On the globalization of Riemannian Newton method

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Abstract

In the present paper, in order to find a singularity of a vector field defined on Riemannian manifolds, we present a new globalization strategy of Newton method and establish its global convergence with superlinear rate. In particular, this globalization generalizes for a general retraction the existing damped Newton’s method. The presented global convergence analysis does not require any hypothesis on singularity of the vector field. We applied the proposed method to solve the truncated singular value problem on the product of two Stiefel manifolds, the dextrous hand grasping problem on the cone of symmetric positive definite matrices and the Rayleigh quotient on the sphere. Moreover, some academic problems are solved. Numerical experiments are presented showing that the proposed algorithm has better robustness compared with the aforementioned method.

Keywords: Global Convergence · Riemannian Newton Method · Superlinear Rate · Retraction.

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1 Introduction

Iterative methods on manifolds arise in the context of optimizing a real-valued function, dating back to the work of Luenberger [35] in the early 1970s, if not earlier. Luenberger proposed the idea of performing a line search along geodesics that are computationally feasible. Around 1990, the main research issue was to exploit differential-geometric objects in order to formulate optimization strategies on abstract nonlinear manifolds. Gabay in [23] was the first to focus on optimization on manifolds by minimizing a differentiable function defined on a Riemannian manifold. In the 1990s, the field of optimization on manifolds gained considerable popularity, especially with the work of Edelman et al. [18]. Recent years have witnessed a growing interest in the development of numerical algorithms for nonlinear manifolds, as there are many numerical problems posed in manifolds arising in various natural contexts. For example, eigenvalue problems [14,34,46,50,51], low-rank matrix completion [49], loss minimization problem [42] and dextrous hand grasping problem [16,24,25]. For such problems, the solutions of a system of equations often have to be computed or the zeros

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of a vector field have to be found. Because these problems are naturally posed on Riemannian manifolds, we can use the specific underlying geometric and algebraic structures to significantly reduce the computational cost of finding the zeros of a vector field. In this work, instead of focusing on finding singularities of gradient vector fields on Riemannian manifolds, which includes finding local minimizers, we consider the more general problem of finding singularities of vector fields. Newton’s method is known to be a powerful tool for finding the zeros of nonlinear functions in Banach spaces. It also serves as a powerful theoretical tool with a wide range of applications in pure and applied mathematics [13, 37, 38]. These factors have motivated several studies to investigate the issue of generalizing Newton’s method from a linear setting to the Riemannian setting [2, 7, 20, 22, 32, 33, 43, 47]. Although Newton’s method shows fast local convergence, it is highly sensitive to the initial iterate and may diverge if the initial iterate is not sufficiently close to the solution. Thus, Newton’s method does not converge in general. To overcome this drawback, some strategies have been introduced for using Newton’s method in optimization problems, such as the Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm, Levenberg–Marquardt algorithm, and trust region algorithm [8, 15]. When the objective function is twice continuously differentiable and strongly convex, the Newton direction is a descent direction of the objective function. Hence, by adjusting the step size in the Newton direction using, e.g., the Armijo rule, we can ensure convergence of Newton’s method. This strategy of dumping the step size to globalize Newton’s method is known as damped Newton’s method. For a comprehensive study of this method, see [8, 12, 15, 30]. For the problem of finding a zero of a nonlinear equation in a Euclidean setting, this strategy of dumping the Newton step size can also be adopted by using a merit function for which the Newton direction is a descent direction. This strategy was generalized from Euclidean context to Riemannian context, see [11].

The generalization to Riemannian setting of damped Newton’s method by using a merit function was obtained by using the notion of continuously moving in the Newton direction while staying on a geodesic curve in the manifold until we reach a point where the vector field vanishes. By using the geodesic curve, we can define the exponential mapping that can be used to give a short notation for a geodesic with a given starting point and initial velocity. However, the geodesic, and consequently the exponential mapping, is defined as the solution of a nonlinear ordinary differential equation, whose efficient computation generally involves significant numerical challenges. Nevertheless, an approximation of the geodesic is sufficient to guarantee the desired convergence properties. Actually, to obtain the next iterate of an iterative method on a manifold, it is sufficient to use the notion of moving in the direction of a tangent vector while staying on the manifold. It is generalized by the notion of a retraction mapping that may generate a curve on the manifold with greater computational efficiency compared to the exponential mapping. The idea of using computationally efficient alternatives to the exponential mapping was introduced in [36]. The strategy of using approximations of classical geometric concepts to obtain efficient iterative algorithms has attracted considerable attention lately in the context of Riemannian optimization; see, e.g., [1, 2, 6, 10, 13, 39]. Obtaining an iterative method using retraction is becoming increasingly common, as such algorithms are faster and possibly more robust than existing algorithms. Recent studies on the development of geometric optimization algorithms that exploit the mapping retraction on nonlinear manifolds include [26, 29, 52]. A toolbox for building retractions on manifolds can be found in [3].

Our main contribution is to present a Newton type algorithm with global convergence. From the theoretical point of view this algorithm generates a sequence that converges without any assumption on singularity of the vector field in consideration, which improves the convergence analysis of [5, 11]. Besides, this algorithm uses general retractions instead of only the exponential mapping. In addition, numerical experiments are presented showing that the proposed algorithm has better...
robustness compared with the one presented in [11] and better performance than the one presented in [11]. In order to present a numerical performance for proposed algorithm we have submitted it to the task to solve the truncated singular value problem on the product of two Stiefel manifolds [11], the Rayleigh quotient on the sphere and the dextrous hand grasping problem, see [16, 24, 25]. Also, we yet analyse the problem to find the singularity of a nonconservative vector field on the sphere and to minimize an academic function on the cone of symmetric definite positive matrices.

The remainder of this paper is organized into five sections. The basic concepts and auxiliary results are developed in Section 2. In Section 3 we present a local superlinear convergence of the Newton method with retraction. The main result of the paper is presented in Section 4. Concrete examples and numerical experiments of the new gained insights of the proposed method are presented in Section 5. Concluding remarks are presented in Section 6.

2 Preliminaries

In this section, we recall some notations, definitions, and basic properties of Riemannian manifolds used throughout the paper, which can be found in many introductory books on Riemannian geometry, for example [17] and [10].

For a smooth manifold $\mathbb{M}$, denote the tangent space of $\mathbb{M}$ at $p$ by $T_p\mathbb{M}$ and the tangent bundle of $\mathbb{M}$ by $T\mathbb{M} = \bigcup_{p \in \mathbb{M}} T_p\mathbb{M}$. The corresponding norm associated with the Riemannian metric $\langle \cdot, \cdot \rangle$ is denoted by $\| \cdot \|$. The Riemannian distance between $p$ and $q$ in a finite-dimensional Riemannian manifold $\mathbb{M}$ is denoted by $d(p, q)$, and it induces the original topology on $\mathbb{M}$. An open ball of radius $r > 0$ centered at $p$ is defined as $B_r(p) := \{ q \in \mathbb{M} : d(p, q) < r \}$. Let $\Omega \subset \mathbb{M}$ be an open set, and let $\mathcal{X}(\Omega)$ denote the space of $C^1$ vector fields on $\Omega$. Let $\nabla$ be the Levi-Civita connection associated with $(\mathbb{M}, \langle \cdot, \cdot \rangle)$. The covariant derivative of a vector field $X \in \mathcal{X}(\Omega)$ denoted by $\nabla$ defines at each $p \in \Omega$ a linear map $\nabla X(p) : T_p\mathbb{M} \to T_p\mathbb{M}$ given by $\nabla X(p)v := \nabla_Y X(p)$, where $Y$ is a vector field such that $Y(p) = v$. For $f : \mathbb{M} \to \mathbb{R}$, a twice-differentiable function the Riemannian metric induces the mappings $f \mapsto \text{grad} f$ and $f \mapsto \text{Hess} f$, which associate its gradient and Hessian via the rules $d f(X) := \langle \text{grad} f, X \rangle$ and $d^2 f(X, X) := \text{Hess} f(X, X)$, for all $X \in \mathcal{X}(\Omega)$, respectively. Therefore, $\text{Hess} fX = \nabla \text{grad} f$, for all $X \in \mathcal{X}(\Omega)$. The norm of a linear map $A : T_p\mathbb{M} \to T_p\mathbb{M}$ is defined by $\|A\| := \sup \{ \|Av\| : v \in T_p\mathbb{M}, \|v\| = 1 \}$. A vector field $V$ along a differentiable curve $\gamma$ in $\mathbb{M}$ is said to be parallel iff $\nabla_{\gamma'} V = 0$. For each $t \in [a, b]$, the operator $\nabla$ induces an isometry relative to $\langle \cdot, \cdot \rangle$, $P_{\gamma, a, t} : T_{\gamma(t)}\mathbb{M} \to T_{\gamma(t)}\mathbb{M}$, defined by $P_{\gamma, a, t}v = V(t)$, where $V$ is the unique vector field on $\gamma$ such that $\nabla_{\gamma'}(t)V(t) = 0$ and $V(a) = v$, the so-called parallel transport along of a segment of curve $\gamma$ joining the points $\gamma(a)$ and $\gamma(t)$. Further note that $P_{\gamma, b, b_2} \circ P_{\gamma, a, b_1} = P_{\gamma, a, b_2}$ and $P_{\gamma, b, a} = P_{\gamma, a, b}^{-1}$. As long as there is no confusion, we will consider the notation $P_{pq}$ instead of $P_{\gamma, a, b}$ when $\gamma$ is the unique segment of curve joining $p$ and $q$. The following lemma ensures that, if $\nabla X(p)$ is nonsingular then there exists a neighborhood of $p$ such that $\nabla X$ is also nonsingular.

Lemma 1. Assume that $\nabla X$ is continuous at $p$. Then, $\lim_{p \to p} \| P_{pq} \nabla X(p)P_{pq} - \nabla X(p) \| = 0$. Moreover, if $\nabla X(p)$ is nonsingular, then there exists $0 < \delta < \delta_p$ such that $B_{\delta}(p) \subset \Omega$, and for each $p \in B_{\delta}(p)$, $\nabla X(p)$ is nonsingular and $\| \nabla X(p)^{-1} \| \leq 2 \| \nabla X(p)^{-1} \|$.

Proof. See [20, Lemma 3.2] \hfill \square

In the following we present the concept of retraction which has been introduced by [36].

Definition 1. A retraction on a manifold $\mathbb{M}$ is a smooth mapping $R$ from the tangent bundle $T\mathbb{M}$ onto $\mathbb{M}$ with the following properties: If $R_p$ denote the restriction of $R$ to $T_p\mathbb{M}$, then
(i) \( R_p(0_p) = p \), where \( 0_p \) denotes the origin of \( T_pM \);

(ii) With the canonical identification \( T_0 T_pM \simeq T_pM, \) \( R_p'(0_p) = I_p \), where \( I_p \) is the identity mapping on \( T_pM \), and \( R_p' \) denotes the differential of \( R_p \).

The Definition 1 implies that the exponential map is a retraction, see [2]. Since \( R_p'(0_p) = I_p \), by the Inverse Function Theorem, \( R_p \) is a local diffeomorphism. Hence, we define the injectivity radius of \( \mathbb{M} \) at \( p \) with respect to \( R \) as follow \( i_p := \sup \{ r > 0 : R_p|_{B_r(0_p)} \text{ is a diffeomorphism} \} \), where \( B_r(0_p) := \{ v \in T_p\mathbb{M} : \| v - 0_p \| < r \} \).

Remark 1. Let \( \bar{p} \in \mathbb{M} \). The above definition implies that if \( 0 < \delta < i_{\bar{p}} \), then \( R_{\bar{p}}B_\delta(0_{\bar{p}}) = B_\delta(\bar{p}) \). Moreover, for all \( p \in B_\delta(\bar{p}) \) the curve segment \( \gamma_{p\bar{p}}(t) = R_{\bar{p}}(tR_{\bar{p}}^{-1}p) \) joining \( \bar{p} \) to \( p \) belongs to \( B_\delta(\bar{p}) \).

The following result establishes an important relation between the retraction and the Riemannian distance and its proof can be found in [39, Lemma 6].

**Proposition 1.** Let \( \mathbb{M} \) be a Riemannian manifold endowed with a retraction \( R \) having equicontinuous derivatives in a neighborhood of \( \bar{p} \in \mathbb{M} \). Then, there exist \( a_0 > 0, a_1 > 0, \) and \( \delta_{a_0,a_1} \) such that for all \( p \) in a sufficiently small neighborhood of \( \bar{p} \) and all \( v \in T_p\mathbb{M} \) with \( \| v \| \leq \delta_{a_0,a_1} \), the following inequality holds

\[
a_0 \| v \| \leq d(p, R_p(v)) \leq a_1 \| v \|. \tag{1}
\]

Let \( a_0 > 0, a_1 > 0, \) and \( \delta_{a_0,a_1} \) be given as in the Lemma [1]. Making \( \delta_{a_0,a_1} \) smaller, if necessary, such that \( \delta_{a_0,a_1} < i_{\bar{p}} \). Let \( v \in B_{\delta_{a_0,a_1}}(0_{\bar{p}}) \) and \( p = R_{\bar{p}}(v) \). Then, by (1) we can conclude

\[
a_0 \| R_{\bar{p}}^{-1}(p) \| \leq d(\bar{p}, p) \leq a_1 \| R_{\bar{p}}^{-1}(p) \|, \quad \forall \ p \in B_\delta(\bar{p}), \tag{2}
\]

where \( \delta < \delta_{a_0,a_1} \). Now, we are ready to define the number \( K_{R,p} \). Letting \( i_{\bar{p}} \) be the radius of injectivity of \( \mathbb{M} \) at \( p \) we define the quantity

\[
\delta_p := \min \{ 1, i_{\bar{p}} \}.
\]

\[
K_{R,p} := \sup \left\{ \frac{d(R_qu, R_qv)}{\| u - v \|} : q \in B_{\delta_p}(p), \ u, v \in T_q\mathbb{M}, \ u \neq v, \ \| v \| \leq \delta_p, \ \| u - v \| \leq \delta_p \right\}. \tag{3}
\]

Let \( i_{\bar{p}} \) be the radius of injectivity of \( \mathbb{M} \) at \( p \) and define the quantity \( \delta_{p} := \min \{ 1, i_{\bar{p}} \} \). Consider \( X \in \mathcal{X}(\Omega) \) and \( \bar{p} \in \Omega \). Assume that \( 0 < \delta < \delta_{\bar{p}} \). From definition of \( \delta_{\bar{p}} \) follows that for any curve \( [0, 1] \ni t \mapsto \gamma(t) = R_{\bar{p}}(t\nu_{\bar{p}}) \) joining \( \bar{p} \) to \( p \in B_\delta(\bar{p}) \) such that \( \gamma'(0) = v_{\bar{p}} \), we have \( v_{\bar{p}} = R_{\bar{p}}^{-1}p \). Moreover, using [22, equality 2.3] we obtain

\[
X(p) = P_{pp}X(\bar{p}) + P_{pp}(\nabla X(\bar{p})R_{\bar{p}}^{-1}p + \| R_{\bar{p}}^{-1}p \| r(p)), \quad \lim_{p \to \bar{p}} r(p) = 0, \tag{4}
\]

for each \( p \in B_\delta(\bar{p}) \).

We end this section by formally presenting the problem of interest in this paper. Let \( X : \mathbb{M} \to T\mathbb{M} \) with \( X(p) \in T_p\mathbb{M} \) be a differentiable vector field. We are interested in to find a \( p \in \mathbb{M} \) such that

\[
X(p) = 0. \tag{5}
\]
3 Local superlinear convergence of Newton method

In this section, we analyse the local convergence of Newton method with a general retraction to solve the problem (5), which generalize the results presented in [20]. We first formally present Newton method with a general retraction. It is described as follows.

Algorithm 1. Newton Method

Step 0. Take an initial point $p_0 \in \mathbb{M}$, and set $k = 0$.

Step 1. Compute search direction $v_k \in T_{p_k} \mathbb{M}$ as a solution of the linear equation

$$X(p_k) + \nabla X(p_k)v = 0.$$  \hfill (6)

If $v_k$ exists go to Step 2. Otherwise, stop.

Step 2. Compute

$$p_{k+1} := R_{p_k}v_k.$$  \hfill (7)

Step 3. Set $k \leftarrow k + 1$ and go to Step 1

When the retraction $R$ is the exponential mapping, a sequence generated by this method converges to a singularity of $X$ with superlinear rate, [20]. Moreover, if the covariant derivative is Lipschitz continuous around the singularity then the method has $Q$-quadratic convergence rate, see [21]. It is well known that the convergence of a sequence generated by Algorithm 1 is ensured when the initial guess is sufficiently close to a solution at which the covariant derivative is nonsingular. Otherwise, the equation (6) may not have a solution. In this case, the Algorithm 1 stops. In the next section, we present a new algorithm that overcome this. Now, our aim is to prove a generalization of [20, Theorem 3.1], it is, under the assumption of nonsingularity of the covariant derivative at the solution $\bar{p}$, the iteration (7) starting in a suitable neighborhood of $\bar{p}$ is well defined and converges superlinearly to $\bar{p}$. Before to obtain that generalization some results are required.

Consider $\delta > 0$ given by Lemma 1 and define Newton’s iterate mapping $N_{R,X} : B_\delta(\bar{p}) \rightarrow \mathbb{M}$ by

$$N_{R,X}(p) := R_{\bar{p}}(-\nabla X(p)^{-1}X(p)).$$  \hfill (8)

The next lemma ensures existence of a neighborhood of $\bar{p}$ where Newton’s iterate given by (7) belong to the same neighborhood.

Lemma 2. Let $\bar{p} \in \mathbb{M}$ a solution of (5). Assume that $\nabla X$ is continuous at $\bar{p}$ and $\nabla X(\bar{p})$ is nonsingular. Then,

$$\lim_{p \to \bar{p}} \frac{d(N_{R,X}(p), \bar{p})}{d(p, \bar{p})} = 0.$$  \hfill (9)

Proof. Define $r(p) := X(p) - P_{pp}X(\bar{p}) - P_{pp}\nabla X(\bar{p})R_{\bar{p}}^{-1}p$, for each $p \in B_\delta(\bar{p})$, where $\tilde{\delta}$ is given by Lemma 1. By using some algebraic manipulations we obtain the following equality

$$\nabla X(p)^{-1}X(p) + R_{\bar{p}}^{-1}\bar{p} = \nabla X(p)^{-1}[r(p) + [P_{pp}\nabla X(\bar{p}) - \nabla X(p)P_{pp}]R_{\bar{p}}^{-1}p].$$
Thus, using the above equality, the definition of \( r \), and some properties of the norm, we conclude
\[
\frac{\|\nabla X(p)^{-1}X(p) + R_{p}^{-1}\bar{p}\|}{d(p, \bar{p})} \leq \frac{\|\nabla X(p)^{-1}\|}{a_0} \left( \|r(p)\| + \|P_{pp}\nabla X(\bar{p}) - \nabla X(p)P_{pp}\| \right) \frac{\|R_{p}^{-1}p\|}{d(p, \bar{p})}.
\]
By using (2) we obtain \( \|R_{p}^{-1}p\|/d(p, \bar{p}) \leq 1/a_0 \). Combining these two last inequalities we have
\[
\frac{\|\nabla X(p)^{-1}X(p) + R_{p}^{-1}\bar{p}\|}{d(p, \bar{p})} \leq \frac{\|\nabla X(p)^{-1}\|}{a_0} \left( \|r(p)\| + \|P_{pp}\nabla X(\bar{p}) - \nabla X(p)P_{pp}\| \right) \frac{\|R_{p}^{-1}p\|}{d(p, \bar{p})}.
\]
Since \( p \in B_{\delta}(\bar{p}) \), \( P_{pp}P_{pp} = I_p \) where \( I_p \) denotes the identity operator on \( T_pM \), and the parallel transport is an isometry, Lemma \( \text{I} \) combined with this last inequality implies
\[
\|\nabla X(p)^{-1}X(p) + R_{p}^{-1}\bar{p}\| \leq \frac{1}{a_0} \|\nabla X(\bar{p})^{-1}\| \left( \|r(p)\| + \|P_{pp}\nabla X(\bar{p}) - \nabla X(p)P_{pp}\| \right) d(p, \bar{p}).
\]
Owing to Lemma \( \text{I} \) and \( \lim_{p \to \bar{p}} r(p) = 0 \), the right-hand side of the last inequality tends to zero, as \( p \) goes to \( \bar{p} \). Recalling that \( \delta_{\bar{p}} = \min\{1, i_p\} \), we can shrink \( \delta \), if necessary, to obtain
\[
\|\nabla X(p)^{-1}X(p) + R_{p}^{-1}\bar{p}\| \leq \delta_{\bar{p}}, \quad \forall \ p \in B_{\delta}(\bar{p}).
\]
Hence, from definitions of \( N_{R,X} \) in (8) and \( K_{R,\bar{p}} \) in (3), we can conclude
\[
d(N_{R,X}(p), \bar{p}) \leq K_{\bar{p}} \|\nabla X(p)^{-1}X(p) - R_{p}^{-1}\bar{p}\|, \quad \forall \ p \in B_{\delta}(\bar{p}).
\]
Therefore, by combining (9) with the last inequality we obtain for all \( p \in B_{\delta}(\bar{p}) \) that
\[
\frac{d(N_{R,X}(p), \bar{p})}{d(p, \bar{p})} \leq \frac{2}{a_0} K_{\bar{p}} \|\nabla X(\bar{p})^{-1}\| \left( \|r(p)\| + \|P_{pp}\nabla X(p)P_{pp} - \nabla X(p)\| \right).
\]
By letting \( p \) tend to \( \bar{p} \) in the last inequality, by considering Lemma \( \text{I} \) and that \( r(p) \) tends to zero, as \( p \) goes to \( \bar{p} \), the desired result follows. \( \square \)

In the next we show that whenever the vector field is continuous and has nonsingular covariant derivative at a solution, there exist a neighborhood around of it which is invariant by the Newton’s iterate mapping associated. Its proof is a direct consequence from Lemma \( \text{I} \) and Lemma \( \text{II} \)

**Lemma 3.** Let \( \bar{p} \in M \) such that \( X(\bar{p}) = 0 \). If \( \nabla X \) is continuous at \( \bar{p} \) and \( \nabla X(\bar{p}) \) is nonsingular, then there exists \( 0 < \delta < \delta_{\bar{p}} \) such that \( B_{\delta}(\bar{p}) \subset \Omega \) and \( \nabla X(p) \) is nonsingular for each \( p \in B_{\delta}(\bar{p}) \). Moreover, \( N_{R,X}(p) \in B_{\delta}(\bar{p}) \), for all \( p \in B_{\delta}(\bar{p}) \).

The main result this section is presented as follow. It is a generalization of [20] Theorem 3.1 for a general retraction. Its proof can be made by adaptations of the idea used in that result. For this reason, we do not present it here.

**Theorem 1.** Let \( M \) be a Riemannian manifold with a retraction \( R \) and \( \Omega \subset M \) be an open set. Let \( X : \Omega \to TM \) be a differentiable vector field and \( \bar{p} \in \Omega \). Consider the Newton sequence \( \{p_k\} \) generated by Algorithm \( \text{I} \). Suppose that \( \bar{p} \) is a singularity of \( X \) and \( \nabla X \) is continuous and nonsingular at \( \bar{p} \). Then, there exists \( \delta > 0 \) such that, for all \( p_0 \in B_{\delta}(\bar{p}) \), the sequence \( \{p_k\} \) is well defined, contained in \( B_{\delta}(\bar{p}) \), and it converges superlinearly to \( \bar{p} \).

Let \( X = \text{grad} \ f \), then the following result is a version of Theorem \( \text{I} \) for finding critical points of a twice-differentiable function.
Corollary 1. Let $\mathcal{M}$ be a Riemannian manifold with a retraction $R$ and $\Omega \subset \mathcal{M}$ be an open set. Let $f : \Omega \to \mathbb{R}$ be a twice-differentiable function and $\bar{p} \in \Omega$. Suppose that $\bar{p}$ is a critical point of $f$ and $\text{Hess} f$ is continuous and nonsingular at $\bar{p}$. Then, there exists $\delta > 0$ such that, for all $p_0 \in B_\delta(\bar{p})$, a sequence generated by Algorithm 1,

$$p_{k+1} = R_{p_k}(-\text{Hess} f(p_k)^{-1} \text{grad} f(p_k)), \quad k = 0, 1, \ldots \quad (10)$$

is well defined, contained in $B_\delta(\bar{p})$ and converges superlinearly to $\bar{p}$.

4 Globalization of Newton method

In [11] has been presented a global version of the Newton method with the iterations being updated by the exponential mapping. In this section, we present a version of that method for a general retraction, see Algorithm 2 below. Our numerical experiments in the present paper have shown that this method is quite sensitive with respect to retractions used, having effect on its robustness. To correct this drawback, we will also present a new version of this method, see Algorithm 3. Besides, its convergence analysis is carried out under weaker conditions. In order to present both algorithms, we consider a merit function $\varphi : \mathcal{M} \to \mathbb{R}$ associated to the vector field $X$, which is defined as

$$\varphi(p) = \frac{1}{2} \| X(p) \|^2. \quad (11)$$

4.1 Damped Newton method

In the following we present a version of the algorithm introduced in [11] for a general retraction. This algorithm is similar to the one presented in [11], for the sake of completeness and support in the next section, we have included it here. The formal statement of the algorithm is as follows.

Algorithm 2. Damped Newton method

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**Step 0.** Choose a scalar $\sigma \in (0, 1/2)$, take an initial point $p_0 \in \mathcal{M}$, and set $k = 0$;

**Step 1.** Compute search direction $v_k \in T_{p_k} \mathcal{M}$ as a solution of the linear equation

$$X(p_k) + \nabla X(p_k) v = 0. \quad (12)$$

If $v_k$ exists go to **Step 2.** Otherwise, set the search direction as $v_k = -\text{grad} \varphi(p_k)$, where $\varphi$ is defined by (11), i.e.,

$$v_k = -\nabla X(p_k)^* X(p_k). \quad (13)$$

If $v_k = 0$, stop.

**Step 2.** Compute the stepsize by the rule

$$\alpha_k := \max \left\{ 2^{-j} : \varphi(R_{p_k}(2^{-j} v_k)) \leq \varphi(p_k) + \sigma 2^{-j} \langle \text{grad} \varphi(p_k), v_k \rangle, \ j \in \mathbb{N} \right\}; \quad (14)$$

and set the next iterated as

$$p_{k+1} := R_{p_k}(\alpha_k v_k); \quad (15)$$

**Step 3.** Set $k \leftarrow k + 1$ and go to **Step 1.**
We can see that Algorithm 2 is a generalized version of the algorithm considered in [11], by using a general retraction in Step 2. To analyze a sequence generated by the method studied in [11] it was necessary to assume nonsingularity of covariant derivative of the vector field at its cluster points. This assumption is also required here, it allows us to obtain the same result of the ones obtained in [11]. Next we state the convergence theorem to sequence generated by Algorithm 2. Since its proof can be made by adaptations of the idea used in [11] to general retraction, we do not present it here.

**Theorem 2.** Let $M$ be a Riemannian manifold, $\Omega \subset M$ be an open set and $X : \Omega \to TM$ be a differentiable vector field. Take $R$ a retraction in $M$. Assume $\{p_k\}$, generated by Algorithm 2, has an accumulation point $p \in \Omega$ and $\nabla X$ is continuous and nonsingular at $p$. Then, $\{p_k\}$ converges superlinearly to $p$ and is a singularity of $X$.

It is well known that the superlinear rate of Newton method just can be reached when the covariant derivative is nonsingular at the solution. However, this assumption is not necessary to obtain convergence of the damped Newton method. On the other hand, the equation (12) at points far away a singularity may have more than one solution. In that case, a sufficient decreasing of the merit function is not guaranteed, which implies a great computational effort of linear search in Step 2. Consequently, the robustness of the method is affected. In the next section, we will present a condition that excludes those solutions of (12) that do not ensure sufficient decreasing of the merit function.

### 4.2 Modified damped Newton method

In this section, we state the main algorithm of present paper and its global convergence analysis. This algorithm has an extra condition on the Newtonian direction in order to improve the theoretical results and numerical performance of Algorithm 2. The statement of the algorithm is as follows.

**Algorithm 3.** Modified damped Newton method

**Step 0.** Choose a scalar $\sigma \in (0, 1/2)$, $\theta \in [0, 1]$, take an initial point $p_0 \in M$, and set $k = 0$;

**Step 1.** Compute search direction $v_k \in T_{p_k}M$ as a solution of the linear equation

$$X(p_k) + \nabla X(p_k)v = 0. \tag{16}$$

If $v_k$ exists and

$$\langle \text{grad } \varphi(p_k), v_k \rangle \leq -\theta \| \text{grad } \varphi(p_k) \| \| v_k \| \tag{17}$$

go to **Step 2**. Otherwise, set the search direction as $v_k = -\text{grad } \varphi(p_k)$, where $\varphi$ is defined by (11), i.e.,

$$v_k = -\nabla X(p_k)^* X(p_k). \tag{18}$$

If $v_k = 0$, stop.
Step 2. Compute the stepsize by the rule
\[ \alpha_k := \max \left\{ 2^{-j} : \varphi \left( R_{p_k} (2^{-j} v_k) \right) \leq \varphi(p_k) + \sigma 2^{-j} \langle \nabla \varphi(p_k), v_k \rangle, \ j \in \mathbb{N} \right\}; \] (19)
and set the next iterated as
\[ p_{k+1} := R_{p_k} (\alpha_k v_k); \] (20)

Step 3. Set \( k \leftarrow k + 1 \) and go to Step 1.

Let us describe the main features of Algorithm 3. We first compute \( v_k \) a solution of (16) if any, and then we check if it satisfies (17). In this case, we use it as a search direction in Step 2. On the other hand, if \( v_k \) does not satisfy either (16) or (17), then we set the steepest descent direction \( v_k = -\nabla \varphi(p_k) \) as the search direction in Step 2. In fact, is the steepest descent direction for the merit function (11). Finally, we use the Armijo’s linear search (19) to compute a step-size \( \alpha_k \).

Then, for a given retraction fixed previously, from the current \( p_k \) we compute the next iterated \( p_{k+1} \) by (20).

Remark 2. We point out for \( \theta = 0 \), Algorithm 3 with the retraction being the exponential map retrieve the algorithm considered in [11]. Indeed, if \( v_k \neq 0 \) satisfies (16), then we have
\[ \langle \nabla \varphi(p_k), v_k \rangle = -\|X(p_k)\|^2 < 0, \]
which implies that the condition (17) holds trivially for \( \theta = 0 \). Also, note that the condition \( \theta = 1 \) is the most restrictive among all those in the range \( [0, 1] \). Because, the condition (17) happens only when \( \nabla \varphi(p_k) \) and \( v_k \) are collinear.

Before studying the properties of the sequence generated by the Algorithm 3 it is need some preliminaries results. We begin with a useful result for establishing the well-definition of this sequence, which the proof can be found in [11, Lemma 3].

Lemma 4. Let \( p \in \Omega \) such that \( X(p) \neq 0 \). Assume that \( v = -\nabla X(p)^* X(p) \) or that \( v \) is a solution of the linear equation \( X(p) + \nabla X(p)v = 0 \). If \( v \neq 0 \), then \( \langle \nabla \varphi(p), v \rangle < 0 \).

Under suitable assumptions the following result guarantees that the conditions (16) and (17) are satisfied in a neighbourhood of a point where the covariant derivative is nonsingular.

Lemma 5. If \( \nabla X \) is continuous at \( \bar{p} \in \Omega \) and \( \nabla X(\bar{p}) \) is nonsingular, then there exists \( 0 < \delta < \delta_{\bar{p}} \) such that \( B_{\delta}(\bar{p}) \subset \Omega \), \( \nabla X(p) \) is nonsingular for \( p \in B_{\delta}(\bar{p}) \). Moreover, for all \( p \in B_{\delta}(\bar{p}) \) the vector \( v = -\nabla X(p)^{-1} X(p) \) is the unique solution of the linear equation \( X(p) + \nabla X(p)v = 0 \) and, for \( 0 \leq \theta < 1/\text{cond}(\nabla X(p)) \), there holds
\[ \langle \nabla \varphi(p), v \rangle \leq -\|\nabla \varphi(p)\||v||, \quad \forall \ p \in B_{\delta}(\bar{p}). \] (21)

Proof. The first part of the proof follows from Lemma 3. Whenever \( X(p) = 0 \), the inequality (21) holds. Assume that \( X(p) \neq 0 \), for all \( p \in B_{\delta}(\bar{p}) \). Letting \( p \in B_{\delta}(\bar{p}) \), we obtain that \( \nabla X(p) \) is nonsingular. Thus, \( v = -\nabla X(p)^{-1} X(p) \) is the unique solution of \( X(p) + \nabla X(p)v = 0 \), and due to \( \nabla \varphi(p) = \nabla X(p)^{*} X(p) \) and \( \|\nabla X(p)^{*}\| = \|\nabla X(p)\| \) we conclude that
\[ \frac{\langle \nabla \varphi(p), -v \rangle}{\|\nabla \varphi(p)\||v||} = \frac{\|X(p)\|}{\|\nabla X(p)^{*} X(p)\||\nabla X(p)^{-1} X(p)||} \geq \frac{1}{\|\nabla X(p)^{*}\||\nabla X(p)^{-1}||} = \frac{1}{\text{cond}(\nabla X(p))}. \]
Thus, using (25) and (2) we conclude that
\[
\lim_{p \to \bar{p}} \frac{\langle \text{grad} \, \varphi(p), -v \rangle}{\| \text{grad} \, \varphi(p) \| \| v \|} \geq \frac{1}{\text{cond}(\nabla X(\bar{p}))} > \theta.
\]
Therefore, there exists \( \delta < \bar{\delta} \) such that \( \langle \text{grad} \, \varphi(p), -v \rangle / \| \text{grad} \, \varphi(p) \| \| v \| > \theta \), for all \( p \in B_{\delta}(\bar{p}) \), and (21) also holds for \( X(p) \neq 0 \).

Next lemma shows, in particular, that for \( k \) sufficiently large \( \alpha_k \equiv 1 \) given by (19). Consequently, (20) becomes the Newton iteration (7).

**Lemma 6.** Let \( \bar{p} \in \mathbb{M} \) such that \( X(\bar{p}) = 0 \). If \( \nabla X \) is continuous at \( \bar{p} \) and \( \nabla X(\bar{p}) \) is nonsingular, then there exists \( 0 < \bar{\delta} < \delta \), such that \( B_{\bar{\delta}}(\bar{p}) \subset \Omega \), \( \nabla X(p) \) is nonsingular for each \( p \in B_{\bar{\delta}}(\bar{p}) \) and
\[
\lim_{p \to \bar{p}} \frac{\varphi(N_{R,X}(p))}{\| X(p) \|^2} = 0.
\]

As a consequence, there exists a \( \delta > 0 \) such that, for all \( \sigma \in (0, 1/2) \) and \( \delta < \bar{\delta} \) there holds
\[
\varphi(N_{R,X}(p)) \leq \varphi((p)) + \sigma \langle \text{grad} \, \varphi(p), -\nabla X(p)^{-1}X(p) \rangle, \quad \forall \ p \in B_{\delta}(\bar{p}).
\]

**Proof.** Using Lemma 1 we obtain that there exists \( 0 < \bar{\delta} < \delta \), such that \( B_{\bar{\delta}}(\bar{p}) \subset \Omega \) and \( \nabla X(p) \) is nonsingular for each \( p \in B_{\bar{\delta}}(\bar{p}) \). We proceed to prove (22). To simply the notation we define
\[
v_p = -\nabla X(p)^{-1}X(p), \quad p \in B_{\delta}(\bar{p}).
\]
Since \( X(\bar{p}) = 0 \) and \( \nabla X \) is continuous at \( \bar{p} \) and nonsingular we have \( \lim_{p \to \bar{p}} v_p = 0 \). Moreover, since the parallel transport is an isometry and taking into account (2) and (4) we can conclude that
\[
\varphi(N_{R,X}(p)) = \frac{1}{2} \| X(R_p v_p) - P_{\bar{p}R_p}X(\bar{p}) \|^2 \leq \frac{1}{2a_0^2} \left( \| \nabla X(\bar{p}) \| + \| r(R_p v) \| \right)^2 d^2(R_p v, \bar{p}).
\]
Hence, after some simples algebraic manipulations we can conclude from the last inequality that
\[
\frac{\varphi(N_{R,X}(p))}{\| X(p) \|^2} \leq \frac{1}{2a_0^2} \left( \| \nabla X(\bar{p}) \| + \| r(R_p v) \| \right)^2 \frac{d^2(R_p v, \bar{p})}{d^2(p, \bar{p})} \frac{d^2(p, \bar{p})}{\| X(p) \|^2}, \quad \forall \ p \in B_{\delta}(\bar{p}) \setminus \{ \bar{p} \}.
\]
On the other hand, owing that \( X(\bar{p}) = 0 \) and \( \nabla X(\bar{p}) \) is nonsingular, it is easy to see that
\[
\| R_p^{-1} - p \| \leq \| \nabla X(\bar{p})^{-1} [P_{pp}X(p) - X(\bar{p}) - \nabla X(\bar{p})R_p^{-1}p] \| + \| \nabla X(\bar{p})^{-1}P_{pp}X(p) \|.
\]
Since \( \nabla X(\bar{p}) \) is nonsingular, using (2) and (4), and taking into account that \( \lim_{p \to \bar{p}} r(p) = 0 \), we can take \( \delta > 0 \) with \( 0 < \delta < \delta \), such that
\[
\| \nabla X(\bar{p})^{-1} [P_{pp}X(p) - X(\bar{p}) - \nabla X(\bar{p})R_p^{-1}p] \| \leq \frac{a_0}{2a_1} \| R_p^{-1}p \|
\leq \frac{1}{2a_1} d(p, \bar{p}), \quad \forall \ p \in B_{\delta}(\bar{p}).
\]
Thus, using (25) and (2) we conclude that \( d(p, \bar{p}) \leq d(p, \bar{p})/2 + a_1 \| \nabla X(\bar{p})^{-1}P_{pp}X(p) \| \), for all \( p \in B_{\delta}(\bar{p}) \), which is equivalent to
\[
\frac{d(\bar{p}, p)}{\| X(p) \|} \leq 2a_1 \| \nabla X(\bar{p})^{-1} \|, \quad \forall \ p \in B_{\delta}(\bar{p}).
\]
Let \( \delta = \min\{\delta', \delta\} \) we conclude from (24) and last inequality that, all \( p \in B_\delta(\bar{p}) \setminus \{\bar{p}\} \), holds

\[
\frac{\varphi (N_{R, X}(p))}{\| X(p) \|^2} \leq \frac{2a^2_0}{a_0^2} \| \nabla X(\bar{p}) \|^{-1} (\| \nabla X(\bar{p}) \| + \| r(R_p v_p) \|) \frac{d^2(r(\bar{p}, v_p))}{d^2(p, \bar{p})}.
\]

Therefore, using Lemma 2 and considering \( \lim_{p \to \bar{p}} r(R_p v_p) = 0 \), the equality (23) follows by taking limit, as \( p \) goes to \( \bar{p} \), in the latter inequality. For proving (23), we first use (22) for concluding that there exists a \( \delta > 0 \) such that, \( \delta < \delta' \) and for \( \sigma \in (0, 1/2) \) we have

\[
\varphi (N_{R, X}(p)) \leq \frac{1 - 2\sigma}{2} \| X(p) \|^2, \quad \forall \ p \in B_\delta(\bar{p}).
\]

Since \( \text{grad} \, \varphi(p) = \nabla X(p)^* X(p) \) we obtain \( \langle \text{grad} \, \varphi(p), -\nabla X(p)^{-1} X(p) \rangle = -\| X(p) \|^2 \), then the last inequality is equivalent to (23) and the proof is concluded. \( \square \)

### 4.3 Convergence Analysis

In this section we establish our main results, namely, the global convergence and superliner rate of the sequence generated by Algorithm 3. Before presenting these results, we remark that the well-definition of the sequence generated by Algorithm 3 follows from Lemma 4, see [11, Lemma 6]. It is worth noting that, if the sequence generated by Algorithm 3 is finite, then the last point generated is a solution of (5) or it is critical point of \( \varphi \) defined in (11). Thus, from now on, we assume that \( \{p_k\} \) is infinite. In this case, we have \( v_k \neq 0 \) and \( X(p_k) \neq 0 \), for all \( k = 0, 1, \ldots \).

**Theorem 3.** Let \( \mathbb{M} \) be a Riemannian manifold, \( \Omega \subset \mathbb{M} \) be an open set and \( X : \Omega \to T\mathbb{M} \) be a continuously differentiable vector field. Take \( R \) a retraction in \( \mathbb{M} \). If \( \bar{p} \in \Omega \) is an accumulation point of a sequence \( \{p_k\} \) generated by Algorithm 3 then \( \bar{p} \) is a critical point of \( \varphi \). Moreover, assuming that \( \nabla X \) is nonsingular at \( \bar{p} \), the convergence of \( \{p_k\} \) to \( \bar{p} \) is superlinear and \( X(\bar{p}) = 0 \).

**Proof.** Assume that \( \{p_k\} \) generated by Algorithm 3 has an accumulation point \( \bar{p} \). First, we show that \( \bar{p} \) is a critical point of \( \varphi \). We can assume \( \text{grad} \, \varphi(p_k) \neq 0 \) for all \( k = 0, 1, \ldots \). Hence, from (19)

\[
\varphi(p_k) - \varphi(p_{k+1}) \geq -\sigma \alpha_k \langle \text{grad} \, \varphi(p_k), v_k \rangle = \begin{cases} \sigma \alpha_k \| X(p_k) \|^2 > 0, & \text{if } v_k \text{ satisfies (16) and (17)}; \\ \sigma \alpha_k \| \text{grad} \, \varphi(p_k) \|^2 > 0, & \text{else}. \end{cases}
\]

Thus, \( \{\varphi(p_k)\} \) is strictly decreasing. Since \( \varphi \) is bounded from below by zero, it converges. Therefore,

\[
0 = \lim_{k \to \infty} \alpha_k \langle \text{grad} \, \varphi(p_k), v_k \rangle = \begin{cases} \sigma \lim_{k \to \infty} \alpha_k \| X(p_k) \|^2 = 0, & \text{if } v_k \text{ satisfies (16) and (17)}; \\ \sigma \lim_{k \to \infty} \alpha_k \| \text{grad} \, \varphi(p_k) \|^2 = 0, & \text{else}. \end{cases}
\]

In this equality we have two possibilities, namely, \( \liminf_{k \to \infty} \alpha_k > 0 \) and \( \liminf_{k \to \infty} \alpha_k = 0 \). First, we assume that \( \liminf_{k \to \infty} \alpha_k > 0 \). Let \( \{p_k\} \) be a subsequence of \( \{p_k\} \) such that \( \lim_{k \to \infty} p_k = \bar{p} \) and \( \lim_{j \to \infty} \alpha_{k_j} = \bar{\alpha} > 0 \). Taking into account \( \lim_{j \to \infty} p_k = \bar{p} \) and \( X \) is continuous at \( \bar{p} \) we conclude \( X(\bar{p}) = 0 \) or \( \text{grad} \, \varphi(\bar{p}) = 0 \). Since \( \text{grad} \, \varphi(\bar{p}) = \nabla X(\bar{p})^* X(\bar{p}) \), \( \bar{p} \) is a critical point of \( \varphi \). Now, we assume that \( \liminf_{j \to \infty} \alpha_{k_j} = 0 \). We analyze the following two possibilities: the sequence \( \{v_k\} \) is unbounded or bounded. Firs we assume \( v_k \) is unbounded. Since \( \lim_{j \to \infty} p_k = \bar{p} \) and \( X \) is continuous \( \bar{p} \), the direction \( v_k \) satisfies (18) just for finite indexes, otherwise \( \lim_{j \to \infty} v_k = -\lim_{j \to \infty} \nabla X(p_k)^* X(p_k) = -\nabla X(\bar{p})^* X(\bar{p}) \), which contradicts the assumption.
Thus, making \( \hat{\mathbf{v}} \) converges superlinearly to \( \bar{\mathbf{v}} \). Finally, to obtain the superlinear convergence of the algorithms studied in the previous sections. The examples are established on spheres, product of

5 Numerical Experiments

In this section, some examples are presented in order to examine the numerical behavior of algorithms studied in the previous sections. The examples are established on spheres, product of
two Stiefel manifolds and cones of symmetric positive definite matrices. All numerical experiments have been developed by using MATLAB R2015b and were performed on an Intel Core Duo Processor 2.26 GHz, 4 GB of RAM, and OSX operating system. We have been considered convergence at the iterate \( k \) when \( p_k \in M \) satisfies \( \| \nabla f(p_k) \| < 10^{-6} \), where \( \| \cdot \| \) is the norm associated to metric of the considered manifold. The algorithms were interrupted when the step length reached a value less than \( 10^{-10} \) or the maximum number of 2000 iterates was reached. Moreover, we have been assumed \( \sigma = 10^{-3} \). All codes are freely available at [http://www2.uesb.br/professor/mbortoloti/wp-content/uploads/2020/08/public_codes.zip](http://www2.uesb.br/professor/mbortoloti/wp-content/uploads/2020/08/public_codes.zip).

5.1 Problems on the sphere

The aim of this section is to present problems on the sphere \( M := (S^n, \langle \cdot, \cdot \rangle) \), where \( S^n := \{ p := (p_1, ..., p_{n+1}) \in \mathbb{R}^{n+1} : \| p \| = 1 \} \) is endowed with the Euclidian inner product \( \langle \cdot, \cdot \rangle \) and its corresponding norm \( \| \cdot \| \). The tangent hyperplane in \( M \) at \( p \) is given by \( T_pM := \{ v \in \mathbb{R}^{n+1} : \langle p, v \rangle = 0 \} \).

It is worth noting that problems have already studied in [11]. They were solved by using Algorithm 2 where the exponential

\[
\exp_p v = \cos(\| v \|) p + \sin(\| v \|) \frac{v}{\| v \|}, \quad p \in S^n, \ v \in T_pM/\{0\},
\]  

(27)

were used to update the iterates. Here we compare the performance of Algorithm 2 by using the exponential and the following retraction

\[
R_p v = \frac{p + v}{\| p + v \|}, \quad p \in S^n, \ v \in T_pM/\{0\}.
\]  

(28)

It is worth to point out that, for all problems studied in this section, all results obtained show that Algorithm 2 with the retraction (28) has a better performance than the exponential (27). We also note that retraction (28) has performed better than (27) in others algorithms, see for example [44].

5.1.1 Non conservative vector field

In this section, we consider the problem of finding a singularity of a non conservative vector field on the sphere. For that fix a point \( \bar{p} \in M \) and \( Q \) a \( n \times n \) skew-symmetric matrix, and define the vector field \( X \) by

\[
X(p) = Q(p - \bar{p}) - \langle p, Q(p - \bar{p}) \rangle p.
\]

Note that \( \bar{p} \) is a singularity of \( X \), i.e., \( X(\bar{p}) = 0 \). We recall the covariant derivative of \( X \) is given by

\[
\nabla X(p) = \left[ I + pp^T \right] Q - p (Q(p - \bar{p}))^T - \langle p, Q(p - \bar{p}) \rangle I.
\]

Since \( Q \) is not symmetric neither is \( \nabla X(p) \), consequently, \( X \) is not a conservative vector field. We present a comparative study between retractions (27) and (28) for Algorithm 2. We have performed numerical experiments for dimensions \( n = 2, 50, 500, 1000 \). For each dimension, we consider a skew matrix, \( Q \), defined as \( Q = A - A^T \), where \( A \) is a random matrix generated by code \( A = \text{randn}(n,n) \). We have taken one initial guess on sphere for dimension, in order to start algorithm. Our numerical results are presented in Table 1 where Iter and EX denote the iteration numbers and evaluation of vector field, respectively. It can be seen that the exponential mapping presents a greater number of vector fields evaluations than retraction. Moreover, the retraction (28) solves the problems with a smaller number of iterations than exponential map (27). We also remark that the quantities Iter and EX do not depend on the dimension of the problem.
Table 1: Comparison between retractions (27) and (28) for Algorithm 2.

| n     | 
|-------|-------|-------|-------|-------|-------|
| exp_p | exp_p | R_p  | R_p  |
|-------|-------|-------|-------|
| 2     | 7     | 7     | 14    | 14    |       |
| 50    | 22    | 21    | 75    | 64    |       |
| 500   | 27    | 26    | 71    | 61    |       |
| 1000  | 15    | 12    | 31    | 25    |       |

5.1.2 Rayleigh quotient

Numerical results to minimizer the Rayleigh quotient on the sphere is presented in this section. Let $A$ be an $n \times n$ symmetric and positive definite matrix and $f : \mathbb{S}^n \to \mathbb{R}$ be the Rayleigh quotient, $f(p) = p^T Ap$.

The gradient and the hessian of $f$ are given by, respectively, by

$$\text{grad } f(p) = -2 [I + pp^T] Ap, \quad \text{Hess } f(p) = [I + pp^T] [A - p^T ApI].$$

In order to develop our numerical experiments, we define the Rayleigh quotient mapping by considering symmetric positive definite matrices $A$, given by the following codes

1. $A = \text{gallery('poisson',ceil(sqrt(n))+1)}$,
2. $A = \text{ones(n,n)}; A = A*\text{diag(diag(A))} + \text{diag(2*n*ones(n,1))}$,
3. $e = \text{ones(n,1)}; A = \text{spdiags([e 10*e e], -1:1, n, n)}$,
4. $v = \text{rand(n,1)}; A = \text{diag(v)}; A(1,n) = 1; A(n,1) = 1$,
5. $A = \text{sprandsym(n,0.7,0.1,1)}$.

For each type of matrix above, simulations were performed for dimensions $n = 500, 750, 1000, 1250, 1500$, where we considered, for each one, 10 initial guesses randomly taken on sphere, totaling 250 problems.

In figure 1 can be seen that the retraction (28) solves all problems faster than exponential (27). We can also observe that Algorithm 2 with (28) solves all problems before 0.2 CPU time ratio. This behaviour can be assigned to the simple form of retraction (28) so that fewer calculations are needed to generate the next point in the sequence, when considered the classical exponential.

5.2 The truncated singular value problem on Stiefel manifold

In this section, we study the globality of Algorithm 3 to solve a truncated singular value problem. This problem, analyzed in [41], consists of

$$\min F(P, Q) = \text{Tr}(-P^T A Q N)$$

subject to $(P, Q) \in St(p, m) \times St(p, n)$ (29)
where, Tr (X) denotes the trace of X, \( St(p,n) = \{ P \in \mathbb{R}^{n \times p} : P^T P = I_p \} \) is the Stiefel manifold endowed with the Frobenius metric, \( A \in \mathbb{R}^{m \times n} \) with \( m \geq n \) is a given matrix, and \( N = \text{diag}(\mu_1, \mu_2, \ldots, \mu_p) \) is a diagonal matrix with \( \mu_1 > \mu_2 > \ldots > \mu_p > 0 \) for \( p \leq n \).

Considering \( P \in St(p,m) \), the tangent space of \( St(p,m) \), at \( P \), is given by
\[
T_P St(p,m) = \{ PB + P_\perp C : B \in \text{Skew}(p), C \in \mathbb{R}^{(m-p) \times p} \}
\]
where \( \text{Skew}(p) \) denotes the set of all \( p \times p \) skew-symmetric matrices and \( P_\perp \) is an \( n \times (n-p) \) orthonormal matrix such that \( PP^T + P_\perp P_\perp^T = I_m \).

In order to implement the Algorithm 2 to solve problem (29), we present the Newton equation (12) and the safeguard direction (18). The Newton equation at \((P,Q) \in St(p,m) \times St(p,n)\) in the variables \( U,V \in T_P St(p,m) \times T_Q St(p,n) \) is written as
\[
\begin{align*}
VS_1 - AUN - P \text{ sym} (P^T (VS_1 - AUN)) &= AQN - PS_1, \\
US_2 - ATVN - Q \text{ sym} (Q^T (US_2 - ATVN)) &= A^T PN - QS_2,
\end{align*}
\]
see [5]. The safeguard direction (18) is given by
\[
\text{grad } \varphi (P,Q) (V,U) = (VS_1 - AUN - P \text{ sym} (P^T (VS_1 - AUN)), \\
US_2 - ATVN - Q \text{ sym} (Q^T (US_2 - ATVN)) ),
\]
where \( \text{sym} (X) = (X + X^T)/2 \) denotes the symmetric part of a square matrix \( X \), \( S_1 = \text{sym} (P^T AQN) \) and \( S_2 = \text{sym} (Q^T A^TPN) \). To compute the iterates on Stiefel manifold, we have considered the following retractions:

- Exponential map, [19], given by
\[
R_P(V) = PM + QN,
\]
where \( QR \) is the compact decomposition of \((I_n - PP^T)V\) such that \( Q \) is \( n \)-by-\( p \), \( R \) is \( p \)-by-\( p \) and \( M,N \) are \( p \)-by-\( p \) matrices given by the \( 2p \)-by-\( 2p \) matrix exponential
\[
\begin{pmatrix}
M \\
N
\end{pmatrix} = \exp \begin{pmatrix}
PP^T & -R^T \\
R & 0
\end{pmatrix} \begin{pmatrix}
I_p \\
0
\end{pmatrix}.
\]
• Cayley map, [48], written as

\[ R_P(V) = P + M \left( I_{2p} - \frac{1}{2} N^T M \right)^{-1} M^T P, \]  

where \( M = [\Pi_V P, P] \) and \( N = [P, -\Pi_P V] \), with \( \Pi_P = I_p - PP^T / 2 \).

• Polar map, [2], given by

\[ R_P(V) = (P + V) \left( I_p + V^T V \right)^{-1/2}. \]  

• qf retraction, [2], written as

\[ R_P(V) = qf(P + V), \]  

where \( qf(P) \) denotes the Q factor of the QR decomposition with nonnegative elements on the diagonal of the upper triangle matrix.

In order to solve the equations in (30) we used the ideas presented in [5]. The numerical experiments were performed on the product of two Stiefel manifolds, \( St(p, m) \times St(p, n) \), with \((m, n, p) = (5, 3, 2), (7, 5, 2), (10, 5, 3), (20, 10, 3) \). For each \((m, n, p)\), the generated problem has \((P^*, Q^*) \in St(p, m) \times St(p, n)\) as critical point and \( A = P^* N Q^* T \), where \( N = \text{diag}(p, p - 1, \ldots, 1) \) and \( P^*, Q^* \) are given by the Q factors of the QR decompositions of two random matrices. It were taken 10 initial guesses \((P_0, Q_0)\), for each dimensions \((m, n, p)\), by considering the matrices \( P_0 = qf(P^* + \text{randn}(m, p) \varepsilon) \) and \( Q_0 = qf(Q^* + \text{randn}(n, p) \varepsilon) \) with \( \varepsilon = 10^{-4}, 10^{-3}, \ldots, 10^3 \).

In figures 2(a)-2(d) we present the percentage of solved problems when the initial guesses are taken by considering the values from \( \varepsilon = 10^{-4} \) to \( \varepsilon = 10^3 \). As it can seen, the Algorithm 3 is not sensitive to increasing of \( \varepsilon \) solving 100% of the problems for each retraction given in (31)-(34).

5.3 Academic problem on the cone of symmetric positive definite matrices

The aim of this section is to present some numerical experiments to illustrate the behavior of Algorithms 2 and 3. For that, we have considered the problem for minimizing two different functions defined on the cone of symmetric positive definite matrices, \( \mathbb{P}^n_{++} \), endowed with the inner product given by \( \langle U, V \rangle = \text{tr}(V P^{-1} U P^{-1}) \), \( P \in \mathbb{P}^n_{++}, U, V \in T_P \mathbb{P}^n_{++} \approx \mathbb{P}^n \) where, \( \mathbb{P}^n \) denotes the set of symmetric matrices. Consider \( f_1, f_2 : \mathbb{P}^n_{++} \rightarrow \mathbb{R} \) defined by

\[ f_1(P) = \ln \det P + \text{tr} P^{-1}, \quad f_2(P) = \ln \det P - \text{tr} P, \]  

where \( \det P \) and \( \text{tr} P \) denote the determinant and trace of \( P \), respectively. The function \( f_2 \) can be related to robotics, see [10, 24, 25]. It is worth noting that these problems have already studied in [11]. In order to implement the Algorithms 2 and 3 to minimize the functions in (35), we first present the Newton equation and the safeguard direction associated to them. The Newton equations for \( f_1 \) and \( f_2 \) are, respectively, given by

\[ PV + VP = 2 (P^2 - P^3), \quad P^{-1} V + VP^{-1} = 2 (P^{-1} - I), \]  

where \( I \) denotes the \( n \times n \) identity matrix. On the other hand, the gradient of merit function for \( f_1 \) and \( f_2 \) can be, respectively, written as

\[ \text{grad } \varphi_1(P) = I - P^{-1}, \quad \text{grad } \varphi_2(P) = P^3 - P^2. \]
For all $P \in \mathbb{P}^{n+}++$ and $V \in T_P \mathbb{P}^{n+}+$ we compute the iterates in (15) and (20) by using the following retractions

\[ R_P V = P^{1/2} \exp \left( P^{-1/2} V P^{-1/2} \right) P^{1/2}, \tag{36} \]
\[ R_P V = P \exp \left( P^{-1} V \right), \tag{37} \]
\[ R_P V = P + V + 1/2VP^{-1}V, \tag{38} \]
\[ R_P V = P + V. \tag{39} \]

The map presented in (36) is the classical exponential and (37) is obtained from (36), see [45]. For (38) and (39), see [31] and [9], respectively.

For both functions given by (35) we consider dimensions $n = 100, 200, \ldots, 1000$ and 5 initial guesses for each dimension, totaling 50 problems for each retraction. The initial guesses were generated by considering the same type of symmetric positive definite matrices presented in Section 5.1.2. Figure 3 shows a performance of Algorithm 2 with the retractions (36) and (37) for minimizing the function $f_1$. It can be seen that the retraction (37) is much better than the second one. This behaviour can be justified by the smaller number of operations required to generate each iterate of the method.

In order to highlight the improvement of the Algorithm 3 related to robustness, we compare it with Algorithm 2 by using $\theta = 0.9999$. It can be seen in figures 4(a) and 4(b) that Algorithm 2 provided with retractions (34) and (35), did not solve all problems. This has happened because the step length has became too small. On the other hand, Algorithm 3 was able to solve all problems because the inequality given by (17) prevents an inappropriate decreasing of step length.
Figure 3: Performance profiles comparing retractions (36) and (37) for $f_1$ in the Algorithm 2.

(a) $R\rho V = P + V$

(b) $R\rho V = P + V + \frac{1}{2}V P^{-1}V$

Figure 4: Comparison between Algorithms 2 and 3 with retractions (39) and (38) for $f_1$.

For minimizing the function $f_2$, we compare retractions (36)-(38) in the Algorithm 2 as can be seen in the figure 5. It shows that the retraction (39) is much better than the other.

Figure 5: Performance profiles comparing retractions (36)-(38) for $f_2$ in the Algorithm 2.
6 Conclusions

In this work, in order to find a singularity of a vector field defined on Riemannian manifolds, we presented a globalization of Newton method and established its global convergence with superlinear rate. The Algorithm 2 was designed with a general retraction in order to improve the performance of the analogous presented in [11]. As it can be seen in the Section 5, the numerical performance of Algorithm 2 is better than the one presented in [11]. We point out that the convergence analysis presented in [11] requires nonsingularity of covariant derivative at cluster point. On the other hand, the condition (17) in the Algorithm 3 ensures that this hypothesis on the covariant derivative is not necessary to establish convergence, as it can be seen in the Theorem 3. In addition, it is worth mentioning that condition (17) seems to avoid Newton directions that can generate quite small step lengths. As a consequence, Algorithm 3 is more robust than Algorithm 2 in number of solved problems as we can see in the experiments presented in Sections 5.2 and 5.3.

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