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Solving Weighted Orthogonal Procrustes Problems via a Projected Gradient Method

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ABSTRACT. This paper proposes a family of line–search methods to deal with weighted orthogonal procrustes problems. In particular, the proposed family uses a search direction based on a convex combination between the Euclidean gradient and the Riemannian gradient of the cost function. The non–monotone line–search of Zhang and Hager, and an adaptive Barzilai–Borwein step–size are the chosen tools, in order to speed up the convergence of the new family of methods. One of the extremes of that convex combination is reduced to well–known spectral projected gradient method, while the another one can be interpreted as a Riemannian steepest descent method. To preserve feasibility of all the iterates, we use a projection operator based on the singular value decomposition, which can be computed efficiently via the spectral decomposition of an appropriate matrix. In addition, we prove that the entire uncountable collection of search directions satisfies a descent condition. Some numerical experiments are provided in order to demonstrate the effectiveness of the new approach.

Keywords: continuous optimization, constrained optimization, Stiefel manifold, procrustes analysis, projected gradient method.

1 INTRODUCTION

In this paper, we consider the following equality constrained least–square problem

$$\min_{X\in\mathbb{R}^{m\times n}} \frac{1}{2}\|AXC-B\|_F^2, \quad \text{subject to} \quad X^\top X = I, \tag{1.1}$$

where $n \leq m$, $A \in \mathbb{R}^{p\times m}$, $B \in \mathbb{R}^{p\times q}$ and $C \in \mathbb{R}^{n\times q}$ are three given data matrices. This optimization problem is known as *the weighted orthogonal procrustes problem* (WOPP) [21, 23]. The set formed by the constraints, that is $St(m,n) := \{X \in \mathbb{R}^{m\times n} : X^\top X = I\}$ is called the *Stiefel manifold* [6]. The Stiefel manifold is a compact set, which guarantees that (1.1) has at least a global

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optimum. This set can be regarded as an embedded Riemannian sub–manifold of $\mathbb{R}^{m\times n}$ with dimension equals to $mn-\frac{1}{2}n(n+1)$, see [1].

The optimization model (1.1) has many applications such as, body rigid movements [22], psychometry [9], global positioning system [3] and trace minimization [24]. In addition, some dimension reduction techniques very useful in statistical pattern recognition such as laplacean eigenmaps, locality preserving projections, orthogonal neighborhood preserving projection, orthogonal locality preserving projections can be posed as problem (1.1), for details see [11].

Some special cases of the non–convex quadratic optimization problem with quadratic equality constraints (1.1) have closed expressions for their solution. In particular, if $B=0$ and $C=I_{n,q}$ (i.e. the rectangular diagonal matrix with diagonal entries equal one) then any global solution correspond to a matrix X^* whose columns span the eigenspace of $A^\top A$ associated with the n–smallest eigenvalues of $A^\top A$, and the optimal value is $0.5\|AX\|_F^2=(\sum_{i=1}^n\lambda_i)/2$, where $\lambda_1\leq\lambda_2\leq\cdots\lambda_m$ denotes the eigenvalues of $A^\top A$. In addition, if $C=I_{n,q}$, and $m=n$ then the optimization problem (1.1) is known as the *orthogonal procrustes problem* (OPP) [21, 23, 28] or also *balanced procrustes problem* [28] and an explicit solution can be derived by using the singular value decomposition (SVD) of $B^\top A$, [21, 23]. The general case when $C=I_{n,q}$, and $n<m$ is known as *unbalanced procrustes problem* [28]. Unfortunately, both the unbalanced procrustes problem and the weighted version of the orthogonal procrustes problem, i.e. the optimization model (1.1) do not have closed expressions for their solutions. Moreover, compute a solution of the more general problem (1.1) is a costly task, due to the non–linearity and non–convexity of the constraints set $St(m,n)$, which may generate that the WOPP problem have multiple local or global solutions. In fact, Viklands in [23] conjectured that the WOPP problem has at most 2^n unconnected minima. Therefore, a solution is possible only computationally by using an iterative procedure. There are several iterative algorithms, in the literature, that can be used to solve the problem (1.1), see [8, 13, 15, 16, 18, 20, 25, 29]. The vast number of applications of the optimization problem (1.1) and the difficulty to solve it motivates the design of new iterative methods to obtain approximations of at least its local minimizers.

In this paper, we develop a new iterative algorithm to tackle the optimization problem (1.1). In particular, we design a new projected gradient–type method, which uses a search direction based on a convex combination between the Euclidean gradient and the Riemannian gradient of the quadratic cost function. To improve the efficiency of the method, we consider a self–adaptive step size based on the Barzilai–Borwein step sizes, in combination with an inaccurate non-monotone line–search. In order to preserve the feasibility of all the iterates, we use the standard projection operator on the Stiefel manifold. Finally, we present some numerical experiments to illustrate the efficacy and fast convergence of the new approach.

This paper is organized as follows. In the next section, we present some notations and tools necessary for a good understanding of this paper. In subsection 2.1, we establishes the first–order necessary optimality conditions corresponding with (1.1). Section 3 exhibits our proposed algorithm, and comment its convergence properties. Section 4 presents some numerical results. Finally, we provide the conclusions in Section 5.

2 NOTATIONS AND TOOLS

In the rest of the present manuscript, we say that $W \in \mathbb{R}^{n\times n}$ is skew–symmetric if $W = -W^\top$. The expression $\mathscr{M}_n(\mathbb{R}^{m\times n})$ will be denote the following set $\mathscr{M}_n(\mathbb{R}^{m\times n}) := \{X \in \mathbb{R}^{m\times n} : \texttt{rank}(X) = n\}$, where $\texttt{rank}(X)$ denotes the rank of the matrix X. The objective function of problem (1.1) will be denoted by $\mathscr{F}(X) := \frac{1}{2}\|AXC - B\|_F^2$. The trace of X is defined as the sum of the diagonal elements which we denote by $tr[X]$. The Frobenius inner product of two matrices $A, B \in \mathbb{R}^{m\times n}$ is given by $\langle A, B\rangle := \sum_{i,j} a_{ij}b_{ij} = tr[A^\top B]$. It is well–known that this inner product induces the norm of Frobenius norm $\|A\|_F = \sqrt{\langle A, A\rangle}$. Let $F : \mathbb{R}^{n\times p} \to \mathbb{R}$ be a differentiable function, we denote by $\nabla F(X) = (\frac{\partial F(X)}{\partial X_{ij}})$ the matrix of partial derivatives of F (the Euclidean gradient of F). By a simple calculation on the objective function of the problem (1.1) we have $\nabla\mathscr{F}(X) = A^\top(AXC - B)C^\top$, for all $X \in \mathbb{R}^{m\times n}$. Additionally, the directional derivative of F along a given matrix Z at X is defined by:

$$\mathscr{D}F(X)[Z] := \lim_{t\to 0} \frac{F(X + tZ) - F(X)}{t} = \langle \nabla F(X), Z\rangle. \tag{2.1}$$

The tangent space $T_X St(m,n)$ of the Stiefel manifold at $X \in St(m,n)$ is given by

$$T_X St(m,n) = \{Z \in \mathbb{R}^{m\times n} : Z^\top X + X^\top Z = 0\}.$$

The orthogonal projection operator onto the Stiefel manifold is defined by the following constrained optimization problem

$$\pi(X) = \arg\min_{P\in St(m,n)} \|X - P\|_F.$$

The proposition below shows that $\pi : \mathscr{M}_n(\mathbb{R}^{m\times n}) \to St(n,p)$ is a well–defined function, and also provides us with an exact formula to evaluate this projection operator.

Proposition 1. *Let $X \in \mathbb{R}^{m\times n}$ be a rank n matrix. Then, $\pi(X)$ is well defined. Moreover, if the singular value decomposition of X is $X = U\Sigma V^\top$, then $\pi(X) = UI_{m,n}V^\top$, where $I_{m,n} \in \mathbb{R}^{m\times n}$ is the rectangular diagonal matrix with diagonal entries equal one.*

Proof. This result can also be found in [13]. In order to make this manuscript self–contained, we briefly write the proof here. Let $X \in \mathbb{R}^{m\times n}$ be a rank n matrix. Let us suppose that $X = U\Sigma V^\top$ is the singular value decomposition of X. Since the Frobenius norm is invariant under orthogonal transformations, we have

$$\arg\min_{P\in St(m,n)} \|X - P\|_F \equiv \arg\min_{Q\in St(m,n)} \|\Sigma - Q\|_F. \tag{2.2}$$

Hence, it is enough to prove that $Q_* = I_{m,n}$ is the only solution of the following Stiefel manifold constrained optimization problem

$$\min_{Q\in \mathrm{St}(m,n)} \|\Sigma - Q\|_F^2. \tag{2.3}$$

In view of the definition of the Frobenius norm, we have $\|\Sigma - Q\|_F^2 = tr[(\Sigma - Q)^\top(\Sigma - Q)] = p + tr[\Sigma^\top\Sigma] - 2tr[\Sigma^\top Q]$. This relation indicates that solving (2.3) is equivalent to solve the maximization problem presented below

$$\max_{Q\in \mathrm{St}(m,n)} tr[\Sigma^\top Q]. \tag{2.4}$$

Now, let us denote by σ_{ij} and q_{ij} the elements (i,j) of the matrices Σ and Q respectively. Notice that if $Q \in St(m,n)$ is any matrix on the Stiefel manifold then $q_{jj}^2 \leq \sum_{i=1}^m q_{ij}^2 = \|\mathbf{q}_j\|_2^2 = 1$, where $\mathbf{q}_j$ denotes the j–th column of Q. Using this result, and the fact that the matrix Σ is diagonal, we arrive at

$$tr[\Sigma^\top Q] = \sum_{j=1}^n \sigma_{jj} q_{jj} \leq \sum_{j=1}^n \sigma_{jj}|q_{jj}| \leq \sum_{j=1}^n \sigma_{jj} = tr[\Sigma^\top I_{m,n}], \quad \forall Q \in St(m,n). \tag{2.5}$$

From (2.5), we conclude that $I_{m,n}$ is a global solution of problem (2.4), and consequently it is also a global solution of (2.2). Now, by contradiction, suppose that there exists a matrix $Q \in St(m,n)$ such that $Q \neq I_{m,n}$ and $tr[\Sigma^\top Q] = tr[\Sigma^\top I_{m,n}]$. This last condition implies that

$$0 = tr[\Sigma^\top Q] - tr[\Sigma^\top I_{m,n}] = tr[\Sigma^\top (Q - I_{m,n})] = \sum_{j=1}^n \sigma_{jj}(q_{jj} - 1). \tag{2.6}$$

Since $\mathtt{rank}(X) = n$ then it must be verified that $\sigma_{ii} > 0$, for all $i \in \{1,\ldots,n\}$. In addition, since $|q_{jj}| \leq 1$, for all j, and $\sigma_{jj} > 0$, for all j; then the equality (2.6) leads to $q_{jj} = 1$, for all j. However, $I_{m,n}$ is the unique matrix on the Stiefel manifold with diagonal elements equals one. Thus $Q = I_{m,n}$, which is a contradiction. This last fact demonstrates that $I_{m,n}$ is the unique global solution to (2.2). □

Remark 2. *In view of $n \leq m$, we can compute the projection $\pi(X)$ efficiently using the spectral–decomposition based SVD computation. Particularly,*

$$\pi(X) = XVD^{-1/2}V^\top,$$

where $V \in \mathbb{R}^{n\times n}$ is an orthogonal matrix and D is a diagonal matrix satisfying the spectral decomposition $X^\top X = VDV^\top$. This strategy is suggested in [7] to save computations in the calculation of SVD factorizations.

2.1 The Karush–Khun–Tucker conditions

The Lagrangian function related to the optimization problem (1.1) is

$$\mathscr{L}(X,\Lambda) = \mathscr{F}(X) - tr[\Lambda^\top(X^\top X - I_p)], \tag{2.7}$$

where Λ is the Lagrange multipliers matrix (the dual variable), which is symmetric because the constraint $X^\top X$ is also symmetric. By computing the derivative of $\mathscr{L}(X,\Lambda)$ with respect to X and Λ, we obtain the Karush–Khun–Tucker conditions for problem (1.1):

$$\nabla_X \mathscr{L}(X,\Lambda) \equiv \nabla\mathscr{F}(X) - 2X\Lambda = 0, \tag{2.8}$$

$$\nabla_{\Lambda}\mathscr{L}(X,\Lambda) \equiv X^{\top}X - I_p = 0. \tag{2.9}$$

Notice that if (X,Λ) is any critical point of the Lagrangian function then by multiplying by $X^{\top}$ in both side of equation (2.8) and using (2.9), we have an analytical formula for the dual variable Λ

$$\Lambda = \frac{1}{2}X^{\top}\nabla\mathscr{F}(X) = \frac{1}{2}\nabla\mathscr{F}(X)^{\top}X, \tag{2.10}$$

where the last equality is obtained from the symmetry of the Lagrange multiplier matrix.

The following proposition provides us with an important tool to identify critical points of Lagrangian function.

Proposition 3. *Let $X \in St(m,n)$ be any orthogonal matrix satisfying that $(1-\theta)\|\nabla\mathscr{F}(X)\|_F^2 + \theta\|W(X)\|_F^2 = 0$, for a given $\theta \in [0,1]$, where $W : \mathbb{R}^{m\times n} \to \mathbb{R}^{m\times m}$ is the function defined by $W(X) = \nabla\mathscr{F}(X)X^{\top} - X\nabla\mathscr{F}(X)^{\top}$. Then there exists $\Lambda \in \mathbb{R}^{n\times n}$ such that the pair (X,Λ) is stationary point of the Lagrangian function.*

Proof. Let us assume that $\bar{X} \in St(m,n)$ is a matrix such that $(1-\theta)\|\nabla\mathscr{F}(\bar{X})\|_F^2 + \theta\|W(\bar{X})\|_F^2 = 0$, for some $\theta \in [0,1]$. Since $X \in St(m,n)$ then the second condition (2.9) holds. Thus it is enough to prove that (2.8) is also satisfied for some Lagrange multiplier. In fact, notice that if $\theta = 0$ then the hypothesis implies that $\nabla\mathscr{F}(\bar{X}) = 0$. In this case, we have directly that the point $(\bar{X},\bar{\Lambda}) = (\bar{X},0)$ verifies the condition (2.9). Now, if $0 < \theta \leq 1$ then the equality $(1-\theta)\|\nabla\mathscr{F}(\bar{X})\|_F^2 + \theta\|W(\bar{X})\|_F^2 = 0$ leads to $W(\bar{X}) = 0$. Hence, by selecting $\bar{\Lambda} = \frac{1}{2}\nabla\mathscr{F}(\bar{X})^{\top}\bar{X}$, we arrive at

$$\begin{aligned}
\nabla\mathscr{F}(\bar{X}) - 2\bar{X}\bar{\Lambda} &= \nabla\mathscr{F}(\bar{X}) - \bar{X}\nabla\mathscr{F}(\bar{X})^{\top}\bar{X} \\
&= \nabla\mathscr{F}(\bar{X})\bar{X}^{\top}\bar{X} - \bar{X}\nabla\mathscr{F}(\bar{X})^{\top}\bar{X} \\
&= \left(\nabla\mathscr{F}(\bar{X})\bar{X}^{\top} - \bar{X}\nabla\mathscr{F}(\bar{X})^{\top}\right)\bar{X} \\
&= W(\bar{X})\bar{X} = 0,
\end{aligned}$$

which means that the pair $\left(\bar{X},\bar{\Lambda}\right) = \left(\bar{X},\frac{1}{2}\nabla\mathscr{F}(\bar{X})^{\top}\bar{X}\right)$ solve the equation (2.9). Therefore the proposition is proved. □

Remark 4. *Let $X \in St(m,n)$ be an arbitrary matrix. If we equip the Stiefel manifold with the Riemannian metric given by*

$$\langle\xi_X,\eta_X\rangle_c := tr\left[\xi_X^{\top}\left(I - \frac{1}{2}XX^{\top}\right)\eta_X\right], \quad \forall\xi_X,\eta_X \in T_X St(m,n),$$

then the matrix $W(X)X$ reduces to the Riemannian gradient of the cost function $\mathscr{F}(\cdot)$, for an entire description about this fact see [1, 6].

In the next section, we will introduce a new projected line–search method whose search direction is inspired by the convex combination of the matrices involved in Proposition 3. Furthermore, Proposition 3 will be important to ensure the global convergence of our proposed method.

3 A NEW GRADIENT PROJECTION METHOD

Now, we introduce our iterative algorithm to deal with the optimization problem (1.1). However, the approach presented below can also be used to minimize any smooth function on the Stiefel manifold. Since we have available a projection operator on the feasible set of problem (1.1), then the family of projected line–search methods become an interesting alternative for solving (1.1). In particular, the projected line–search methods construct a sequence of feasible points $\{X_k\} \subset St(m,n)$ through the following recursive scheme

$$X_{k+1} = \pi(X_k + \alpha_k Z_k), \tag{3.1}$$

where $\alpha_k > 0$ represents the step–size, and Z_k must be some descent direction for $\mathscr{F}(\cdot)$ at X_k.

From Proposition 1, we known that the function $\pi(X)$ is well defined if and only if $X \in \mathbb{R}^{m\times n}$ is a full rank matrix. Now, observe that

$$Y(\alpha) \equiv (X_k + \alpha Z_k)^\top (X_k + \alpha Z_k) = I + \alpha(X_k^\top Z_k + Z_k^\top X_k) + \alpha^2 Z_k^\top Z_k. \tag{3.2}$$

Since $Y(0) = I$ is positive definite, then it follows from the continuity of the quadratic function $Y(\alpha)$ that there must exists an interval $\mathscr{I}_k = [0, \alpha_k^{\max}]$, with $\alpha_k^{\max} > 0$ such that $Y(\alpha) = (X_k + \alpha Z_k)^\top (X_k + \alpha Z_k)$ is positive definite, for all $\alpha \in \mathscr{I}_k$. This last relation implies that $\operatorname{rank}(X_k + \alpha Z_k) = n$, for every $\alpha \in \mathscr{I}_k$. Therefore, we can always project $X_k + \alpha_k Z_k$ uniquely over $St(m,n)$ if the step–size is small enough.

A natural idea for the search direction in (3.1), is to select Z_k as the negative of the gradient of the objective function that is $Z_k^1 = -\nabla\mathscr{F}(X_k)$, since this direction gives rise to a successful and very efficient method called *spectral projected gradient method* [4,5], which was originally designed to minimize smooth functions on convex and closed sets, but it was later extended to minimize continuously differentiable functions on arbitrary closed domains [8]. On the other hand, the equations (2.8) and (2.10) suggest the search direction $Z_k^2 = -\left(\nabla\mathscr{F}(X_k) - X_k\nabla\mathscr{F}(X_k)^\top X_k\right) = -W(X_k)X_k$, which is closely related to the gradient of the Lagrangian function with respect to the primal variable. In order to take advantage of these two directions, we propose to select Z_k as the following weighed sum

$$\begin{aligned} Z_k &= -[(1-\theta_k)\nabla\mathscr{F}(X_k) + \theta_k W(X_k)X_k] \\ &= -\nabla\mathscr{F}(X_k) + \theta_k X_k \nabla\mathscr{F}(X_k)^\top X_k, \end{aligned} \tag{3.3}$$

where $\{\theta_k\} \subset [0,1]$ is any convergent sequence of non–negative real numbers such that $\lim_{k\to\infty}\theta_k = \theta \in [0,1]$. Notice that Z_k is a convex combination of Z_k^1 and Z_k^2. The lemma below indicates that (3.3) is indeed a descent direction for $\mathscr{F}$ at X_k.

Lemma 1. *The search direction $Z_k \in \mathbb{R}^{m\times n}$ defined in* (3.3) *is a descent direction for $\mathscr{F}(\cdot)$ at X_k. In particular, we have*

$$\mathscr{D}\mathscr{F}(X_k)[Z_k] = -(1-\theta_k)\|\nabla\mathscr{F}(X_k)\|_F^2 - \frac{\theta_k}{2}\|W(X_k)\|_F^2 < 0.$$

Proof. By using the trace properties an the feasibility of X_k, we have

$$\begin{aligned}
\mathscr{D}\mathscr{F}(X_k)[Z_k] &= tr[\nabla\mathscr{F}(X_k)^\top(-(1-\theta_k)\nabla\mathscr{F}(X_k)-\theta_k W(X_k)X_k)]\\
&= -(1-\theta_k)\|\nabla\mathscr{F}(X_k)\|_F^2-\frac{\theta_k}{2}tr[2\nabla\mathscr{F}(X_k)^\top W(X_k)X_k]\\
&= -(1-\theta_k)\|\nabla\mathscr{F}(X_k)\|_F^2-\frac{\theta_k}{2}tr[2\nabla\mathscr{F}(X_k)^\top(\nabla\mathscr{F}(X_k)X_k^\top-X_k\nabla\mathscr{F}(X_k)^\top)X_k]\\
&= -(1-\theta_k)\|\nabla\mathscr{F}(X_k)\|_F^2-\frac{\theta_k}{2}\left(2\|\nabla\mathscr{F}(X_k)\|_F^2-2tr[\nabla\mathscr{F}(X_k)^\top X_k\nabla\mathscr{F}(X_k)^\top X_k]\right)\\
&= -(1-\theta_k)\|\nabla\mathscr{F}(X_k)\|_F^2-\frac{\theta_k}{2}(2\|\nabla\mathscr{F}(X_k)\|_F^2-tr[X_k\nabla\mathscr{F}(X_k)^\top X_k\nabla\mathscr{F}(X_k)^\top]\\
&\quad -tr[\nabla\mathscr{F}(X_k)X_k^\top\nabla\mathscr{F}(X_k)X_k^\top])\\
&= -\frac{\theta_k}{2}tr[(X_k\nabla\mathscr{F}(X_k)^\top-\nabla\mathscr{F}(X_k)X_k^\top)(\nabla\mathscr{F}(X_k)X_k^\top-X_k\nabla\mathscr{F}(X_k)^\top)]\\
&\quad -(1-\theta_k)\|\nabla\mathscr{F}(X_k)\|_F^2\\
&= -(1-\theta_k)\|\nabla\mathscr{F}(X_k)\|_F^2-\frac{\theta_k}{2}\|W(X_k)\|_F^2, \qquad (3.4)
\end{aligned}$$

which completes the proof. □

Lemma 1 guarantees that we will be able to decrease the value of the objective function throughout the iterations. In addition, note that if we select $\theta_k = 1$ then the update scheme (3.3)–(3.1) reduces to the Riemannian steepest descent method (RSD) proposed by Manton in [13], while if we choose $\theta_k = 0$ then we recover the spectral gradient projection method (SPG), (see equation (2.5) in [10]). Therefore, the convex combination (3.3) constitutes a unified framework that incorporates the SPG and RSD methods in the extreme values of the parameter θ_k, while the intermediate values $\theta_k \in (0,1)$ correspond to new non–Riemannian gradient type methods. In general, the approach (3.1)–(3.3) defines a non–countable family of effective projected gradiente–type methods for the solution of problem (1.1).

Example 3.1. *Now we present an example to illustrate the numerical behavior of our update scheme by considering $\theta_k = \theta$ constant along the iterations but using several values of θ. In this example, the WOPP problems are generated by the following Matlab commands:* $\texttt{randn}('seed',5)$; $A = \texttt{diag}(\texttt{diag}(\texttt{ones}(m)/\texttt{sqrt}(n)))$; $B = \texttt{rand}(m,n)/\texttt{sqrt}(m)$; $C = \texttt{eye}(n)$; *and* $[X_0,\sim] = \texttt{qr}(\texttt{randn}(m,n),0)$. *In addition, we set $m = 100$, $n = 10$ and $\varepsilon = 1e\text{-}5$. We solve this toy experiment with our porposed iterative scheme given by* (3.1)–(3.3)*, for $\theta \in \{0, 0.25, 0.5, 0.75, 1\}$. The convergence behavior of the logarithm of the gradient norm* $\texttt{log}(\|\nabla\mathscr{F}(X)\|_F)$ *along the iteration is presented in Figure 1. In this figure, we note that the performance of the Algorithm 1 changes for different values of θ.*

On the other hand, we have not yet explained how we determine the scalar $\alpha_k > 0$ in our developed projected line–search procedure (3.1)–(3.3). In practice, we employ a non–monotone globalization strategy combined with an adaptive Barzilai–Borwein step–size. It is well–known that the Barzilai–Borwein [2, 19] step–sizes (BB–steps) can greatly speed up the convergence of

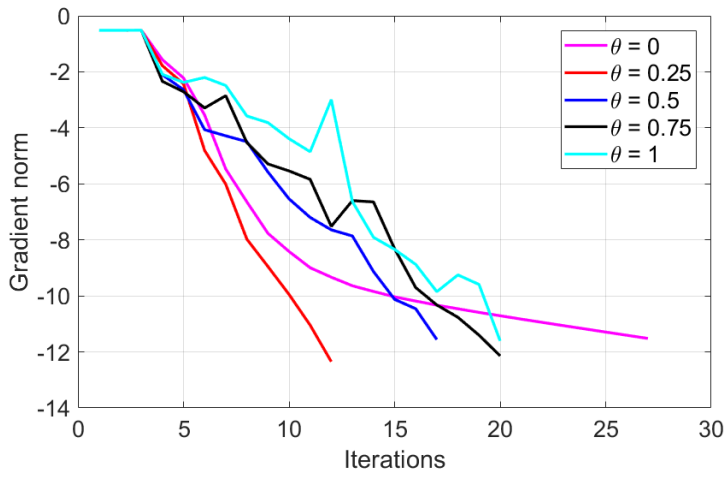


Figure 1: Behavior of the Algorithm 1 varying θ. The y–axis represents the logarithm of the gradient norm, that is $\log(\|\nabla\mathscr{F}(X_k) - X_k\nabla\mathscr{F}(X_k)^\top X_k\|_F)$

the gradient–type methods, without increasing the computational cost too much. In view of these numerical advantages, we use the recently published cyclic delayed weighted steplength [17]

$$\alpha_k^{ACSDMG} = \begin{cases} \min\{\alpha_i^{CSDMG} : i \in \mathscr{S}_k^m\} & \text{if } \alpha_k^{CSDMG} < \kappa\alpha_k^{BB1} \\ \alpha_k^{CSDMG} & \text{otherwise,} \end{cases} \tag{3.5}$$

where $\mathscr{S}_k^m = \{\max\{1,\ldots,k-m\},\ldots,k\}$, $m \in \mathbb{N}$, $\kappa \in (0,1)$ and α_k^{CSDMG} is given by

$$\alpha_k^{CSDMG} = \alpha_k^{BB2}\left(\frac{(1-\mu)\alpha_k^{BB1} + 2\mu}{(1-\mu)\alpha_k^{BB2} + 2\mu}\right). \tag{3.6}$$

where $\mu \in [0,1]$ is a fixed value. In addition, in (3.6) the parameters α_k^{BB1} and α_k^{BB2} refer to the classical Brazilai–Borwein step–sizes [2], i.e.

$$\alpha_k^{BB1} = \frac{\|S_{k-1}\|_F^2}{|\,tr[S_{k-1}^\top Y_{k-1}]\,|} \quad \text{and} \quad \alpha_k^{BB2} = \frac{|\,tr[S_{k-1}^\top Y_{k-1}]\,|}{\|Y_{k-1}\|_F^2}, \tag{3.7}$$

where $S_{k-1} = X_k - X_{k-1}$ and $Y_{k-1} = \nabla\mathscr{F}(X_k) - \nabla\mathscr{F}(X_{k-1})$. Because the inner product $tr[S_{k-1}^\top Y_{k-1}]$ can be equal to zero (or very close to zero); or it can even be very large, we will consider the following safeguard to avoid numerical errors

$$\hat{\alpha}_k^{ACSDMG} = \max\{\min\{\alpha_k^{ACSDMG}, \alpha_M\}, \alpha_m\},$$

where $0 < \alpha_m \leq \alpha_M < 1e^{16}$ are two global parameters chosen by the user. In addition, since the BB–type step–sizes do not necessary guarantee descent of the cost function along the iterative process, these step–sizes are generally used in combination with some globalization technique

Algorithm 1 Gradient projection method

Require: $X_0 \in St(n,p)$, $\alpha > 0$, $0 < \alpha_m \leq \alpha_M$, $\eta \in [0,1)$, $\mu, \kappa, \rho_1, \varepsilon, \delta \in (0,1)$, $m \in \mathbb{N}$, $Q_0 = 1$, $C_0 = \mathscr{F}(X_0)$, $k = 0$.

Ensure: X^* an ε–KKT point.

while $\|\nabla \mathscr{F}(X_k) - X_k \nabla \mathscr{F}(X_k)^\top X_k\|_F > \varepsilon$ **do**
  Select $\theta_k \in [0,1]$.
  $Z_k = -\nabla \mathscr{F}(X_k) + \theta_k X_k \nabla \mathscr{F}(X_k)^\top X_k$.
  while $\mathscr{F}(\pi(X_k + \alpha Z_k)) > C_k + \rho_1 \alpha \mathscr{D}\mathscr{F}(X_k)[Z_k]$ **do**
    $\alpha = \delta \alpha$,
  end while
  $X_{k+1} = \pi(X_k + \alpha Z_k)$.
  $Q_{k+1} = \eta Q_k + 1$ and $C_{k+1} = (\eta Q_k C_k + \mathscr{F}(X_{k+1}))/Q_{k+1}$.
  Choose $\alpha = \alpha_{k+1}^{ACSDMG}$ with α_{k+1}^{ACSDMG} according to (3.5).
  $\alpha = \max(\min(\alpha, \alpha_M), \alpha_m)$.
  $k \leftarrow k + 1$.
end while
$X^* = X_k$.

in order to ensure the global convergence. For this end, we use the non–monotone globalization technique proposed by Zhang and Hager in [26]. The above description leads us to Algorithm 1.

It follows from Lemma 1 and Proposition 3 that the sequence of search directions $\{Z_k\}$ generated by Algorithm 1 is a sequence of gradient–related directions (see Definition 4.2.1 in [1]), hence if we set $\eta = 0$ (in this case the Zhang–Hager condition is reduced to the Armijo rule [12]) then we can repeat the steps of the proof of Theorem 4.3.1 and Corollary 4.3.2 that appear in [1] to obtain the global convergence of our proposal. Similarly, to derive the global convergence of Algorithm 1 for the case $\eta \in (0,1)$, we can replicate the steps of the proofs of Lemma 2 and Theorem 1 that appear in [14].

Now let us consider the particular case of (1.1) when $C = I_n$ is the n-by-n identity matrix and $A \in \mathbb{R}^{m\times m}$ is a square matrix, that is, let us consider the following problem

$$\min_{X\in\mathbb{R}^{m\times n}} \frac{1}{2}\|AX - B\|_F^2, \quad \text{subject to} \quad X^\top X = I, \tag{3.8}$$

where B is a known real matrix of correct dimensions. This problems is known as "unbalanced orthogonal procrustes problem" (OPP), [23, 27, 28]. In general, this problem does not have an analytical solution, except in the case when $m = n$, see [21, 23, 28]. However, if A is positive definite matrix then we can derive a problem similar to (3.8) with closed–form solution.

Lemma 2. *Let $A \in \mathbb{R}^{m\times m}$ be a positive definite matrix, $B \in \mathbb{R}^{m\times n}$. Let us consider the the non–convex constrained optimization problem*

$$\min_{X\in\mathbb{R}^{m\times n}} \frac{1}{2}\|AX - B\|_{A^{-1}}^2, \quad \textit{subject to} \quad X^\top X = I, \tag{3.9}$$

where $\|P\|_{A^{-1}} := \sqrt{tr[P^\top (AA^\top)^{-1}P]} = \|A^{-1}P\|_F$*, for any* $P \in \mathbb{R}^{m\times n}$*. Then, the global solution of* (3.9) *is* $\hat{X} = \pi(A^{-1}B) = UI_{m,n}V^\top$*, where* $A^{-1}B = U\Sigma V^\top$ *represents the singular value decomposition of* $A^{-1}B$*.*

Proof. Let $H(X) = \frac{1}{2}\|AX - B\|^2_{A^{-1}}$ be the cost function of (3.9). Notice that

$$\begin{aligned} H(X) &= \frac{1}{2}tr[(AX-B)^\top (AA^\top)^{-1}(AX-B)] \\ &= \frac{1}{2}tr[(AX-B)^\top A^{-\top}A^{-1}(AX-B)] \\ &= \frac{1}{2}tr[(X^\top - B^\top A^{-\top})(X - A^{-1}B)] \\ &= \frac{1}{2}tr[(X-A^{-1}B)^\top (X-A^{-1}B)] \\ &= \frac{1}{2}\|X - A^{-1}B\|^2_F. \end{aligned} \tag{3.10}$$

So, the optimization problem (3.9) is equivalent to

$$\min_{X\in St(m,n)} \frac{1}{2}\|X - A^{-1}B\|^2_F.$$

Thus, by applying Proposition 1, we have that the global minimizer of (3.9) is $\hat{X} = \pi(A^{-1}B)$, completing the proof. □

It follows from the lemma above that if we replace the Frobenius norm in (3.8) by the $\|\cdot\|_{A^{-1}}$ then the new procrustes problem has an analytical solution. This result can be used to initialize Algorithm 1 with the point $X_0 = \pi(A^{-1}B)$, for the case when A is positive definite and C is the identity matrix.

4 COMPUTATIONAL EXPERIMENTS

In order to give further insight into the Algorithm 1, we present some numerical comparisons. For benchmarking, we compare our method with the Riemannian gradient method based on the Cayley transform *OptSt* developed in [25][1], the Riemannian steepest descent method (Manton–SD) introduced by Manton in [13], and the Riemannian conjugate gradient methods *Algor.1a* and *Algor.1b* proposed in [29][2]. All the experiments have been performed on a intel(R) CORE(TM) i7-4770, CPU 2.20 GHz with 1TB HD and 16GB RAM. The algorithm was coded in Matlab (version 2017b).

In this section, *Time*, *Nfe*, *Nitr* and *Grad* will denote the averaged total computing time in seconds, the average number of function evaluations, the average number of iterations, the averaged residual $\|\nabla\mathscr{F}(X^*)\|_F$ where X^* is the optimum estimated by each method, respectively. In addition, we stop the methods if one of the following conditions holds: (i) $k \geq N$; (ii)

[1]The OptSt Matlab code is available in `https://github.com/wenstone/OptM`

[2]The Riemannian conjugate gradient methods Algor.1a, Algor.1b and Algor.1b+ZH can be downloaded from `http://www.optimization-online.org/DB_HTML/2016/09/5617.html`

$\|\nabla\mathscr{F}(X_k) - X_k\nabla\mathscr{F}(X_k)^\top X_k\|_F \leq \varepsilon$, where the values of N and ε will be specificated for each experiment. In our Algorithm 1, we set $\alpha_m = 1e\text{-}15$, $\alpha_M = 1e{+}15$, $\rho_1 = 1e\text{-}4$, $\eta = 0.85$, $\delta = 0.2$, $(m,\kappa) = (9, 0.8)$ and $\mu \equiv \mu_k = (k+1)/(k+2)$ varying along the iterations.

For the first experiment, we consider the following optimization problem

$$\min_{x\in\mathbb{R}^n} x^\top Lx, \quad \text{s.t.} \quad x^\top x = 1, \tag{4.1}$$

where $L \in \mathbb{R}^{n\times n}$ is a symmetric matrix. Problem (4.1) can be seen as a particular version of problem (1.1) obtained by substituting $C = 1$ and $B = (0,0,\ldots,0)^\top$ in (1.1); and considering the identification $L = A^\top A$. It is well–known that the global solution of (4.1) corresponds to the eigenvector associated with the smallest eigenvalue of L. In fact, problem (4.1) is equivalent to minimizing the Rayleigh quotient of L. For this experiment, we solve (4.1) for the following 20 values of n, $n \in \{500, 1000, 1500, \ldots, 9500, 10000\}$. In order to make this experiment replicable, we construct the matrix L as the discrete Laplacian operator, generated with the following Matlab command $L = \texttt{gallery}('\text{tridiag}', n, -1, 2, -1)$, and the initial vector $x_0 \in \mathbb{R}^n$ is chosen as $x_0 = v/\|v\|_2$, where $v = (1,2,3,\ldots,n)^\top$. In this computational study, we use $N = 15000$, choose $\varepsilon = 1e\text{-}6$; and $\theta_k = k/(k+1)$ in our algorithm. The accuracy of the computed eigenvalue and its associated eigenvector of L are measured by using the absolute error

$$\texttt{error} = \|L\hat{x} - (\hat{x}^\top L\hat{x})\hat{x}\|_2,$$

and the absolute residual in the objective value

$$\texttt{residual} = |\, f(\hat{x}) - \lambda_{\min}\,|,$$

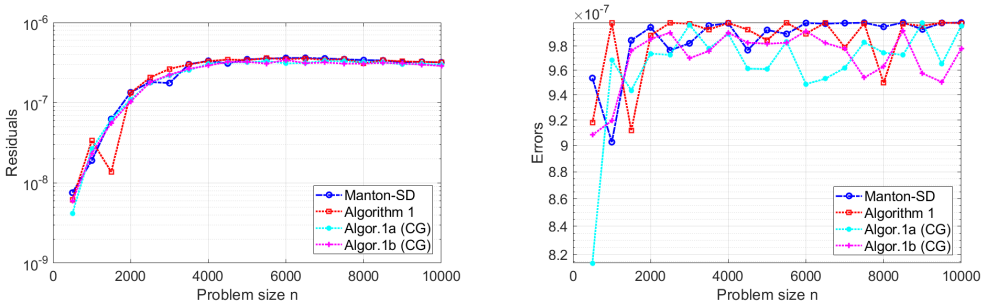
where $\hat{x}$ denote the estimated solution of (4.1) obtained by each method, and $\lambda_{\min}$ is the smallest eigenvalue of L.

Table 1 summarizes the average values *Time*, *Nfe*, *Nitr* and *Grad* obtained by every method. As shown in Table 1, the most efficient methods in terms of computational time and number of iterations are Algorithm 1 and the Riemannian gradient method proposed by Manton in [13]. In Figure 2, we show the absolute error and the absolute residual for each method and for each value of n. From Figure 2, we can see that all the methods obtain the global solution of problem (4.1), for all the considered values of n, with the pre–established precision. Furthermore, we observe that Algorithm 1 converges to the solution faster than the Riemannian conjugate gradient methods Algor.1a and Algor.1b.

Our second experiment was taken from [20]. Let $n = q$, $p = m$, $A = PSR^\top$ and $C = Q\Lambda Q^\top$, where P, Q and R are orthogonal matrices randomly generated such that $Q \in \mathbb{R}^{n\times n}$, $R, P \in \mathbb{R}^{m\times m}$, $\Lambda \in \mathbb{R}^{n\times n}$ is a diagonal matrix with entries generated from a uniform distribution in the range $[\frac{1}{2}, 2]$ and S is a diagonal matrix defined for each type of problem, see below for details. When not specified, the entries of the matrix were generated using the standard Gaussian distribution. The matrix B was randomly generated with entries follow a normal standard distribution. Finally, for the different tested problems the diagonal matrix S is described below.

Table 1: Numerical results computing the smallest eigenvalue of tridiagonal matrices.

Method	Nitr	Nfe	Time	Grad
Manton–SD	3790.1	3894.2	0.51	9.87e-7
Algor.1a (CG)	12821.0	12854.0	3.16	9.65e-7
Algor.1b (CG)	12971.0	12971.0	3.12	9.71e-7
Algorithm 1	3530.7	3634.2	0.37	9.85e-7



(a) Residuals

(b) Errors

Figure 2: The residuals of the computed eigenvalues (a) and the corresponding absolute errors (b), of a tridiagonal matrix. The y–axis is in logarithmic scale.

Structure 1: The diagonal elements of S were generated by a normal distribution in the interval [10,12].

Structure 2: The diagonal of S is given by $S_{ii} = i + 2r_i$, where r_i was a random number uniformly distributed in the interval $[0,1]$.

Structure 3: Each diagonal element of S was generated as follows: $S_{ii} = 1 + \frac{99(i-1)}{m+1} + 2r_i$, with r_i uniformly distributed in the interval $[0,1]$.

In this experiment, we use $N = 50000$ and choose $\varepsilon = 1e\text{-}6$; and $\theta_k = 1/(k+9)$ for our algorithm. For all experiments, we randomly generate the starting point X_0 using the following Matlab command $[X_0, \sim] = \texttt{qr}(\texttt{randn}(n,p),0)$. In all the experiments, we solve 10 independent instances for the different values of (n,p) and then we report the average values *Time*, *Nfe*, *Nitr* and *Grad*. The numerical results concerning this test are contained in Table 2. From Table 2, we can see that all the methods obtain an approximated solution with the required precision. In addition, we note that our procedure obtains competitive results compared to the existing methods in the literature. Finally, we notice that the most efficient methods, in terms of computational time, were the OptSt method and our Algorithm 1.

Table 2: Numerical results on weighted orthogonal procrustes problems.

Method	Nitr	Nfe	Time	Grad	Nitr	Nfe	Time	Grad
	Structure 1 with $n = 500$ and $p = 70$				Structure 1 with $n = 1000$ and $p = 100$			
OptSt	37.4	38.4	0.12	6.40e-6	37.0	39.0	0.35	5.68e-6
Algor.1a (CG)	43.6	46.6	0.17	7.16e-7	40.9	43.1	0.53	6.97e-7
Algor.1b (CG)	34.0	36.0	0.12	6.90e-7	44.7	47.4	0.56	8.14e-7
Algorithm 1	31.2	34.2	0.07	6.58e-6	34.2	35.2	0.31	6.23e-6
	Structure 2 with $n = 100$ and $p = 50$				Structure 2 with $n = 100$ and $p = 100$			
OptSt	2942.5	3112.0	1.87	1.94e-6	2290.7	2494.0	1.96	8.41e-6
Algor.1a (CG)	4640.5	7735.2	6.00	1.07e-3	3033.5	4870.1	9.94	7.85e-7
Algor.1b (CG)	4488.8	7453.7	5.00	1.48e-4	3440.5	5607.5	8.97	8.49e-7
Algorithm 1	2293.8	2434.0	1.11	9.24e-6	2275.6	2377.1	2.51	9.55e-6
	Structure 3 with $n = 300$ and $p = 20$				Structure 3 with $n = 1000$ and $p = 100$			
OptSt	3397.2	3556.5	1.78	9.10e-6	957.4	999.5	2.56	8.42e-6
Algor.1a (CG)	6741.9	11863.0	5.93	2.55e-4	1136.5	1869.5	3.32	9.12e-7
Algor.1b (CG)	7289.0	12784.0	5.92	1.13e-3	1134.2	1876.3	3.35	8.61e-7
Algorithm 1	2865.8	3010.5	0.97	8.93e-6	751.4	789.7	1.41	9.21e-6

5 CONCLUDING REMARKS

In the present work, we have proposed a novel feasible line–search algorithm for solving a class of linear least–square optimization problems on the Stiefel manifold. In particular, we have introduced a projected gradient–type method with mixed direction, which uses the non–monotone globalization strategy of Zhang and Hager combine with an alternate Barzilai-Borwein step–size. All operations are performed with matrices to preserve the structure of the problem and avoiding vectorization. The search direction used by our method involves the Riemannian gradient in order to exploit the geometric information of the Stiefel manifold. In addition, the search directions computed by our algorithm were proved to satisfy the sufficient descent condition, which guarantees that the method reduces the value of the cost function throughout the iterative process. A numerical study with problems taken from the literature shows the reliability of adopting this new approach for solving weighted orthogonal procrustes problems.

Our numerical results show that the new family of methods works very well for any selection of the parameter θ in the interval $[0,1]$. But, since θ may be a problem dependent parameter, then it will remain as future work, to develop and investigate self–adaptive strategies to select this parameter along the iterative process, possibly using local information of the objective function, in order to improve the performance of the new collection of methods.

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