or (we recall that $g_k^T s_k \leq 0$ and $s_k^T H_k s_k \leq 0$)

$$\begin{cases} \lim_{k \rightarrow \infty, k \in \mathcal{K} \cap \mathcal{K}_3} g_k^T s_k = 0 \\ \lim_{k \rightarrow \infty, k \in \mathcal{K} \cap \mathcal{K}_3} s_k^T H_k s_k = 0. \end{cases} \quad (5.32)$$

If (5.31) holds we have from **Step 2.2**

$$f\left(x_k + \frac{\alpha_k}{\beta} s_k\right) - f(x_k) > \mu \left(\frac{\alpha_k}{\beta} g_k^T s_k + \frac{1}{2} \left(\frac{\alpha_k}{\beta}\right)^2 s_k^T H_k s_k \right), \quad k \in \mathcal{K} \cap \mathcal{K}_3,$$

and the Mean Value Theorem eventually gives

$$\frac{\alpha_k}{\beta} g_k^T s_k + \frac{1}{2} \left(\frac{\alpha_k}{\beta}\right)^2 s_k^T H(u_k) s_k > \mu \left(\frac{\alpha_k}{\beta} g_k^T s_k + \frac{1}{2} \left(\frac{\alpha_k}{\beta}\right)^2 s_k^T H_k s_k \right), \quad k \in \mathcal{K} \cap \mathcal{K}_3, \quad (5.33)$$

where $H(u_k) = H(x_k + \omega_k \alpha_k / \beta s_k)$, $\omega_k \in [0, 1]$. Now, from (5.33), Proposition 2.1 and considering that $s_k^T H_k s_k < 0$, for $k \in \mathcal{K} \cap \mathcal{K}_3$ we have

$$0 \leq (\mu - 1) \left[g_k^T s_k + \frac{1}{2} \frac{\alpha_k}{\beta} s_k^T H_k s_k \right] < \frac{1}{2} \frac{\alpha_k}{\beta} s_k^T [H(u_k) - H_k] s_k, \quad (5.34)$$

so that, since $\alpha_k \rightarrow 0$, $k \in \mathcal{K} \cap \mathcal{K}_3$, relation (5.34) yield

$$\lim_{k \rightarrow \infty, k \in \mathcal{K} \cap \mathcal{K}_3} g_k^T s_k + \frac{1}{2} \frac{\alpha_k}{\beta} s_k^T H_k s_k = 0,$$

so that

$$\lim_{k \rightarrow \infty, k \in \mathcal{K} \cap \mathcal{K}_3} g_k^T s_k = 0. \quad (5.35)$$

Furthermore, recalling that $g_k^T s_k \leq 0$ and $s_k^T H_k s_k \leq 0$, relation (5.34) yields

$$0 \leq \frac{1}{2} (\mu - 1) \frac{\alpha_k}{\beta} s_k^T H_k s_k \leq (\mu - 1) \left[g_k^T s_k + \frac{1}{2} \frac{\alpha_k}{\beta} s_k^T H_k s_k \right].$$

The latter relation along with relation (5.34) yield

$$\lim_{k \rightarrow \infty, k \in \mathcal{K} \cap \mathcal{K}_3} s_k^T H_k s_k = 0. \quad (5.36)$$

Therefore, recalling (5.35) and (5.36), condition (5.31) implies (5.32). Finally, for $k \in \mathcal{K} \cap \mathcal{K}_3$ Proposition 2.1 and relation $s_k^T H_k s_k < 0$ yield

$$\left| g_k^T s_k + \frac{1}{2} s_k^T H_k s_k \right| \geq c_2 \|g_k\|^2. \quad (5.37)$$

Thus, relations (5.35), (5.36) and (5.37) yield $g_k \rightarrow 0$, $k \in \mathcal{K} \cap \mathcal{K}_3$, which again proves (a).

In order to prove the point (b), suppose by contradiction that the subsequence $\{x_k\}_{\mathcal{K}}$ converges to the limit point x^* , with $g(x^*) = 0$ and $H(x^*) \not\prec 0$, i.e.

$$\lim_{k \rightarrow \infty, k \in \mathcal{K}} x_k = x^*, \quad g(x^*) = 0 \quad \text{and} \quad H(x^*) \prec 0. \quad (5.38)$$

Then, from (5.38) and *ii*) of Proposition 2.2 an index $\bar{k} \in \mathcal{K}$ exists such that for $k > \bar{k}$ and $k \in \mathcal{K}$ then

$$q(x_k + s_k) < -\tilde{\epsilon}/4, \quad (5.39)$$

where $\tilde{\epsilon}$ was defined in Assumption 2. On the other hand, from the Proposition 2.1 and (5.38) we have

$$\lim_{k \in \mathcal{K}} q(x_k + d_k) = 0,$$

so that for $k > \bar{k}$ and $k \in \mathcal{K}$ then

$$q(x_k + s_k) < q(x_k + d_k).$$

This implies that for $k > \bar{k}$ and $k \in \mathcal{K}$ then $k \in \mathcal{K}_3$. Finally, recalling (5.35)-(5.36) we obtain a contradiction with (5.39), since

$$-\frac{\tilde{\epsilon}}{4} > \lim_{k \rightarrow \infty, k \in \mathcal{K} \cap \mathcal{K}_3} q(x_k + s_k) = 0.$$

□

References

- [1] R. S. Dembo and T. Steihaug. Truncated-Newton algorithms for large-scale unconstrained optimization, *Mathematical Programming*, 26:190–212, 1983.
- [2] E. D. Dolan and J. J. Moré. Benchmarking Optimization Software with Performance Profiles, Mathematics and Computer Science Division, Preprint ANL/MCS-P861-1200.
- [3] G. Fasano and M. Roma. Iterative Computation of Negative Curvature Directions in Large Scale Optimization, *Computational Optimization and Applications*, 38(1):81–104, 2007.
- [4] M. C. Ferris, S. Lucidi and M. Roma. Nonmonotone curvilinear linesearch methods for unconstrained optimization, *Computational Optimization and Applications*, 6:117–136, 1996.
- [5] A. Forsgren. On the Behavior of the Conjugate-Gradient Method on Ill-conditioned Problems, Technical Report TRITA-MAT-2006-OS1, Department of Mathematics, Royal Institute of Technology.
- [6] D. Goldfarb. Curvilinear path steplength algorithms for minimization which use directions of negative curvature, *Mathematical Programming*, 18:31–40, 1980.
- [7] N. I. M. Gould, S. Lucidi, M. Roma and Ph. L. Toint. Exploiting Negative Curvature Directions in Linesearch Methods for Unconstrained Optimization, *Optimization Methods and Software*, 14:75–98, 2000.
- [8] N. I. M. Gould, D. Orban and Ph. L. Toint. CUTEr: Constrained and unconstrained testing environment, revised, *Transactions of the ACM on Mathematical Software*, 29(4):353–372, 2003.
- [9] N. I. M. Gould, D. Orban and Ph. L. Toint. GALAHAD, a library of thread-safe Fortran 90 packages for large-scale nonlinear optimization, *ACM Trans. Math. Software*, 29(4):353–372, 2004.

- [10] N. I. M. Gould, C. Sainvitu and Ph. L. Toint. A Filter-Trust-Region Method for Unconstrained Optimization, *SIAM Journal on Optimization*, 16(2):341–357, 2005.
- [11] L. Grippo, F. Lampariello and S. Lucidi. A truncated Newton method with nonmonotone linesearch for unconstrained optimization, *Journal of Optimization Theory and Applications*, 60:401–419, 1989.
- [12] L. Grippo, F. Lampariello and S. Lucidi. A class of nonmonotone stabilization methods in unconstrained optimization, *Numer. Math.*, 59:779-805, 1991.
- [13] S. Lucidi, F. Rochetich and M. Roma. Curvilinear stabilization techniques for truncated Newton methods in large scale unconstrained optimization, *SIAM Journal on Optimization*, 8:916–939, 1998.
- [14] S. Lucidi and M. Roma. Numerical experiences with new truncated Newton methods in large scale unconstrained optimization, *Computational Optimization and Applications*, 7:71–87, 1997.
- [15] G. P. McCormick. A Modification of Armijo’s Stepsize Rule for Negative Curvature, *Mathematical Programming*, 13:111-115, 1977.
- [16] J. J. More’ and D. C. Sorensen. On the Use of Directions of Negative Curvature in a Modified Newton Method, *Mathematical Programming*, 16:1-20, 1979.
- [17] H. Mukai and E. Polak. A second-order method for unconstrained optimization, *Journal of Optimization Theory and Applications*, 26:501–513, 1978.
- [18] S. G. Nash and A. Sofer. Assessing a Search Direction within a Truncated Newton Method, *Operations Research Letters*, 9:219–221, 1990.
- [19] G. A. Shultz, R. B. Schnabel and R. H. Byrd. A family of trust-region-based algorithms for unconstrained minimization, *SIAM Journal on Numerical Analysis*, 22:47–67, 1985.

ALA (Adaptive Linesearch Algorithm)

Step 0. **Choose** $x_0 \in \mathbb{R}^n$, $\beta \in (0, 1)$, $\Delta_0 > 0$, $\delta \in (0, 1)$, $N > 0$, $M \geq 0$, $\mu \in (0, \frac{1}{2})$.
Set $k = \ell = j = 0$, $\Delta = \Delta_0$, $f_0^M = f_0 = f(x_0)$.

Step 1. **Computation and choice of the search direction.** If direction d_k is chosen in **Scheme 2** then execute Step 2, otherwise execute Step 3.

Step 2. **Linesearch along the negative curvature direction.**

Step 2.1. **Check on the function.** If $k \neq \ell$ compute $f(x_k)$ and
if $f(x_k) \geq f_j^M$, backtrack to x_ℓ , set $d_k = d_\ell$ and go to Step 3.3;
else, set $j = j + 1$, $\ell(j) = k$, $f_j = f(x_k)$ and update f_j^M by

$$f_j^M = \max_{0 \leq i \leq m(j)} f_{j-i}, \quad \text{where } m(j) = \min\{m(j-1) + 1, M\}; \quad (3.1)$$

Step 2.2. **Monotone linesearch.** Choose $\sigma_k > 0$. If

$$f(x_k + \sigma_k s_k) \leq f(x_k) + \mu \left(\sigma_k g_k^T s_k + \frac{1}{2} \sigma_k^2 s_k^T H_k s_k \right), \quad (3.2)$$

then set $\alpha_k = \beta^h \sigma_k$, where h is the largest non-positive integer such that

$$f(x_k + \alpha_k s_k) \leq f(x_k) + \mu \left(\alpha_k g_k^T s_k + \frac{1}{2} \alpha_k^2 s_k^T H_k s_k \right) \quad (3.3)$$

$$f\left(x_k + \frac{\alpha_k}{\beta} s_k\right) > f(x_k) + \mu \left(\frac{\alpha_k}{\beta} g_k^T s_k + \frac{1}{2} \left(\frac{\alpha_k}{\beta}\right)^2 s_k^T H_k s_k \right) \quad (3.4)$$

otherwise set $\alpha_k = \beta^h \sigma_k$, where h is the smallest positive integer such that (3.3) holds.
Set $x_{k+1} = x_k + \alpha_k s_k$, $k = k + 1$, $j = j + 1$, $\ell(j) = k$, $f_j = f(x_k)$, update f_j^M by (3.1) and go to Step 1.

Step 3. **Linesearch along the Truncated Newton direction.**

Step 3.1. **Function control every N steps.** If $k = \ell + N$ compute $f(x_k)$ then:
if $f(x_k) \geq f_j^M$, backtrack to x_ℓ , set $d_k = d_\ell$ and go to Step 3.3;
else, set $j = j + 1$, $\ell(j) = k$, $f_j = f(x_k)$ and update f_j^M by (3.1).

Step 3.2. **Test for acceptance.** If $\|d_k\| \leq \Delta$, set $x_{k+1} = x_k + d_k$, $k = k + 1$, $\Delta = \delta \Delta$
and go to Step 1; otherwise, if $k \neq \ell$ compute $f(x_k)$ and
if $f(x_k) \geq f_j^M$, backtrack to x_ℓ , set $d_k = d_\ell$ and go to Step 3.3;
else set $j = j + 1$, $\ell(j) = k$, $f_j = f(x_k)$ and update f_j^M by (3.1).

Step 3.3. **Nonmonotone linesearch.** Set $\alpha_k = \beta^h$ where h is the smallest nonnegative integer such that

$$f(x_k + \alpha_k d_k) \leq f_j^M + \alpha_k \mu g_k^T d_k, \quad (3.5)$$

set $x_{k+1} = x_k + \alpha_k d_k$, $k = k + 1$, $j = j + 1$, $\ell(j) = k$, $f_j = f(x_k)$, update f_j^M by (3.1) and go to Step 1.

Table 3.1: The algorithm ALA (Adaptive Linesearch Algorithm).

ARGLINA	200	ARGLINB	200	ARGLINC	200	ARWHEAD	5000	BDQRTIC	5000
BROWNAL	200	BRYBND	5000	CHAINWOO	4000	CLPLATEA	9900	CLPLATEB	4970
CLPLATEC	4970	COSINE	10000	CRAGGLVY	5000	CURLY10	10000	CURLY20	10000
CURLY30	1000	DIXMAANA	9000	DIXMAANB	9000	DIXMAANC	9000	DIXMAAND	9000
DIXMAANE	9000	DIXMAANF	9000	DIXMAANG	9000	DIXMAANH	9000	DIXMAANI	9000
DIXMAANJ	9000	DIXMAANK	9000	DIXMAANL	9000	DIXON3DQ	10000	DQDRTIC	5000
DQRTIC	5000	EDENSCH	10000	EG2	1000	EIGENALS	2550	EIGENBLS	2550
EIGENCLS	2652	ENGVAl1	10000	EXTROSNB	1000	FMINSRF2	5625	FMINSURF	49
FREUROTH	5000	GENROSE	500	HYDC20LS	99	LIARWHD	5000	LMINSURF	5329
MANCINO	100	MOREBV	5000	MSQRTALS	1024	MSQRTBLS	1024	NCB20	5010
NCB20B	5000	NLMSURF	5329	NONCVXU2	5000	NONCVXUN	5000	NONDIA	5000
NONDQUAR	5000	NONMSQRT	100	ODC	4900	PENALTY1	1000	PENALTY2	200
PENALTY3	120	POWELLSG	5000	POWER	100	QUARTC	5000	RAYBENDL	2046
RAYBENDL	2046	RAYBENDS	2046	SBRYBND	500	SCHMVETT	5000	SCOSINE	5000
SCURLY10	100	SCURLY20	100	SCURLY30	100	SENSORS	100	SINQUAD	10000
SPARSINE	5000	SPARSQR	10000	SPMSRTLS	4900	SROSENBR	5000	SSC	4900
TESTQUAD	5000	TOINTGSS	5000	TQUARTIC	5000	TRIDIA	5000	VARDIM	200
VAREIGVL	50	WOODS	10000						

Table 4.1: List of our test problems from CUTEr [8].