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Nonmonotone algorithm for minimization on closed sets with applications to minimization on Stiefel manifolds

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ABSTRACT

A nonmonotone Levenberg–Marquardt-based algorithm is proposed for minimization problems on closed domains. By preserving the feasible set's geometry throughout the process, the method generates a feasible sequence converging to a stationary point independently of the initial guess. As an application, a specific algorithm is derived for minimization on Stiefel manifolds and numerical results involving a weighted orthogonal Procrustes problem are reported.

1. Introduction

Constrained optimization problems play an important role in numerous applications in science and engineering. All practical methods for these problems are iterative and generate a (feasible) sequence of iterates hopefully approximating a (local) extremum of the objective function. In this paper, we are concerned with the problem

$$\begin{aligned} &\text{minimize} && f(x) \\ &\text{s.t.} && x \in \Gamma, \end{aligned} \tag{1}$$

where Γ is closed and $f : \mathbb{R}^n \to \mathbb{R}$ is a continuously differentiable function defined on an open convex set Γ_c that contains Γ.

We introduce a new algorithm for (1), which can be viewed as a Levenberg–Marquardt variation of the method devised by Birgin et al. in [1] for the case when Γ is convex. The idea behind the algorithm presented here is to compute a trial point by solving the subproblem

$$\begin{aligned} &\text{minimize} && Q_\rho(x) \equiv \langle \nabla f(y), x - y\rangle + \frac{1}{2}(x-y)^T(B + \rho A)(x-y) \\ &\text{s.t.} && x \in \Gamma, \end{aligned} \tag{2}$$

where $\rho > 0$ is a regularization parameter and $A, B \in \mathbb{R}^{n\times n}$ are symmetric matrices which may vary at every iteration, and A is positive definite. Once the subproblem (2) is solved, the decision to accept or reject the trial point will depend

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on whether the decrease of the objective function (with respect to a proper iterated) is meaningful when compared to the predicted reduction of the quadratic model. A globally convergent algorithm for the electronic structure calculation problem which solves (2) at each iteration within a monotone trust-region framework is proposed in [2]. In the present work, our algorithm extends the ideas of [2] to more general optimization problems and convergence to stationary points is obtained by incorporating a nonmonotone trust-region-like framework into the scheme. Besides, we include a rigorous globally convergence proof which does not require a regularity assumption used in [2]. As far as we know, nonmonotone line search approaches were first introduced in [3] in connection with a Newton-like method. Afterward, several more papers have appeared highlighting the efficacy of the procedure for unconstrained and constrained problems. For further contributions concerning nonmonotone strategies the reader is referred to [1,4–8] and references therein. Despite the extensive literature, we emphasize that nonmonotone schemes for minimization on arbitrary closed sets have not been sufficiently investigated so far.

Summarizing, our algorithm generates a feasible sequence such that all of its accumulation points are stationary points of (1) irrespective of the initial approximation chosen. With respect to its potentiality, a globally convergent nonmonotone gradient-like scheme for minimization on Stiefel manifolds is proposed and verified through numerical tests involving a weighted orthogonal Procrustes problem.

This paper is organized as follows. In Section 2 we include preliminary material and describe our algorithm. Section 3 is concerned with the theoretical analysis of the method; a global convergence proof is done there. Section 4 states a globally convergent method for minimization on Stiefel manifolds including numerical results on the weighted orthogonal Procrustes problem that verify the theoretical properties of the algorithm. The paper ends with some conclusions in Section 5.

Notation. The gradient of f will be denoted by g, that is, $g(x) = \nabla f(x)$. For all function $\beta : [a, b] \to \mathbb{R}^n$, $\beta \in C^1[a, b]$ means that β is a continuously differentiable function in the interval $[a, b]$. $\mathbb{N} = \{0, 1, 2, \ldots\}$. Assuming $K \subseteq \mathbb{N}$ is an infinite subset of $\mathbb{N}$, $K_1 \subseteq^{\infty} K$ means that K_1 is an infinite set as well. Additionally, if $\{x^k\}_{k\in K_1}$ is an infinite sequence, $\lim_{k\in K_1} x^k$ denotes $\lim_{k\to\infty} x^k$ restricted to $k \in K_1$. Throughout this paper $\|\cdot\|$ denotes the euclidean norm in $\mathbb{R}^n$, $\langle\cdot,\cdot\rangle$ the euclidean inner product and $\|\cdot\|_F$ the Frobenius norm in $\mathbb{R}^{m\times n}$. Assuming $A \in \mathbb{R}^{n\times n}$, $\mathrm{Tr}(A)$ means the trace of matrix A and $\mathrm{diag}(A) \in \mathbb{R}^n$ means its diagonal.

2. Preliminaries and model algorithm

We start by recalling the well-known definition of stationary points through feasible arcs.

Definition 1. Given $x \in \Gamma$ and $b > 0$, $\alpha : [0, b] \to \mathbb{R}^n$ is said to be a feasible arc emanating from x if $\alpha(t) \in \Gamma$ for all $t \in [0, b]$, $\alpha \in C^1[0, b]$, $\alpha(0) = x$ and $\alpha'(0) \neq 0$. Furthermore, a point $x^* \in \Gamma$ is a *stationary point* of (1) if and only if all feasible arc α emanating from x^* satisfies $\langle \nabla f(x^*), \alpha'(0)\rangle \geq 0$.

The following result provides a connection between local minimizers of (1) and the definition above. Its proof can be easily checked and is omitted.

Theorem 1. *If $x^* \in \Gamma$ is a local minimizer of (1), it is a stationary point.*

Throughout the paper we denote:

$$\mathbb{S}_n = \{A \in \mathbb{R}^{n\times n} \mid A^T = A\}, \qquad \mathbb{S}_n^+ = \{A \in \mathbb{S}_n \mid x^T Ax > 0 \text{ for all } x \in \mathbb{R}^n\}.$$

In addition g is assumed to be Lipschitz continuous in Γ_c, that is, there exists $L_f > 0$ such that

$$\|g(y) - g(x)\| \leq L_f \|y - x\|, \quad \forall x, y \in \Gamma_c. \tag{3}$$

Hence

$$|f(y) - f(x) - \langle g(x), y - x\rangle| = \left| \int_0^1 \langle g(x + t(y - x)) - g(x), y - x\rangle dt \right| \leq \frac{L_f}{2}\|y - x\|^2,$$

and thus

$$f(y) \leq f(x) + \langle g(x), y - x\rangle + \frac{L_f}{2}\|y - x\|^2, \quad \forall x, y \in \Gamma_c. \tag{4}$$

We note that assumption (3) can be verified in a wide class of applications, for instance, when the Hessian of f is bounded or twice continuously differentiable and Γ compact.

Since our algorithm works within a nonmonotone framework, we consider $\mathcal{M} \in \mathbb{N}$, $m(0) = 0$ and, for every $k \geq 1$, we set

$$0 \leq m(k) \leq \min\{m(k - 1) + 1, \mathcal{M}\}.$$

Therefore, assuming $\{x^{k-j}\}_{j=0}^{m(k)} \subseteq \Gamma$, we define

$$f_{\max}^k = \max\{f(x^{k-j}) \mid j \in \{0, 1, \ldots, m(k)\}\} \tag{5}$$

and $\nu(k) \in \{k - m(k), \ldots, k - 1, k\}$ such that $f(x^{\nu(k)}) = f_{\max}^k$.

The proposed algorithm is described as follows.

Algorithm 1. Let $x^0 \in \Gamma$ be an arbitrary initial point. The parameters set for the execution of the algorithm are: $\eta \in (0, 1]$, $\mathcal{M} \in \mathbb{N}$, $\beta_1 \in (0, \frac{1}{2}]$, $L_u \geq L_f$, $\rho_{\text{bound}} > 0$, $0 < \rho_{\min} \leq \rho_{\max} < +\infty$ and $1 < \zeta_1 \leq \zeta_2 < +\infty$.
Set $k \leftarrow 0$.

Step 1. Compute $f(x^{v(k)})$ as in (5), $g(x^k)$ and set $\rho \in [\rho_{\min}, \rho_{\max}]$.
Step 2. If $\rho \leq \rho_{\text{bound}}$, pick $B_\rho^k \in \mathbb{S}_n$ and $A_\rho^k \in \mathbb{S}_n^+$; otherwise, set $B_\rho^k = L_u I$ and $A_\rho^k = I$.
Step 3. Compute $\bar{x}_\rho^k$, the global solution of

$$\begin{aligned} \text{minimize} \quad & Q_\rho^k(x) \\ \text{s.t.} \quad & x \in \Gamma, \end{aligned} \tag{6}$$

where $Q_\rho^k(x)$ denotes the quadratic defined in (2) with $y = x^k$, $B = B_\rho^k$ and $A = A_\rho^k$.
Step 4. Compute $x_\rho^k \in \Gamma$ such that $Q_\rho^k(x_\rho^k) \leq \eta Q_\rho^k(\bar{x}_\rho^k)$.
If $Q_\rho^k(x_\rho^k) = 0$, terminate the execution setting x_ρ^k as a stationary point of (1).
Step 5. Define

$$\Psi_k(x) = \langle g(x^k), x - x^k \rangle + \frac{1}{2}(x - x^k)^T B_\rho^k (x - x^k), \tag{7}$$

$\text{Ared}_\rho^k = (f(x^{v(k)}) - f(x_\rho^k))$ and $\text{Pred}_\rho^k = -\Psi_k(x_\rho^k)$.
If

$$\frac{\text{Ared}_\rho^k}{\text{Pred}_\rho^k} \geq \beta_1, \tag{8}$$

define $\rho^k = \rho$, $x^{k+1} = x_\rho^k$, set $k \leftarrow k + 1$ and go back to Step 1.
Else, choose $\rho_{\text{new}} \in [\zeta_1 \rho, \zeta_2 \rho]$, set $\rho = \rho_{\text{new}}$ and go back to Step 2.

It is worth mentioning that the choice $\eta < 1$ in Algorithm 1 corresponds to the case when subproblem (6) is solved inexactly. This choice, firstly introduced in [1], is suitable for problems where global solutions of (6) are difficult to compute. Independently of which η is chosen, we shall assume that $\bar{x}_\rho^k$ computed at Step 3 is well defined for each k and ρ. Such an assumption clearly will depend on the set Γ and the choice of matrices B_ρ^k and A_ρ^k. Also, note that if $H^k = (B_\rho^k + \rho A_\rho^k)$ is assumed to be symmetric definite positive (which holds for ρ large enough), there exists a invertible matrix G such that $H^k = GG^T$ (e.g., the Cholesky factorization of H^k). Hence, subproblem (2) reduces to the more friendly constrained least squares problem

$$\min \|G^T x - (G^T x^k - G^{-1}\nabla f(x^k))\|^2 \quad \text{subject to } x \in \Gamma, \tag{9}$$

which can be handled efficiently in several cases. For example, if $\Gamma = \mathcal{O}_n$, the set of $n \times n$ orthogonal matrices, using the thin SVD of $(H^k X^k - \nabla f(X^k))$ one can determine a closed-form solution to (9) (see, e.g., [9]) and the proposed algorithm can be employed to minimize functions over the set of orthogonal matrices. Another example for which (9) has a known closed-form solution is when $\Gamma = \mathbb{S}_n$, (the set of symmetric matrices); the reader is referred to [10] for details.

3. Convergence analysis

In this section we will discuss the theoretical properties of Algorithm 1. Specifically, we will show convergence of the iterated sequence to stationary points of (1), irrespective of the starting point chosen. Let the subsets of matrices chosen at Step 2 be denoted by $\mathbb{B} = \{B_\rho^k\}$ and $\mathbb{A}^+ = \{A_\rho^k\}$ respectively. Our analysis relies on the following assumptions:

A1. $\Gamma^0 = \{x \in \Gamma \mid f(x) \leq f(x^0)\}$ is a bounded subset.
A2. The subsets $\mathbb{B}$ and $\mathbb{A}^+$ are uniformly bounded, that is, there exists $\widetilde{M} > 0$ such that $\|B_\rho^k\|_F \leq \widetilde{M}$ and $\|A_\rho^k\|_F \leq \widetilde{M}$, for all k and ρ.
A3. There exists $\gamma > 0$ such that $x^T A x \geq \gamma \|x\|^2$ for all $A \in \mathbb{A}^+$ and $x \in \mathbb{R}^n$.

Assumption A1 is a standard hypothesis used in nonlinear programming to ensure that a minimum value is reached in Γ^0 as well as to ensure that any sequence in Γ^0 possesses at least one accumulation point. As for A2 and A3, they are mild user-controlled assumptions introduced to maintain stability of the iterates, that is essential for our convergence result.

Lemma 1. *If $A \in \mathbb{A}^+$, then A is a symmetric positive definite matrix and $\gamma \|x\|^2 \leq x^T A x \leq \widetilde{M} \|x\|^2$ $\forall x \in \mathbb{R}^n$.*

Proof. The proof follows from the spectral decomposition of matrix A. □

Since Q_ρ^k has the same gradient as f at x^k and since $Q_\rho^k(x_\rho^k) \leq \eta Q_\rho^k(\bar{x}_\rho^k) \leq 0$, it follows that $Q_\rho^k(x_\rho^k) < 0$ whenever x^k is not a stationary point of (1). Therefore, either Algorithm 1 stops at Step 4 in a stationary point of (1) or infinitely many iterates x^k are generated. Therefore, without loss of generality, from now on we assume $\{x^k\}$ to be an infinite sequence.

Lemma 2. *Sequence $\{f(x^{\nu(k)})\}_{k\in\mathbb{N}}$ is monotone nonincreasing.*

Proof. From the definition of $f(x^{\nu(k)})$ it follows that

$$\begin{aligned} f(x^{\nu(k+1)}) &= \max\{f(x^{k+1-j}) \mid j \in \{0, 1, \ldots, m(k+1)\}\} \\ &= \max\{f(x^{k+1}), \max\{f(x^{k-j}) \mid j \in \{0, \ldots, m(k+1)-1\}\}\} \\ &\leq \max\{f(x^{k+1}), f(x^{\nu(k)})\}. \end{aligned}$$

Also, since $\text{Ared}_{\rho^k}^k/\text{Pred}_{\rho^k}^k \geq \beta_1$, we have that $f(x^{k+1}) \leq f(x^{\nu(k)}) + \beta_1\Psi_k(x^{k+1}) < f(x^{\nu(k)})$, which leads to $f(x^{\nu(k+1)}) \leq f(x^{\nu(k)})$, and the lemma is proved. □

Lemma 3. *Sequence $\{x^k\} \subset \Gamma^0$.*

Proof. We will prove by induction on k. Note that for all $k \in \mathbb{N}$, $\text{Ared}_{\rho^k}^k \geq \beta_1\text{Pred}_{\rho^k}^k$, leads to $f(x^{k+1}) \leq f(x^{\nu(k)}) + \beta_1\Psi_k(x^{k+1})$. Thus, $f(x^1) \leq f(x^0) + \beta_1\Psi_1(x^1) \leq f(x^0)$, that is, $x^1 \in \Gamma^0$. If by inductive hypothesis we assume $f(x^i) \in \Gamma^0$, for $0 \leq i \leq j$, then we obtain $f(x^{j+1}) \leq f(x^{\nu(j)}) + \beta_1\Psi_k(x^{j+1}) < f(x^{\nu(j)})$. But, since $j - m(j) \leq \nu(j) \leq j$, then $f(x^{j+1}) < f(x^{\nu(j)}) \leq f(x^0)$. Therefore, $x^{j+1} \in \Gamma^0$ and the proof is complete. □

Using Lemma 3 and Assumption A1 we note that the sequence $\{x^k\}$ admits at least one accumulation point.

The next result deals with the well-definiteness of the Algorithm 1. More precisely, it states that a single iteration of the algorithm finishes after a finite number of cycles.

Theorem 2. *If $x^k \in \Gamma$ is not a stationary point and $\rho > \rho_{\text{bound}}$, then condition (8) is fulfilled.*

Proof. Assume $\rho > \rho_{\text{bound}}$. From Step 2 we have that $Q_\rho^k(x) = \langle g(x^k), x - x^k\rangle + (L_u + \rho)/2\|x - x^k\|^2$ and $\Psi_k(x) = \langle g(x^k), x - x^k\rangle + L_u/2\|x - x^k\|^2$. Hence, from (4) and recalling x_ρ^k from (1), it follows that

$$\begin{aligned} f(x_\rho^k) &\leq f(x^k) + \langle g(x^k), x_\rho^k - x^k\rangle + L_f/2\|x_\rho^k - x^k\|^2 \\ &\leq f(x^k) + \Psi_k(x_\rho^k) \leq f(x^{\nu(k)}) + \Psi_k(x_\rho^k). \end{aligned}$$

Now since $\bar{x}_\rho^k$ solves (6) and $\beta_1 \in (0, 1)$, we have that $\Psi_k(x_\rho^k) \leq \eta\Psi_k(\bar{x}_\rho^k) < 0$ and thus $f(x_\rho^k) \leq f(x^{\nu(k)}) + \beta_1\Psi_k(x_\rho^k)$. Therefore, $\text{Ared}_\rho^k \geq \beta_1\text{Pred}_\rho^k$ whenever $\rho > \rho_{\text{bound}}$. □

Lemma 4. *Sequence $\{\rho^k\}$ is bounded.*

Proof. From Theorem 2, for all $\rho > \rho_{\text{bound}}$ condition (8) is fulfilled and then the loop finishes after a finite number of cycles. Hence, the largest ρ possible at Step 2 is $\zeta_2\rho_{\text{bound}}$ and, consequently, $0 \leq \rho^k \leq \zeta_2\rho_{\text{bound}}$ for all k. □

The main result of this section comes in the following theorem.

Theorem 3. *Let x^* be an accumulation point of the sequence generated by Algorithm 1. Then, x^* is a stationary point of (1).*

For the proof of this theorem we need some technical results.

Lemma 5. *Assume that $\mathcal{K} \subseteq^\infty \mathbb{N}$ and $\lim_{k\in\mathcal{K}} \Psi_k(x^{k+1}) = 0$. Then, $\lim_{k\in\mathcal{K}} \|x^{k+1} - x^k\| = 0$.*

Proof. Since $Q_{\rho^k}^k(x^{k+1}) \leq \eta Q_{\rho^k}^k(\bar{x}_{\rho^k}^k)$, where $\bar{x}_{\rho^k}^k$ is the global minimizer of subproblem (6), then $Q_{\rho^k}^k(x^{k+1}) = \langle g(x^k), x^{k+1} - x^k\rangle + 1/2(x^{k+1} - x^k)^T(B_{\rho^k}^k + \rho^k A_{\rho^k}^k)(x^{k+1} - x^k) < 0$. Consequently, from Lemma 1,

$$\begin{aligned} 0 &< \frac{1}{2}\rho_{\min}\gamma\|x^{k+1} - x^k\|^2 \leq \frac{\rho^k}{2}(x^{k+1} - x^k)^T A_{\rho^k}^k(x^{k+1} - x^k) \\ &< -\langle g(x^k), x^{k+1} - x^k\rangle - \frac{1}{2}(x^{k+1} - x^k)^T B_{\rho^k}^k(x^{k+1} - x^k) = -\Psi_k(x^{k+1}). \end{aligned}$$

Since $\lim_{k\in\mathcal{K}} \Psi_k(x^{k+1}) = 0$, it follows that $\lim_{k\in\mathcal{K}} \|x^{k+1} - x^k\| = 0$, and the proof is complete. □

Lemma 6. *Assume that $\widehat{K} \subseteq^\infty \{\nu(k)\}_{k\in\mathbb{N}}$. Then, for any $j \in \mathbb{N}$,*

$$\lim_{k\in\widehat{K}} \|x^{k-(j-1)} - x^{k-j}\| = 0 \quad \text{and} \quad \lim_{k\in\widehat{K}} f(x^{k-j}) = \lim_{k\to\infty} f(x^{\nu(k)}). \tag{10}$$

Proof. From Lemma 2, $\{f(x^{\nu(k)})\}_{k\in\mathbb{N}}$ is a monotone nonincreasing bounded sequence. Then, $\lim_{k\to\infty} f(x^{\nu(k)})$ exists and $\lim_{k\in\widehat{K}} f(x^k) = \lim_{k\to\infty} f(x^{\nu(k)})$. In a proof by induction, we note that for any $k \in \widehat{K}$, $f(x^k) \leq f(x^{\nu(k-1)}) + \beta_1\Psi_{k-1}(x^k)$, and consequently, $\lim_{k\in\widehat{K}} \Psi_{k-1}(x^k) = 0$. From Lemma 5, it follows that $\lim_{k\in\widehat{K}} \|x^k - x^{k-1}\| = 0$. Furthermore, since f is a uniformly continuous function in Γ^0, then $\lim_{k\in\widehat{K}} f(x^{k-1}) = \lim_{k\in\widehat{K}} f(x^k) = \lim_{k\to\infty} f(x^{\nu(k)})$. Now assume that (10) holds for a fixed j and note that $f(x^{k-j}) \leq f(x^{\nu(k-(j+1))}) + \beta_1\Psi_{k-(j+1)}(x^{k-j})$. Also, by induction hypothesis we have $\lim_{k\in\widehat{K}} f(x^{k-j}) = \lim_{k\to\infty} f(x^{\nu(k)}) = \lim_{k\in\widehat{K}} f(x^{\nu(k-(j+1))})$. Hence, since $\Psi_{k-(j+1)}(x^{k-j}) < 0$, we have that $\lim_{k\in\widehat{K}} \Psi_{k-(j+1)}(x^{k-j}) = 0$. Thus, from Lemma 5, $\lim_{k\in\widehat{K}} \|x^{k-j} - x^{k-(j+1)}\| = 0$. Hence, by using the induction hypothesis and the uniform continuity of f in Γ^0 we complete the proof. □

The next lemma is proved by arguments analogous to those given in [3].

Lemma 7. $\lim_{k\to\infty} f(x^k) = \lim_{k\to\infty} f(x^{\nu(k)})$.

Proof. We define $\widehat{\nu}(k) = \{\nu(k+\mathcal{M}+2)\}_{k\in\mathbb{N}}$ and $\widehat{K} = \{\widehat{\nu}(k)\}_{k\in\mathbb{N}} \subseteq^{\infty} \{\nu(k)\}_{k\in\mathbb{N}}$. Furthermore, $x^{k+1} = x^{\widehat{\nu}(k)} + \sum_{i=1}^{\widehat{\nu}(k)-(k+1)} (x^{\widehat{\nu}(k)-i} - x^{\widehat{\nu}(k)-(i-1)})$. Therefore, $\|x^{k+1} - x^{\widehat{\nu}(k)}\| \leq \sum_{i=1}^{\widehat{\nu}(k)-(k+1)} \|x^{\widehat{\nu}(k)-i} - x^{\widehat{\nu}(k)-(i-1)}\|$. Since $\widehat{\nu}(k) - (k+1) = \nu(k+\mathcal{M}+2) - (k+1) \leq \mathcal{M}+1$, it follows from Lemma 6 that $\lim_{k\to\infty} \|x^{k+1} - x^{\widehat{\nu}(k)}\| = 0$, and, by the uniform continuity of f in Γ^0, we have that $\lim_{k\to\infty} f(x^k) = \lim_{k\to\infty} f(x^{\widehat{\nu}(k)}) = \lim_{k\to\infty} f(x^{\nu(k)})$. □

We are now in a position to prove Theorem 3.

Proof of Theorem 3. Let $\mathcal{K} \subseteq^{\infty} \mathbb{N}$ such that $\lim_{k\in\mathcal{K}} x^k = x^*$. From Lemma 4, there exists $\bar{\rho}$ ($\bar{\rho} = \zeta_2\rho_{\text{bound}}$) such that $\rho^k \leq \bar{\rho}$ for all $k \in \mathcal{K}$. Additionally, from Assumptions A2 and A3, both $\{A^k_{\rho^k}\}$ and $\{B^k_{\rho^k}\}$ are uniformly bounded subsequences. Therefore there exists $\mathcal{K}_1 \subseteq^{\infty} \mathcal{K}$ such that $\lim_{k\in\mathcal{K}_1} A^k_{\rho^k} = \bar{A}$ and $\lim_{k\in\mathcal{K}_1} B^k_{\rho^k} = \bar{B}$. Now, for every $k \in \mathcal{K}_1$, $f(x^{k+1}) \leq f(x^{\nu(k)}) + \beta_1\Psi_k(x^{k+1})$, and so, from Lemma 7, $\lim_{k\in\mathcal{K}_1} \Psi_k(x^{k+1}) = 0$. On the other hand, for all $k \in \mathcal{K}_1$, $\Psi_k(x^{k+1}) \leq Q^k_{\rho^k}(x^{k+1}) \leq \eta Q^k_{\rho^k}(\bar{x}^k_{\rho^k}) \leq 0$. Consequently, $\lim_{k\in\mathcal{K}_1} Q^k_{\rho^k}(\bar{x}^k_{\rho^k}) = 0$.

Now let us define $Q^*(x) = \langle g(x^*), x - x^*\rangle + 1/2(x - x^*)^T(\bar{B} + \bar{\rho}\bar{A})(x - x^*)$ and let $\widehat{x}$ be the solution of minimize $Q^*(x)$ subject to $x \in \Gamma$. Hence, since $\rho^k \leq \bar{\rho}$,

$$\begin{aligned} 0 \geq Q^*(\widehat{x}) &\geq \lim_{k\in\mathcal{K}_1} [\langle g(x^k), \widehat{x} - x^k\rangle + 1/2(\widehat{x} - x^k)^T(B^k_{\rho^k} + \rho^k A^k_{\rho^k})(\widehat{x} - x^k)] \\ &\geq \lim_{k\in\mathcal{K}_1} Q^k_{\rho^k}(\bar{x}^k_{\rho^k}) = 0. \end{aligned}$$

Therefore, $Q^*(\widehat{x}) = 0$ and, since $\nabla Q^*(x^*) = g(x^*)$, it follows that x^* is a stationary point. □

4. Application: minimization on Stiefel manifolds

This section deals with a method for a class of optimization problems whose feasible set is the set of matrices with orthogonal columns, which is straightforwardly related to Stiefel manifolds. Minimizing on Stiefel manifolds appears in a number of applications such as eigenvalue problems, electronic structure calculations, factor analysis and body rigid movements. For details on Stiefel manifolds the reader is referred to [11,12] and references therein. Define $\mathcal{G} : \mathbb{R}^{m\times n} \to \mathbb{R}^{n\times n}$, $m \geq n$, so that $\mathcal{G}(X) = X^TX - I$. Let $f : \mathbb{R}^{m\times n} \to \mathbb{R}$ be a twice continuously differentiable function and $\Omega = \{X \in \mathbb{R}^{m\times n} \mid \mathcal{G}(X) = 0\}$. We are concerned with the problem

$$\begin{aligned} \text{minimize} \quad & f(X) \\ \text{s.t.} \quad & X \in \Omega. \end{aligned} \tag{11}$$

Note that $\nabla f(X) = [\partial f(X)/\partial X_1, \ldots, \partial f(X)/\partial X_N] \in \mathbb{R}^{m\times n}$, where $X_i \in \mathbb{R}^m$ is the ith column of X. Also, since $\|X\|_F = \sqrt{n}\forall X \in \Omega$, note that Ω is a compact set and thus there exists L_f such that $\|\nabla f(X) - \nabla f(Y)\|_F \leq L_f\|X - Y\|_F \forall X, Y \in \{Z \in \mathbb{R}^{m\times n} \mid \|Z\|_F \leq \sqrt{n}\} \supset \Omega$. That is, condition (3) is satisfied. Although the optimization problem (11) is stated in a matrix framework, note that it can be rewritten in terms of mn real variables, and therefore within the context of Algorithm 1.

Since our goal is solving problem (11), we must be able to stop the iterative process when its Karush–Kuhn–Tucker (KKT) conditions are fulfilled within a given tolerance. In the following, using projections onto the tangent subspace of Ω, we will characterize these conditions into the context of minimization problems on Stiefel manifolds.

4.1. A first order optimality condition

Based on the ideas of [11], we will calculate the orthogonal projector onto the tangent subspace of Ω including some details that do not appear in [11] and are included here for completeness. We start by noting that (by a Taylor series expansion) the null-space of $\mathcal{G}'(Y)^T$ is $N(\mathcal{G}'(Y)) = \{X \in \mathbb{R}^{m\times n} \mid X^TY + Y^TX = 0\}$, that is, the tangent subspace of Ω in Y is $N(\mathcal{G}'(Y)) = \{X \in \mathbb{R}^{m\times n} \mid Y^TX \text{ is antisymmetric}\}$.

Lemma 8. *Let $Y \in \Omega$ and $A \in \mathbb{R}^{m\times n}$. Then the solution of*

$$\begin{aligned} \text{minimize} \quad & \|A - X\|_F^2 \\ \text{s.t.} \quad & X \in N(\mathcal{G}'(Y)) \end{aligned} \tag{12}$$

is given by $\widehat{X} = A - Y(Y^TA + A^TY)/2$.

Proof. Let $Y^\perp \in \mathbb{R}^{m\times(m-n)}$ have orthogonal columns such that $V = [Y\ Y^\perp] \in \mathbb{R}^{m\times m}$ is orthogonal, i.e., $YY^T + Y^\perp(Y^\perp)^T = I$. Define $\widetilde{I} = [I_n\ 0]^T \in \mathbb{R}^{m\times n}$ where I_n is the identity matrix of order n and note that $Y = V\widetilde{I}$. Then (12) is equivalent to

$$\begin{aligned} \text{minimize} \quad & \|A - X\|_F^2 \\ \text{s.t.} \quad & \widetilde{I}^TV^TX + X^TV\widetilde{I} = 0, \quad X \in \mathbb{R}^{m\times n}. \end{aligned} \tag{13}$$

Now denoting $Z = [Z_1^T\ Z_2^T]^T \equiv V^TX$, with $Z_1 \in \mathbb{R}^{n\times n}$ and $Z_2 \in \mathbb{R}^{(m-n)\times n}$, it follows that $\widetilde{I}^TV^TX + X^TV\widetilde{I} = 0$ if and only if $Z_1 = -Z_1^T$. Consequently (13) is equivalent to

$$\begin{aligned} \text{minimize} \quad & \left\| V^TA - \begin{bmatrix} 0 \\ Z_2 \end{bmatrix} \right\|_F^2 \equiv \|Y^TA - Z_1\|_F^2 + \|(Y^\perp)^TA - Z_2\|_F^2 \\ \text{s.t.} \quad & Z_2 \in \mathbb{R}^{(m-n)\times n}, \qquad Z_1 \in \mathbb{R}^{n\times n} \quad \text{and} \quad Z_1 + Z_1^T = 0, \end{aligned}$$

the solution of which is $\widehat{Z}_1 = (Y^TA - A^TY)/2$ and $\widehat{Z}_2 = (Y^\perp)^TA$. In addition, since Y has orthogonal columns and $X = VZ$, the solution is $\widehat{X} = Y(Y^TA - A^TY)/2 + (I - YY^T)A = A - Y(Y^TA + A^TY)/2$. □

The next theorem states equivalent conditions for a matrix $X_* \in \Omega$ to be a stationary point of (11).

Theorem 4. *Assume $X_* \in \Omega$. Then following statements are equivalents:*

(i) $X_*(X_*^T\nabla f(X_*) + \nabla f(X_*)^TX_*) - 2\nabla f(X_*) = 0$;
(ii) X_* *satisfies KKT conditions of* (11);
(iii) $\nabla f(X_*) = X_*S$ *for some symmetric matrix* $S \in \mathbb{R}^{n\times n}$.

Proof. Statement (i) is equivalent to statement (ii) since problem (11) has only equality constraints and, then, its KKT conditions are equivalent to say that the projection of $\nabla f(X_*)$ onto the tangent subspace $N(\mathcal{G}'(Y))$ vanishes. Furthermore, from Lemma 8, we have that $\nabla f(X)$ is orthogonal to $N(\mathcal{G}'(X))$ if and only if $\nabla f(X) = X(X^T\nabla f(X) + \nabla f(X)^TX)/2$.

Assume that statement (i) holds so that $X_*(X_*^T\nabla f(X_*) - \nabla f(X_*)^TX_*)/2 + (I - X_*X_*^T)\nabla f(X_*) = 0$. Pre-multiplying this equation by X_*^T and using the fact that $X_*^TX_* = I$, it turns out that $X_*^T\nabla f(X_*)$ is symmetric and thus $(I - X_*X_*^T)\nabla f(X_*) = 0$. Then statement (iii) holds with $S = X_*^T\nabla f(X_*)$. Now, differentiation of the Lagrangian function $\mathcal{L}(X, \Theta) = f(X) + \mathrm{Tr}(\Theta(X^TX - I))$ of (11) with respect to X shows that its KKT conditions are $X_*^TX_* = I$ and $\nabla f(X_*) = X_*(\Theta + \Theta^T)$, where $\Theta \in \mathbb{R}^{n\times n}$ is the matrix containing the Lagrange multipliers. This implies that (ii) is equivalent to (iii) with $S = (\Theta + \Theta^T)$. □

A by-product of statement (i) is a stopping criterion for minimization on Stiefel manifolds at the cost of some matrix multiplications. The reason is that since Lagrange multipliers are not used at all, (i) leads to an easy-to-compute expression which measures "the optimality" of a point $X \in \Omega$. In other words, a matrix $X_* \in \Omega$ is a stationary point of (11) if and only if

$$\|X_*(X_*^T\nabla f(X_*) + (X_*^T\nabla f(X_*))^T) - 2\nabla f(X_*)\|_F = 0. \tag{14}$$

This condition will be used in our tests in Section 4.3.

4.2. The spectral projected gradient method for minimization on Stiefel manifold

From here on we will concentrate on the application of Algorithm 1 to solving problem (11). In this case we take $A_\rho^k = I$ and $B_\rho^k = \sigma_\rho^k I$, where

$$\sigma_\rho^k = \begin{cases} \sigma_{\mathrm{spc}}^k/2, & \text{if } 0 < \rho \le L_u, \\ L_u, & \text{otherwise,} \end{cases} \tag{15}$$

with $\sigma_{\mathrm{spc}}^k \in [\sigma_{\min}, \sigma_{\max}]$, $0 < \sigma_{\min} < \sigma_{\max} < \infty$ and $L_u \ge L_f$. Thus $Q_\rho^k : \mathbb{R}^{m\times n} \to \mathbb{R}$ becomes

$$Q_\rho^k(X) = \mathrm{Tr}(\nabla f(X^k)^T(X - X^k)) + \frac{\sigma_\rho^k + \rho}{2}\|X - X^k\|_F^2. \tag{16}$$

Only for practical purpose (that means enhance the convergence behavior), σ_{spc}^k will be assumed to be the Barzilai–Borwein parameter [13]. Thus, for two consecutive iterates, X^{k-1} and X^k, we define

$$\sigma_{bb}^k = \frac{\text{Tr}\left(\left[\nabla f(X^k) - \nabla f(X^{k-1})\right]^T (X^k - X^{k-1})\right)}{\|X^k - X^{k-1}\|_F^2}, \tag{17}$$

and take $\sigma_{\text{spc}}^k = \min\left\{\max\left\{\sigma_{bb}^k, \sigma_{\min}\right\}, \sigma_{\max}\right\}$ for $k \geq 1$ and $\sigma_{\text{spc}}^k = 1$ for $k = 0$. With this choice our algorithm turns out to be a variation of the nonmonotone spectral projected gradient method for minimization on Stiefel manifolds. In this case, the problem to be solved at Step 3 of Algorithm 1,

$$\text{minimize } Q_\rho^k(X) \quad \text{subject to } X^TX = I \text{ and } X \in \mathbb{R}^{m\times n},$$

can readily be seen to be equivalent to,

$$\begin{aligned} \text{minimize} \quad & \|X - W^k\|_F^2, \quad \text{with } W^k = (X^k - 1/(\rho + \sigma_\rho^k)\nabla f(X^k)), \\ \text{s.t.} \quad & X^TX = I, \quad X \in \mathbb{R}^{m\times n}, \end{aligned} \tag{18}$$

whose solution is analytically obtained via a singular value decomposition (SVD). In fact, if W^k has a thin SVD, $W^k = U\Sigma V^T$ (i.e., U is the matrix containing the n left-singular vectors associated with the n largest singular values), then the global solution of (18) is $\bar{X}^k = UV^T$ [9].

Our proposed scheme for minimization with orthogonality constraints can be stated as follows.

Algorithm 2. Let $X^0 \in \Omega$ be an arbitrary initial point. The parameters set for the execution of the algorithm are: $\eta \in (0, 1]$, $\mathcal{M} \in \mathbb{N}$, $\beta_1 \in (0, 1/2]$, $\sigma_{\min}, \sigma_{\max}, \zeta_1, \zeta_2 \in \mathbb{R}$ such that $0 < \sigma_{\min} < \sigma_{\max} < \infty$ and $1 < \zeta_1 \leq \zeta_2 < +\infty$.
Set $k \leftarrow 0$ and $m(0) \leftarrow 0$.

Step 1. Compute $\nabla f(X^k)$, $f(X^{\nu(k)})$ as in (5) and set $\rho \leftarrow \sigma_{\text{spc}}^k/2$.

Step 2. Set σ_ρ^k as in (15) and compute the thin SVD of W^k given in (18): $W^k = U\Sigma V^T$.

Step 3. Define $\bar{X}_\rho^k = UV^T$ (solution of (16)) as mentioned before and compute $X_\rho^k \in \Omega$ such that $Q_\rho^k(X_\rho^k) \leq \eta Q_\rho^k(\bar{X}_\rho^k)$.
If $Q_\rho^k(X_\rho^k) = 0$, terminate the execution declaring X_ρ^k as stationary.

Step 4. Let $\Psi_k(X) = \text{Tr}(\nabla f(X^k)^T(X - X^k)) + \sigma_\rho^k/2\|X - X^k\|_F^2$. If

$$f(X_\rho^k) \leq f(X^{\nu(k)}) + \beta_1\Psi_k(X_\rho^k), \tag{19}$$

define $\rho^k = \rho$, $X^{k+1} = X_\rho^k$, set $k \leftarrow k + 1$ and go back to Step 1.
Else, choose $\rho_{new} \in [\zeta_1\rho, \zeta_2\rho]$, set $\rho = \rho_{new}$ and go back to Step 2.

The choice $\eta < 1$ is appropriate for problems with $m \gg n$ in which case a recursive approach which relies on inexact SVD decompositions can be used, see [14] for instance. This is not pursued here because we will address only small to medium size problems.

As for global convergence of Algorithm 2, it is guaranteed by Theorem 3 (i.e., $\{X^k\}_{k\in\mathbb{N}}$ converges globally to a stationary point of (11)) because in this case Assumptions A1, A2 and A3 are straightforwardly fulfilled. Furthermore, it is not hard to prove that Ω satisfies the Constant Rank Constraint Qualification (CRCQ) [15] and thus all local minimizer of (11) is a KKT point, which justifies our interest in finding stationary points.

We mention in passing that a great deal of work has been done on methods for optimization problems like (11). A globally convergent algorithm for constrained optimization over matrix manifolds based on line search methods can be found in [16]. Given both a feasible iterate X_k and a tangent descent direction η_k from X_k (with η_k e.g., being the projection of $-\nabla f(X_k)$ onto the tangent set), the method computes $X_{k+1} = R_k(t_k\eta_k)$, where R_k is a retraction on the Stiefel manifold and t_k comes from an Armijo's sufficient decrease condition:

$$f(R_k(t_k\eta_k)) \leq f(X_k) + \sigma t_k\langle\nabla f(X_k), \eta_k\rangle, \tag{20}$$

with $\sigma \in (0, 1)$. A gradient descent type method based on curvilinear line search which results in a nonmonotone SVD-free scheme for minimization with orthogonality constraints is provided in [17]. There, given a feasible iterate X_k and $A_k = X_k\nabla f(X_k)^T - \nabla f(x_k)X_k^T$, the method computes

$$X_{k+1} = Y(t_k) = \left(I + \frac{t_k}{2}A_k\right)^{-1}\left(I - \frac{t_k}{2}A_k\right)X_k,$$

where $t_k > 0$ satisfies the Armijo's sufficient decrease condition (20) with $\eta_k = A_kX_k$ and $R_k(t\eta_k) = Y(t) = (I + \frac{t}{2}A_k)^{-1}(I - \frac{t}{2}A_k)X_k$ being a feasible descent path. Besides a global convergence proof to stationary points, a nonmonotone Barzilai–Borwein based choice of t_k which reduces the number of steepest descent iterations can be found in [17]. As opposed to our proposal, the Barzilai–Borwein parameter in [17] is computed using gradients in the tangent set and the nonmonotone technique introduced in [18]. We emphasize that there is a crucial difference between the methodology of [17] and Algorithm 2 above: while the algorithms in [17] are based on steepest descent methods over tangent sets that adjust the Armijo's parameter t_k to decrease the cost function, Algorithm 2 is a variation of the projected gradient method with orthogonality constraints which adjusts parameter ρ up to a nonmonotone trust-region-like sufficient decrease condition is fulfilled.

4.3. Numerical experiments

For fixed matrices $A \in \mathbb{R}^{p\times m}$, $C \in \mathbb{R}^{n\times q}$ ($m \geq n$) and $B \in \mathbb{R}^{p\times q}$, we are concerned with the following problem:

$$\begin{aligned} \text{minimize} \quad & \|AXC - B\|_F^2 \\ \text{s.t.} \quad & X^TX = I, \quad X \in \mathbb{R}^{m\times n}, \end{aligned} \tag{21}$$

also called *weighted orthogonal Procrustes problem* (WOPP). Following [19], if $m = n$ and $C = I$ the case will be referred to as balanced, while if $n < m$, the case will be refereed to as unbalanced. The problem has attracted the attention of numerous researchers, mainly due to its wide diversity of applications (multivariate data analysis, global positioning systems, neuro and brain imaging and others). Concerning recent numerical approaches for (21), we cite the Successive Projection (SP) algorithm of [20] and the Left/Right Relaxation (LSR/RSR) methods devised in [21]. Roughly speaking, the cost of SP at every iteration involves the solution of n constrained least squares problems followed by a balanced Procrustes problem, whereas the cost of LSR and RSR require the computation of a finite sequence of SVD decompositions of $2 \times n$ matrices and $m \times 2$ matrices, respectively. For a comparative study on the performance of these and other algorithms on WOPP the reader is referred to [20]. For theoretical results on optimality conditions and other theoretical properties on WOPP the reader is referred to [19] and references therein.

It is worth mentioning that whereas the balanced case has analytical solution (given by $X_* = UV^T$, where U and V come from the SVD of $A^TB = U\Sigma V^T$ [9]), the unbalanced case, with $A \neq I$, needs to be solved by an iterative scheme capable of handling difficulties such as several stationary points and nonconvex constraints. Further, as far as we know, the determination of a closed-form solution to the unbalanced case is still a challenge, even if $C = I$, which justifies our interest in the problem.

Let $f : \mathbb{R}^{m\times n} \to \mathbb{R}$ be defined by $f(X) = \|AXC - B\|_F^2$. Then it is easy to see that f is twice continuously differentiable, that $\nabla f(X) = 2A^T(AXC - B)C^T$, and that ∇f is Lipschitz continuous with Lipschitz constant satisfying $L_f \leq 2\|A^TA\|_F\|CC^T\|_F \equiv L_u$. In this case (17) reads

$$\sigma_{bb}^k = 2\frac{\|A(X^k - X^{k-1})C\|_F^2}{\|X^k - X^{k-1}\|_F^2},$$

from which we conclude that $\sigma_{bb}^k \leq 2L_u$. Hence, if $0 < \sigma_{\min} < \sigma_{bb}^k < \sigma_{\max}$ and we set $\rho = \sigma_{\text{spc}}^k/2 = \sigma_{bb}^k/2$ in (16), then

$$\begin{aligned} Q_\rho^k(X^k + t(X^k - X^{k-1})) &= 2t\text{Tr}(2A^T(AX^kC - B)C^T(X^k - X^{k-1})) + t^2\|A(X^k - X^{k-1})C\|_F^2 \\ &= \|A(X^k + t(X^k - X^{k-1}))C - B\|_F^2 - f(X^k) \\ &= f(X^k + t(X^k - X^{k-1})) - f(X^k). \end{aligned}$$

Consequently, since $\rho = \sigma_{\text{spc}}^k/2$ at Step 1 of Algorithm 2, the first loop (Step 2–Step 3–Step 4) is equivalent to minimizing a quadratic model of f restricted to Ω that coincides with f along the direction $(X^k - X^{k-1})$.

We shall now illustrate the effectiveness of Algorithm 2 on some test problems from [20]. The following starting parameters are used in Algorithm 2: $\mathcal{M} = 10$, $\beta_1 = 10^{-4}$, $\zeta_1 = \zeta_2 = 5$, $\sigma_{\min} = 10^{-10}$ and $\sigma_{\max} = L_u$. Based on (14) we will declare convergence of the iterative process when

$$\max\{|[X^k(X^{k^T}\nabla f(X^k) + \nabla f(X^k)^TX^k) - 2\nabla f(X^k)]_{ij}|,\ 1 \leq i, j \leq m\} \leq 10^{-3}.$$

Our experiments were carried out using Matlab 7.6 in an AMD Athlon 64 X2 dual Core 5600+ with 2 GB of RAM. In all cases $n = q$, $p = m$, $C = I$ with A of the type $A = PSR^T$, where both P and R are randomly generated orthogonal matrices and S is diagonal. Four examples are considered:

Example 1. The elements on the main diagonal of S are randomly and normally distributed in the interval [10, 12]. This is a well-conditioned problem.

Example 2. The diagonal elements are $S_{ii} = i + 2r_i$, where r_i are random numbers from a uniform distribution on the interval [0, 1]. In this case the singular values of A are more and more distant each other as m grows.

Example 3. In this case $S_{ii} = (1 + 99(i-1)/(m-1) + 2r_i)$ and r_i are random numbers chosen from a uniform distribution on the interval [0, 1].

Example 4. Matrix S is defined using the Matlab functions `ones` and `rand` by $\text{diag}(S) = ([10*\texttt{ones}(1, m_1) + \texttt{rand}(1, m_1), 5*\texttt{ones}(1, m_2) + \texttt{rand}(1, m_2), 2*\texttt{ones}(1, m_3) + \texttt{rand}(1, m_3), \texttt{rand}(1, m_4)/1000])$, with $m_1 + m_2 + m_3 + m_4 = m$. Thus, A has several small singular values and it is ill-conditioned.

Since the solution for the balanced case without weights is an orthogonal basis for the column subspace of A^TB, the initial guess X^0 was chosen as the n first columns of R. Further, in order to monitor the behavior of the iterates X^k with respect to

Table 1
Performance of the method.

q	NT	NV	TM	RES.	ERR	NT	NV	TM	RES.	ERR
Example 1 ($m = 50$)						Example 1 ($m = 500$)				
10	8	13	0.07	1.3e−12	9.6e−08	7	12	0.59	1.3e−11	2.9e−07
20	10	11	0.07	8.9e−14	2.8e−08	7	12	0.99	2.7e−11	3.9e−07
44	10	11	0.08	1.9e−14	7.9e−09	8	13	2.28	1.2e−12	8.7e−08
70	–	–	–	–	–	8	13	3.70	1.4e−12	9.4e−08
Example 2 ($m = 50$)						Example 2 ($m = 500$)				
10	219	297	0.39	7.8e−09	2.9e−05	1344	1942	98.10	3.2e−09	1.3e−05
20	184	240	0.59	6.9e−09	2.8e−05	1207	1729	157.74	2.9e−09	1.2e−05
44	197	260	1.54	3.5e−09	2.3e−05	1436	2101	382.26	4.1e−09	1.3e−05
70	–	–	–	–	–	2237	3256	945.95	2.1e−09	1.3e−05
Example 3 ($m = 50$)						Example 3 ($m = 500$)				
10	70	78	0.15	5.6e−11	3.9e−07	84	97	5.06	5.7e−10	3.5e−07
20	111	128	0.32	4.2e−11	4.0e−07	92	107	9.88	1.2e−10	7.1e−07
44	60	62	0.41	1.8e−11	2.2e−07	94	111	21.84	2.4e−10	1.0e−06
70	–	–	–	–	–	97	110	33.07	7.2e−12	1.7e−07

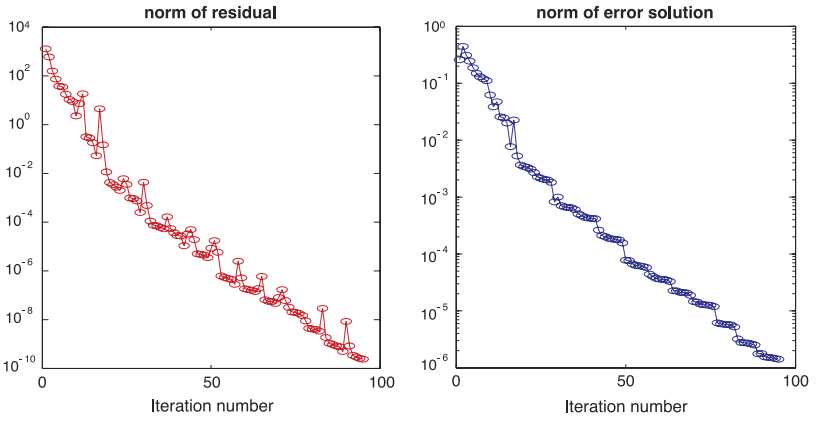

Fig. 1. Plot of $\|AX^kC - B\|_F$ (left) and $\|X^k - \mathcal{Q}_*\|_F$ (right) for Example 3 with $m = 500$ and $q = 44$. The y-axis is on a logarithmic scale.

the exact solution of problem (21), we generate a known solution $\mathcal{Q}_*$ by taking $B = A\mathcal{Q}_*C$, where $\mathcal{Q}_* \in \mathbb{R}^{m\times n}$ has orthogonal columns generated at random. We remark that if the SVD of A, $A = \bar{U}\bar{\Sigma}\bar{V}^T$, is available, problem (21) is equivalent to

$$\begin{aligned} \text{minimize} \quad & \|\bar{\Sigma}ZC - \bar{B}\|_F^2 \\ \text{s.t.} \quad & Z^TZ = I_{n\times n}, \quad Z \in \mathbb{R}^{m\times n}, \end{aligned}$$

where $Z = \bar{V}^TX$ and $\bar{B} = \bar{U}^TB$. Thus after an initial calculation of the SVD of A, in our experiments we use $\bar{\Sigma}$ instead of A and $\bar{B}$ instead of B, which improves performance (a bit).

In Table 1 we summarize the results corresponding to Examples 1–3 for several values of q and m. Although we do not feel important to compare our algorithm with other ones because our goal is just to verify its robustness and theoretical properties, in order to give some idea about its performance we consider some values of q used in [20] for $m = 50$. We use NT, NV and TM to denote, respectively, the number of iterations, the number of evaluations of $f(X)$ needed to reach convergence and the CPU time in seconds (using Matlab's `cputime` function). The Frobenius norm of the residual at approximate solution X_*, $\|AX_*C - B\|_F$, is denoted by RES and its respective error, $\|X_* - \mathcal{Q}_*\|_F$, by ERR.

As for these results, we observe that the number of evaluations is relatively close to the number of iterations and that the residual decays significantly in the first half of the process, see Fig. 1. This behavior is likely a straightforward consequence of the initial ρ satisfying the condition (19) and the use of the spectral parameter choice combined with the nonmonotone trust-region rule. Another fact that must be mentioned here is that our method provided a solution close to the global minimum within an acceptable number of iterations, mainly for well-conditioned problems, as in Example 1 where the singular values are clustered. In order to illustrate the overall behavior of our method, the residual at X^k and corresponding error for Example 3 with $m = 500$ and $q = 44$, are displayed in Fig. 1.

A brief comparison between monotone (M) and nonmonotone (NM) cases (for $\mathcal{M} = 10$) is displayed on Table 2. In order to highlight the performance of the nonmonotone approach, we took $C = Q_1\Lambda Q_1^T$, where $Q_1 \in \mathbb{R}^{n\times n}$ is a random Householder matrix and $\Lambda \in \mathbb{R}^{n\times n}$ is a diagonal matrix with $\{\Lambda_{ii}\}_{i=1}^n$ being uniformly distributed random values in the interval $[1/2, 2]$. This test was ran in a Intel Core 2 Duo 3000 Ghz with 2 Gb of RAM. Row TMR shows the CPU time reduction

Table 2
Comparison of monotone and nonmonotone cases for $m = 50$ and $C = Q_1 \Lambda Q_1^T$.

	q	Example 1				Example 2				Example 3			
		4	10	20	44	4	10	20	44	4	10	20	44
M	NT	18	23	39	38	236	303	336	443	117	195	202	252
	NV	26	32	60	55	450	512	581	746	182	314	337	416
NM	NT	16	24	32	38	270	278	268	408	109	173	177	156
	NV	21	29	37	43	357	383	348	553	130	204	217	195
	TMR(%)	0	0	14	10	10	34	45	23	25	47	26	49

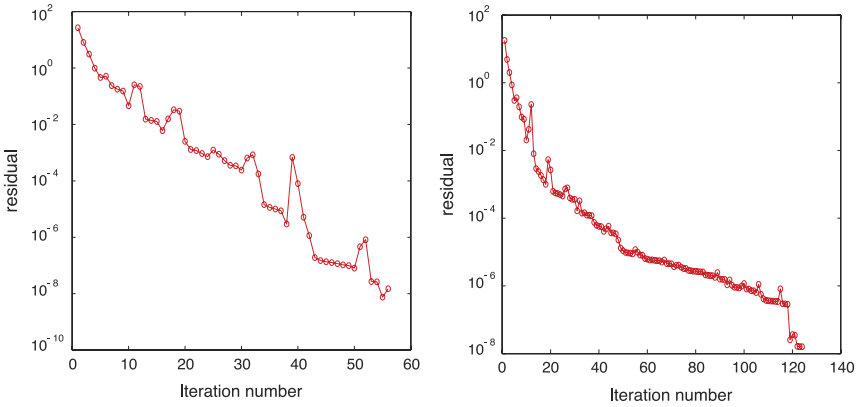

Fig. 2. Plot of $\|AX^kC - B\|_F$ for Example 4. Case 4A (left) and case 4B (right).

(in percent) in the nonmonotone case with relation to the monotone one. Note that the variation was between 0 and 49%. We also note that in general NT and NV are significantly large in the monotone case. This suggests using the nonmonotone approach mainly when evaluation of the objective function is expensive.

For Example 4, we follow [20] and consider two set of parameters:

(4A) $q = 10$, $m_1 = m_2 = 15$, $m_3 = 12$ and $m_4 = 8$, and thus $m = 50$;
(4B) $q = 10$, $m_1 = m_2 = m_3 = 30$ and $m_4 = 5$, and thus $m = 95$.

For this example we only display in Fig. 2 the residual Frobenius norm along the iterations, with the observation that even in this ill-conditioned example, the proposed algorithm declared convergence in an acceptable number of iterations, as we have already noticed in previous examples.

We end the section with the observation that the same experiments were carried out using distinct initialization parameters. Our experience concerning this is that slight variations of the initialization parameters used in this work do not change significantly the values of NT, NV and TM.

5. Conclusions

Combining a regularization approach and nonmonotone trust-region rules we proposed an algorithm for minimizing differentiable functions restricted to an arbitrary closed set. The method is well suited for constrained optimization problems whose feasible set has a special geometry such that a global solution of a quadratic constrained subproblem is easy to compute. In addition, it has the property of computing accumulation points that are stationary, irrespective of the initial approximation chosen. As a consequence, an algorithm for minimization on Stiefel manifolds was presented and its theoretical properties numerically verified. Numerical experiments on small and medium sized weighted orthogonal Procrustes problems show that our technique is a reliable optimization tool for minimization problems with orthogonality constraints.

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