Solving Optimization Problems over the Stiefel Manifold by Smooth Exact Penalty Function

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Abstract

In this paper, we present a novel penalty model called ExPen for optimization over the Stiefel manifold. Different from existing penalty functions for orthogonality constraints, ExPen adopts a smooth penalty function without using any first-order derivative of the objective function. We show that all the first-order stationary points of ExPen with a sufficiently large penalty parameter are either feasible, namely, are the first-order stationary points of the original optimization problem, or far from the Stiefel manifold. Besides, the original problem and ExPen share the same second-order stationary points. Remarkably, the exact gradient and Hessian of ExPen are easy to compute. As a consequence, abundant algorithm resources in unconstrained optimization can be applied straightforwardly to solve ExPen.

1 Introduction

In this paper, we consider the following optimization problem

\[
\min_{X \in \mathbb{R}^{n \times p}} f(X) \quad \text{s.t.} \quad X^T X = I_p, \tag{OCP}
\]

where \(I_p\) denotes the \(p \times p\) identity matrix, and \(f : \mathbb{R}^{n \times p} \rightarrow \mathbb{R}\) satisfies the following assumption throughout this paper.

Assumption 1.1. Blank assumptions on \(f\)

1. \(f\) and \(\nabla f\) are locally Lipschitz continuous in \(\mathbb{R}^{n \times p}\).

The feasible region of the orthogonality constraints \(X^T X = I_p\) is the Stiefel manifold embedded in the \(n \times p\) real matrix space, denoted by \(\mathcal{S}_{n,p} := \{X \in \mathbb{R}^{n \times p} | X^T X = I_p\}\). We also call it as the Stiefel manifold for brevity. Optimization problems with orthogonality constraints have wide applications in statistics [36, 13], scientific computation [27], image processing [5] and many other related areas [17, 31, 49]. Interested readers could refer to some recent works [15, 25, 46, 41], a recent survey [23], and several books [3, 9] for details.

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1.1 Motivation

Optimization over the Stiefel manifold, which is a smooth and compact Riemannian manifold, has been discovered to enjoy a close relationship with unconstrained optimization. Various existing unconstrained optimization approaches, i.e., the approaches for solving nonconvex unconstrained optimization problems, can be extended to their Riemannian versions by the diffeomorphisms between the Stiefel manifold and Euclidean space. The approaches, called Riemannian optimization approaches for brevity hereinafter, include gradient descent with line-search [2, 3, 43, 26, 40], conjugate gradient methods [1], Riemannian accelerated gradient method [48, 47, 38, 11], Riemannian adaptive gradient methods [6], etc. With the frameworks and geometrical materials described in Absil et al. [3], theoretical results of these Riemannian optimization approaches could be established by following almost the same proof techniques as their unconstrained prototypes. These results include the global convergence, local convergence rate, worst-case complexity, saddle-point-escaping properties, etc., see [10, 39, 50, 4, 11, 16, 22] for instances.

The Riemannian optimization approaches usually consist of two fundamental parts. The first one is the so-called “retraction” which maps a point from the tangent space to the manifold. Retractions can be further categorized into two classes: the geodesic-like retractions and the projection-like ones. The former ones require to calculate the geodesics along the manifold and hence expensive. The latter ones enjoy relatively lower computational cost, but still include unparallelizable computation and hence has low scalability when \( p \) is large. The second part is called “parallel transport” which moves a tangent vector along a given curve on a Stiefel manifold “parallelly”. The purpose of parallel transport is to design the manifold version of some advanced unconstrained optimization approaches, such as conjugate gradient methods or gradient methods with momentum. However, as illustrated in [3], computing the parallel transport on Stiefel manifold is equivalent to finding a solution to a differential equation, which is definitely impractical in computation. To this end, the authors of Absil et al. [3] have proposed the concept of vector transport, which can be regarded as an approximation to parallel transport and computationally affordable. Unfortunately, some nice convergence properties can hardly be established for approaches adopting the vector transport strategies. As illustrated in various existing works [48, 47, 10, 50, 4, 11], both parallel transports and geodesics play an essential role in establishing convergence properties. It is still difficult to verify whether their theoretical convergence properties is valid when these approaches are built by retractions and vector transports.

To avoid computing the retractions, parallel transports, or vector transports to the Stiefel manifold, some approaches aim to find smooth mappings from the Euclidean space to the Stiefel manifold, which directly reformulates OCP to unconstrained optimization. Among them, [29, 28] construct equivalent unconstrained problems for OCP by exponential function for square matrices. To efficiently compute the matrix exponential, they apply the iterative approach proposed by Higham and Papadimitriou [20]. Therefore, their approaches require \( O(n^3) \) flops in each iteration for computing the matrix exponential and thus are computationally expensive in practice. Inspired by [29, 28], several recent works use Cayley transformation [18, 34, 12, 30] to avoid computing the matrices exponential. These approaches require computing the inverse of \( n \times n \) matrices in each iterate, which still requires \( O(n^3) \) flops in general. Furthermore, as illustrated in the numerical experiments in [12], when applying nonlinear conjugate gradient methods, the computational time of these approaches is usually much higher than existing Riemannian conjugate gradient approaches.

Recently, some penalty-function-based approaches have been verified to be efficient in solving optimization problems over the Stiefel manifold. They utilize a completely different angle with existing Riemannian optimization approaches. Based on the framework of the augmented Lagrangian method (ALM) [19, 37, 35, 7], the authors of [15] have proposed the proximal linearized augmented Lagrangian method (PLAM) and its column-wise normalization version (PCAL) for (OCP). Both PLAM and PCAL update the multipliers corresponding to the orthogonality constraints by a closed-form expression. Inspired by the closed-form updating scheme in PLAM and PCAL, the authors of [44] have proposed an exact penalty function named PenC,

\[
\min_{\|X\|_F \leq K} h_{\text{PenC}}(X) = f(X) - \frac{1}{2} \left\langle \Phi(X^\top \nabla f(X)), X^\top X - I_p \right\rangle + \frac{\beta}{4} \|X^\top X - I_p\|_F^2
\]
where $K \geq \sqrt{p}$ is a prefixed constant and $\Phi$ is the symmetrization operator defined as

$$
\Phi(M) := \frac{1}{2}(M + M^\top).
$$

In Xiao et al. [44], the authors have illustrated the equivalence between OCP and PenC, which further proposed the corresponding infeasible first-order and second-order methods PenCF and PenCS, respectively. Moreover, successive works [45, 24] have illustrated that PenC could be extended to objective function with special structures. The above-mentioned penalty-function-based approaches are verified to enjoy high efficiency and scalability due to avoiding retractions or parallel transport to the Stiefel manifold. However, their penalty functions involve the first-order derivatives of the original objective, which leads to two limitations. Firstly, the smoothness of the penalty function requires higher-order smoothness of the original objective function. Secondly, calculating an exact gradient of these penalty functions is usually expensive in practice. As a result, many existing unconstrained optimization approaches cannot be directly applied to minimize these penalty functions.

### 1.2 Contributions

The contributions of this paper can be summarized as the following two folds.

**A novel penalty function** We propose a novel penalty function

$$
h(X) := f \left( X \left( \frac{3}{2} I_p - \frac{1}{2} X^\top X \right) \right) + \frac{\beta}{4} \| X^\top X - I_p \|_F^2,
$$

and construct the following unconstrained optimization problem which is abbreviated as ExPen.

$$
\min_{X \in \mathbb{R}^{n \times p}} h(X).
$$

We illustrate that any first-order stationary point (FOSP) of ExPen is either feasible and hence a FOSP of OCP, or far away from the Stiefel manifold. Besides, we prove that any eigenvalue of the Riemannian Hessian at any first-order stationary point $X \in S_{n \times p}$ is an eigenvalue of $\nabla^2 h(X)$. Then we show that any second-order stationary point (SOSP) of ExPen is an SOSP of OCP. We call the above two relationships the *first-order relationship* and *second-order relationship*, respectively, for brevity. These two relationships imply that ExPen can be regarded as an exact penalty function.

**A universal tool** The exact penalty model ExPen builds up a bridge between various existing unconstrained optimization approaches and OCP. Moreover, those rich theoretical results of unconstrained optimization approaches can be directly applied in solving OCP. In particular, some newly developed techniques for unconstrained optimization can be extended to solve optimization over the Stiefel manifold through ExPen. We use the cubic regularization method with momentum as an example. It is difficult to find a compromise between computational efficiency and theoretical guarantee if we adopt Riemannian optimization approaches to achieve this extension.

### 1.3 Notations

We use $S_{n \times p}^+$ to denote the space containing all $p \times p$ real positive semidefinite matrices. The Euclidean inner product of two matrices $X, Y \in \mathbb{R}^{n \times p}$ is defined as $\langle X, Y \rangle = \text{tr}(X^\top Y)$, where $\text{tr}(A)$ is the trace of the square matrix $A$. Besides, $\| \cdot \|_2$ and $\| \cdot \|_F$ represent the 2-norm and the Frobenius norm, respectively. The notations $\text{diag}(A)$ and $\text{Diag}(x)$ stand for the vector formed by the diagonal entries of matrix $A$, and the diagonal matrix with the entries of $x \in \mathbb{R}^n$ to be its diagonal, respectively. We denote the smallest eigenvalue of $A$ by $\lambda_{\text{min}}(A)$. The inner product is set as $\langle X, Y \rangle = \text{tr}(X^\top Y)$ for any $X, Y \in \mathbb{R}^{n \times p}$. We set the Riemannian metric on Stiefel manifold as the metric inherited from the
standard inner product in \( \mathbb{R}^{n \times p} \). We set \( T_X \) as the tangent space of Stiefel manifold at \( X \), which can be expressed as

\[
T_X := \{ D \in \mathbb{R}^{n \times p} \mid \Phi(D^\top X) = 0 \},
\]

while \( N_X \) is denoted as the normal space of Stiefel manifold at \( X \),

\[
N_X := \{ D \in \mathbb{R}^{n \times p} \mid D = X\Lambda, \Lambda = \Lambda^\top \}. 
\]

And \( \text{grad} f(X) \) denotes the Riemannian gradient of \( f \) at \( X \in S_{n,p} \) in Euclidean measure, namely,

\[
\text{grad} f(X) := \nabla f(X) - X\Phi(X^\top \nabla f(X)).
\]

Besides, we use \( \nabla^2 f(X)[D] \) to represent the Hessian-matrix product. The Riemannian Hessian of \( f \) at \( X \in S_{n,p} \) in Euclidean measure is denoted as \( hess f(X) : \mathbb{R}^{n \times p} \to \mathbb{R}^{n \times p} \), which can be expressed by

\[
hess f(X)[D] := \nabla^2 f(X)[D] - D\Phi(X^\top \nabla f(X)), \quad \forall D \in T_X.
\]

Finally, \( \mathcal{P}_{S_{n,p}} = UV^\top \) denotes the orthogonal projection to Stiefel manifold, where \( X = U\Sigma V^\top \) is the economic SVD of \( X^k \) with \( U \in S_{n,p} \), \( V \in S_{p,p} \) and \( \Sigma \) is \( p \times p \) diagonal matrix with the singular values of \( X \) on its diagonal.

### 1.4 Organization

The rest of this paper is organized as follows. In Section 2, we present several preliminaries and useful lemmas. Then we explore the first-order and second-order relationships between OCP and ExPen, respectively, in Section 3. We show how to solve OCP through unconstrained optimization approaches by an illustrative example in Section 4 and draw a brief conclusion in the last section.

### 2 Preliminaries

In this section, we provide several preliminary properties of ExPen. We first introduce the definitions, assumptions and define several constants. Then we give some preliminary properties of ExPen. Finally, we present the computational complexity of calculating the derivatives of ExPen.

#### 2.1 Definitions

The first-order optimality condition of problem OCP can be written as

**Definition 2.1.** [3] Given a point \( X \in S_{n,p} \), we call \( X \) a first-order stationary point of OCP if \( \text{grad} f(X) = 0 \).

According to [14], any \( X \in \mathbb{R}^{n \times p} \) is a first-order stationary point of OCP if and only if it satisfies

\[
\begin{align*}
\nabla f(X) - X\Phi(X^\top \nabla f(X)) &= 0; \\
X^\top X &= I_p.
\end{align*}
\]

Next, we present the definition of the second-order optimality condition of OCP.

**Definition 2.2.** Given a point \( X \in S_{n,p} \), if \( f \) is twice-differentiable, \( X \) is the first-order stationary point of OCP and

\[
\langle D, hess f(X)[D] \rangle \geq 0,
\]

holds for any \( D \in T_X \), then we call \( X \) a second-order stationary point of OCP.
Besides, we present the definitions of first-order and second-order optimality conditions of ExPen. Given a point $X \in \mathbb{R}^{n \times p}$, we say $X$ is a first-order stationary point of a differentiable function $h : \mathbb{R}^{n \times p} \to \mathbb{R}$ if and only if $\nabla h(X) = 0$. And when $h$ is twice-order differentiable, $X$ is a second-order stationary point of $h$ if and only if $X$ is a first-order stationary point of $h$ and

$$\left\langle \nabla^2 h(X)[D], D \right\rangle \geq 0, \quad \forall D \in \mathbb{R}^{n \times p}. \quad (2.1)$$

Next we present the definitions of Łojasiewicz inequality [32, 33] in the following, which coincide with the definitions in [8].

**Definition 2.3.** Let $f$ be a differentiable function. Then $f$ is said to have the (Euclidean) Łojasiewicz gradient inequality at $X \in \mathbb{R}^{n \times p}$ if and only if there exists a neighborhood $U$ of $X$, and constants $\theta \in (0, 1]$, $C > 0$, such that for any $Y \in U$,

$$\| \nabla f(Y) \|_F \geq C | f(Y) - f(X) |^{1-\theta}.$$  

Besides, we present the definitions of Riemannian Łojasiewicz inequality [21].

**Definition 2.4.** Let $f$ be a differentiable function. Then $f$ is said to have the Riemannian Łojasiewicz gradient inequality at $X \in S_{n,p}$ if and only if there exists a neighborhood $U \subset S_{n,p}$ of $X$, and constants $\theta \in (0, 1]$, $C > 0$, such that for any $Y \in U$,

$$\| \nabla f(Y) \|_F \geq C | f(Y) - f(X) |^{1-\theta}.$$  

The constant $\theta$ is usually named as Łojasiewicz exponent in the gradient inequality.

### 2.2 Assumptions

Before presenting some additional assumptions on the objective function $f$ using in some parts of this paper, we first define some set and operators.

- $\Omega := \{ X \in \mathbb{R}^{n \times p} \mid \|X\|_2 \leq 1 + \frac{1}{12} \}$;
- $\overline{\Omega}_r := \{ X \in \mathbb{R}^{n \times p} \mid \|X^T X - I_p\|_F \leq r \}$;
- $G(X) := \nabla f(Y) \big|_{Y = X(\frac{3}{2}I_p - \frac{1}{2}X^T X)}$;
- $H(X) := \nabla^2 f(Y) \big|_{Y = X(\frac{3}{2}I_p - \frac{1}{2}X^T X)}$;
- $J_X(D) := D \left( \frac{3}{2}I_p - \frac{1}{2}X^T X \right) - X\Phi(D^T X)$;
- $g(X) := f \left( X \left( \frac{3}{2}I_p - \frac{1}{2}X^T X \right) \right)$.

Clearly, we have $\overline{\Omega}_{1/12} \subset \overline{\Omega}_{1/6} \subset \Omega$. In addition, we present several constants for the theoretical analysis of ExPen.

- $M_0 := \sup_{X \in \Omega} f(X) - \inf_{X \in \Omega} f(X)$;
- $M_1 := \sup_{X \in \Omega} \| G(X) \|_F$;
- $M_2 := \sup_{X \in \Omega, Y \in \Omega} \frac{\| \nabla g(X) - \nabla g(Y) \|_F}{\| X - Y \|_F}$;
- $\tilde{\beta} := \max \{ 12 M_1, 6 M_2 \}$.

It is worth mentioning that parameters $M_0$, $M_1$, $M_2$ are all independent of the penalty parameter $\beta$. Now, we impose two nice properties on $f$.

**Assumption 2.5.** The lower boundedness and global Lipschitz smoothness of $f$
1. \( f \) is bounded below in \( \mathbb{R}^{n \times p} \);
2. \( g(X) \) is globally Lipschitz smooth in \( \mathbb{R}^{n \times p} \).

Although Assumption 2.5 looks restrictive, it is satisfied by the objective functions of most studied optimization over the Stiefel manifold.

Moreover, under Assumption 2.5, we define several additional constants for ExPen,

- \( \hat{M}_1 := \sup_{X \in \mathbb{R}^{n \times p}} \|G(X)\|_F; \)
- \( \hat{M}_2 := \sup_{X, Y \in \mathbb{R}^{n \times p}} \frac{\|\nabla g(X) - \nabla g(Y)\|_F}{\|X - Y\|_F}; \)
- \( \hat{M}_3 := \sup_{X \in \mathbb{R}^{n \times p}} \|\nabla g(X)\|_F; \)
- \( \hat{\beta} := \max \{12\hat{M}_1, 6\hat{M}_2, 6\hat{M}_3\}. \)

We emphasize that parameters \( \hat{M}_1, \hat{M}_2 \) and \( \hat{M}_3 \) are independent with the penalty parameter \( \beta \). Besides, it follows from Assumption 2.5 that \( \hat{M}_1 \geq M_1 \) and \( \hat{M}_2 \geq M_2 \).

Furthermore, when we analyze the hessian at \( h(X) \), the objective function \( f \) in OCP should be twice-differentiable. As a results, in some cases we assume the objective function \( f \) be twice differentiable.

**Assumption 2.6.** The second-order differentiability of \( f \nabla^2 f(X) \) exists at every \( X \in \mathbb{R}^{n \times p} \).

In the rest of this subsection, we present several useful lemmas for further use. We first show that \( J_X \) is the Jacobian of the mapping \( X \mapsto X \left( \frac{3}{2}I_p - \frac{1}{2}X^\top X \right) \) in the following lemma.

**Proposition 2.7.** For any \( X, Y \in \mathbb{R}^{n \times p} \), let \( D = Y - X \), we have
\[
\left\| Y \left( \frac{3}{2}I_p - \frac{1}{2}Y^\top Y \right) - X \left( \frac{3}{2}I_p - \frac{1}{2}X^\top X \right) - J_X(D) \right\|_F = O(\|D\|_F^2).
\]

Besides,
\[
\left\| Y \left( \frac{3}{2}I_p - \frac{1}{2}Y^\top Y \right) - X \left( \frac{3}{2}I_p - \frac{1}{2}X^\top X \right) - I_X(D) - \left[ D\Phi(D^\top X) + \frac{1}{2}XD^\top D \right] \right\|_F = O(\|D\|_F^3).
\]

**Proof.** Let \( D = Y - X \), from the expression of \( Y \left( \frac{3}{2}I_p - \frac{1}{2}Y^\top Y \right) \) we can conclude that
\[
Y \left( \frac{3}{2}I_p - \frac{1}{2}Y^\top Y \right) = X \left( \frac{3}{2}I_p - \frac{1}{2}X^\top X \right) + D \left( \frac{3}{2}I_p - \frac{1}{2}X^\top X \right) - X\Phi(X^\top D) - D\Phi(D^\top X) - \frac{1}{2}XD^\top D - \frac{1}{2}DD^\top D
\]
\[
= X \left( \frac{3}{2}I_p - \frac{1}{2}X^\top X \right) + J_X(D) - D\Phi(D^\top X) - \frac{1}{2}XD^\top D - \frac{1}{2}DD^\top D,
\]
and thus complete the proof. \( \square \)

In the following Lemma, we present the expression of \( \nabla h(X) \):

**Proposition 2.8.** For any \( X \in \mathbb{R}^{n \times p} \),
\[
\nabla h(X) = G(X) \left( \frac{3}{2}I_p - \frac{1}{2}X^\top X \right) - X\Phi(X^\top G(X)) + \beta X(X^\top X - I_p).
\]
Proof. First, we aim to prove that the linear mapping \( J_X \) is self-adjoint for any \( X \in \mathbb{R}^{n \times p} \). From the expression of \( J_X \), for any \( Z, W \in \mathbb{R}^{n \times p} \), we can have

\[
(J_X(W), Z) = \left\langle W \left( \frac{3}{2} I_p - \frac{1}{2} X^\top X \right) - X \Phi(X^\top W), Z \right\rangle
\]

\[
= \text{tr} \left( Z^\top W \left( \frac{3}{2} I_p - \frac{1}{2} X^\top X \right) \right) - \text{tr} \left( Z^\top X \Phi(X^\top W) \right)
\]

\[
= \text{tr} \left( W^\top Z \left( \frac{3}{2} I_p - \frac{1}{2} X^\top X \right) \right) - \text{tr} \left( W^\top X \Phi(X^\top Z) \right)
\]

\[
= (Z \left( \frac{3}{2} I_p - \frac{1}{2} X^\top X \right) - X \Phi(X^\top Z), W)
\]

\[
= (J_X(Z), W).
\]

Here \((i)\) follows the fact that \( \text{tr} \left( AB \right) = \text{tr} \left( A^\top B \right) \) holds for any square matrix \( A \) and any symmetric matrix \( B \). By Proposition 2.7, for any \( X, Y \in \mathbb{R}^{n \times p} \), let \( D = Y - X \), we have

\[
f \left( Y \left( \frac{3}{2} I_p - \frac{1}{2} Y^\top Y \right) \right) - f \left( X \left( \frac{3}{2} I_p - \frac{1}{2} X^\top X \right) \right)
\]

\[
= (G(X), J_X(D)) + O(\|D\|_F^2)
\]

\[
= (D, J_X(G(X))) + O(\|D\|_F^2)
\]

\[
= \left\langle D, G(X) \left( \frac{3}{2} I_p - \frac{1}{2} X^\top X \right) - X \Phi(X^\top G(X)) \right\rangle + O(\|D\|_F^2),
\]

which illustrates that

\[
\nabla g(X) = G(X) \left( \frac{3}{2} I_p - \frac{1}{2} X^\top X \right) - X \Phi(X^\top G(X)).
\]

Then from the fact that \( h(X) = g(X) + \beta \|X^\top X - I_p\|_F^2 \), we could conclude that

\[
\nabla h(X) = G(X) \left( \frac{3}{2} I_p - \frac{1}{2} X^\top X \right) - X \Phi(X^\top G(X)) + \beta X(X^\top X - I_p),
\]

and complete the proof. \( \Box \)

We can conclude from the definition of \( M_1 \) and Proposition 2.8 that \( \|\nabla g(X)\|_F \leq 2M_1 \) for any \( X \in \Omega \). Besides, from the expression of \( h(X) \) illustrated in Lemma 2.8, we can conclude that \( \nabla h(X) = \text{grad} f(X) \) holds for any \( X \in \mathcal{S}_{n,p} \). Furthermore, the following proposition illustrates the expression of \( \nabla^2 h(X) \).

**Proposition 2.9.** Suppose \( f(X) \) satisfies the conditions in Assumption 2.6, then

\[
\nabla^2 g(X)[D] = J_X(\mathcal{H}(X)[J_X(D)]) - D \Phi(X^\top G(X)) - X \Phi(D^\top G(X)) - G(X) \Phi(D^\top X).
\]

Moreover,

\[
\nabla^2 h(X)[D] = \nabla^2 g(X)[D] + \beta(X \Phi(X^\top D) + D (X^\top X - I_p)).
\]

**Proof.** As illustrated in (2.2) from Lemma 2.8, the mapping \( J_X \) is self-adjoint for any \( X \in \mathbb{R}^{n \times p} \). Then
by Proposition 2.7, for any $Y \in \mathbb{R}^{n \times p}$ and let $D = Y - X$, we have
\[
    f \left( Y \left( \frac{3}{2} I_p - \frac{1}{2} Y^T Y \right) \right) - f \left( X \left( \frac{3}{2} I_p - \frac{1}{2} X^T X \right) \right)
\]
\[
    = f \left( X \left( \frac{3}{2} I_p - \frac{1}{2} X^T X \right) + f_j(D) - \left[ D \Phi(D^T X) + \frac{1}{2} XD^T D \right] \right) - f \left( X \left( \frac{3}{2} I_p - \frac{1}{2} X^T X \right) \right) + O(\|D\|_F^3)
\]
\[
    = \left\langle G(X), f_j(D) \right\rangle - \frac{1}{2} \left\langle D \Phi(D^T X), D^T D \right\rangle + O(\|D\|_F^3)
\]
\[
    = \left\langle D, \nabla g(X) \right\rangle - \left\langle \Phi(D^T G(X)), \Phi(D^T X) \right\rangle - \frac{1}{2} \left\langle D^T D, X^T G(X) \right\rangle + O(\|D\|_F^3).
\]

Therefore, the hessian of $g(X)$ can be expressed as
\[
    \nabla^2 g(X)[D] = f_j(\langle H(X)[f_j(D)], f_j(D) \rangle) - D \Phi(X^T G(X)) - X \Phi(D^T G(X)) - G(X) \Phi(D^T X).
\]

Moreover, since
\[
    \left\| X^T Y - I_p \right\|^2_F - \left\| X^T X - I_p \right\|^2_F
\]
\[
    = \left\langle 4D, X(X^T X - I_p) \right\rangle + 4 \left\langle \Phi(D^T X), \Phi(D^T X) \right\rangle + 2 \left\langle D^T D, X^T X - I_p \right\rangle + O(\|D\|_F^3),
\]
the hessian of $h(X)$ can be expressed as
\[
    \nabla^2 h(X)[D] = \nabla^2 g(X)[D] + \beta \left[ 2 X \Phi(X^T D) + D(X^T X - I_p) \right].
\]

Next, we give an important equality.

**Lemma 2.10.** For any $X \in \mathbb{R}^{n \times p}$, we have
\[
    \left\langle X(X^T X - I_p), \nabla g(X) \right\rangle = -\frac{3}{2} \left\langle \left( X^T X - I_p \right)^2, \Phi(X^T G(X)) \right\rangle.
\]

**Proof.** Consider the inner product of $\nabla g(X)$ and $X(X^T X - I_p)$, the following equality holds for any $X \in \mathbb{R}^{n \times p},$
\[
    \left\langle X(X^T X - I_p), \nabla g(X) \right\rangle
\]
\[
    = \left\langle X(X^T X - I_p), G(X) \left( \frac{3}{2} I_p - \frac{1}{2} X^T X \right) \right\rangle - \left\langle X(X^T X - I_p), X \Phi(X^T G(X)) \right\rangle
\]
\[
    = \left\langle \left( X^T X - I_p \right) \left( \frac{3}{2} I_p - \frac{1}{2} X^T X \right), \Phi(X^T G(X)) \right\rangle - \left\langle (X^T X - I_p) X^T X, \Phi(X^T G(X)) \right\rangle
\]
\[
    = -\frac{3}{2} \left\langle \left( X^T X - I_p \right)^2, \Phi(X^T G(X)) \right\rangle.
\]

Finally, we arrive at the main proposition in this preliminary section.

**Proposition 2.11.** Suppose Assumption 2.5 holds, and $\hat{X}$ is a first-order stationary point of ExPen, then
\[
    \|\hat{X}\|_2 \leq 1 + \frac{M_p}{2\beta}.\quad \text{Furthermore, when } \beta \geq \hat{\beta}, \text{we can conclude that all the first-order stationary points of ExPen are contained in } \Omega.
\]
Proof. Let $\tilde{X} = U\Sigma V^T$ be the singular value decomposition of $\tilde{X}$, namely, $U \in \mathbb{R}^{n \times p}$ and $V \in \mathbb{R}^{n \times p}$ are the orthogonal matrices and $\Sigma$ is a diagonal matrix with singular values of $\tilde{X}$ on its diagonal and $\sigma_1 \leq \cdots \leq \sigma_p$. Suppose the statement to be proved is no true, we achieve $\sigma_p > 1 + \frac{M_3}{2p}$. Let $D := U\text{Diag}(0, \ldots, 0, 1)V^T$, then from the first-order optimality condition, we have

$$\langle \nabla h(\tilde{X}), \tilde{D} \rangle = 0.$$ 

Besides, Assumption 2.5 illustrates that $\|\nabla g(X)\|_F$ is bounded and thus

$$|\langle \tilde{D}, \nabla g(\tilde{X}) \rangle| \leq \|\tilde{D}\|_F \|\nabla g(\tilde{X})\|_F \leq M_3.$$

On the other hand, from the definition of $\tilde{D}$, we can conclude that

$$\langle \tilde{X}(\tilde{X}^\top I_p), \tilde{D} \rangle = \sigma_p (\sigma_p^2 - 1).$$

Therefore, when $\beta \geq 6M_3$, we achieve

$$\langle \nabla h(\tilde{X}), \tilde{D} \rangle \geq \beta \langle \tilde{X}(\tilde{X}^\top I_p), \tilde{D} \rangle - |\langle \tilde{D}, \nabla g(\tilde{X}) \rangle| \geq (\sigma_p^2 - 1)(\beta \sigma_p) - M_3 > 0,$$

which contradicts to the first-order optimality. Therefore, we can conclude that $\|\tilde{X}\|_2 \leq 1 + \frac{M_3}{2p}$. \qed

### 2.3 Computational complexity of the first-order oracle

In this subsection, we analyze the cost of calculating the first-order derivative of $h(X)$, which takes the main computational cost in each iterate of a first-order algorithm such as gradient descent methods, nonlinear conjugate gradient methods, etc. Then we compare it with the fundamental operations in Riemannian optimization approaches. From the expression for $\nabla h(X)$ illustrated in Lemma 2.8, we find that computing $\nabla h(X)$ only involves computing $\nabla f$ and matrix-matrix multiplication. The computational cost of the basic linear algebra operations and the overall costs of computing the gradient of $h$ are listed in Table 1, while a comparison between several fundamental operations in Riemannian optimization and their corresponding operations for $h(X)$ are listed in Table 2. Here, FO denotes the computational of computing the gradient of $f$, and those terms in bold stand for the operations that cannot be parallelized.

| Compute $\nabla f \left( X \left( \frac{3}{2}I_p - \frac{1}{2}X^\top X \right) \right) \left( \frac{3}{2}I_p - \frac{1}{2}X^\top X \right)$ | $X^\top X$ | $X(\tilde{X}^\top I_p)$ | $\nabla f(X) = \nabla f(y)|_{y = X(\frac{3}{2}I_p - \frac{1}{2}X^\top X)}$ | $\Phi \left( X^\top G(X) \right)$ | $\Phi \left( X^\top G(X) \right)$ |
|-----------------|-----------------|-----------------|---------------------------------|-----------------|-----------------|
| Compute $X\Phi \left( X^\top G(X) \right)$ | $\nabla f(X) = \nabla f(y)|_{y = X(\frac{3}{2}I_p - \frac{1}{2}X^\top X)}$ | $\Phi \left( X^\top G(X) \right)$ | $\Phi \left( X^\top G(X) \right)$ |
| In total | $\nabla f(X) = \nabla f(y)|_{y = X(\frac{3}{2}I_p - \frac{1}{2}X^\top X)}$ | $\nabla f(X) = \nabla f(y)|_{y = X(\frac{3}{2}I_p - \frac{1}{2}X^\top X)}$ | $\nabla f(X) = \nabla f(y)|_{y = X(\frac{3}{2}I_p - \frac{1}{2}X^\top X)}$ |

Table 1: Computational complexity the first-order oracle in ExPen.

### 2.4 Postprocessing

We usually terminate an algorithm when achieving mild accuracy. When we implement an infeasible approach, the returned solution only reaches a mild accuracy in feasibility as well. Sometimes we pursue high accuracy for the feasibility at the same time. To this end, we impose an orthonormalization as a postprocess after obtaining a solution $X$ with mild accuracy by applying an unconstrained optimization approach to solve ExPen. Namely,

$$X \to \mathcal{P}_{S_{n,p}}(X), \quad (2.3)$$

where $\mathcal{P}_{S_{n,p}} : \mathbb{R}^{n \times p} \to S_{n,p}$ is the projection on Stiefel manifold defined in Section 1.3.
Lemma 2.12. For any $X \in \overline{\Omega}_{1/6}$, we have

$$\|\nabla h(X)\|_F^2 \geq \|\nabla g(X)\|_F^2 + \left(\frac{2}{3} \beta^2 - 4 \beta M_1\right)\|X^\top X - I_p\|_F^2.$$  

Proof. Since $h(X) = g(X) + \frac{\beta}{4} \|X^\top X - I_p\|_F^2$, we have

$$\langle \nabla h(X), \nabla h(X) \rangle = \langle \nabla g(X), \nabla g(X) \rangle + 2 \beta \langle \nabla g(X), X(X^\top X - I_p) \rangle + \beta^2 \|X(X^\top X - I_p)\|_F^2$$

$$= \|\nabla g(X)\|_F^2 - 3 \beta \langle \Phi(X^\top G(X)), (X^\top X - I_p)^2 \rangle + \beta^2 \|X(X^\top X - I_p)\|_F^2$$

$$\geq \|\nabla g(X)\|_F^2 + \left(\frac{2}{3} \beta^2 - 4 \beta M_1\right)\|X^\top X - I_p\|_F^2.$$  

Here the second equality directly follows Lemma 2.10. □

The following lemma illustrates the relationship between $\|\nabla h(X)\|_F$ and $\|\text{grad } f(\mathcal{P}_{S_n,p}(X))\|_F$.

Lemma 2.13. Suppose $\beta \geq \beta$, $X \in \overline{\Omega}_{1/6}$, then it holds that

$$\|\nabla h(X)\|_F \geq \frac{1}{2} \|\text{grad } f(\mathcal{P}_{S_n,p}(X))\|_F + \frac{\beta}{4} \|X^\top X - I_p\|_F.$$  

Proof. Suppose $X$ has singular value decomposition as $X = U \Sigma V^\top$, we can conclude that

$$\|X - \mathcal{P}_{S_n,p}(X)\|_F = \|\Sigma - I_p\|_F \leq \frac{6}{11} \|\Sigma^2 - I_p\|_F = \frac{6}{11} \|X^\top X - I_p\|_F.$$  

Therefore, the results in Lemma 2.12 illustrates that

$$\|\nabla h(X)\|_F \geq \frac{1}{2} \|\nabla g(X)\|_F + \frac{\sqrt{6} \beta^2 - 36 \beta M_1}{3} \|X^\top X - I_p\|_F$$

$$\geq \frac{1}{2} \|\nabla g(\mathcal{P}_{S_n,p}(X))\|_F - \frac{3M_2}{11} \|X^\top X - I_p\|_F + \frac{\sqrt{6} \beta^2 - 36 \beta M_1}{3} \|X^\top X - I_p\|_F$$

$$\geq \frac{1}{2} \|\text{grad } f(\mathcal{P}_{S_n,p}(X))\|_F + \frac{\beta}{4} \|X^\top X - I_p\|_F.$$  

□

The following lemma guarantees that the postprocess (2.3) can further reduce the function value if the current iterate is sufficiently close to the Stiefel manifold.

Proposition 2.14. Suppose $X \in \overline{\Omega}_{1/6}$, then it holds that

$$h(\mathcal{P}_{S_n,p}(X)) \leq h(X) - \left(\frac{\beta}{4} - \frac{M_1}{2}\right) \|X^\top X - I_p\|_F^2.$$
Proof. By the SVD of $X$, we first conclude that

$$
\left\| X \left( \frac{3}{2} I_p - \frac{1}{2} X^\top X \right) - P_{S_{n,p}}(X) \right\|_F = \left\| U \Sigma \left( \frac{3}{2} I_p - \frac{1}{2} \Sigma^2 \right) V^\top - U V^\top \right\|_F
$$

$$
\leq \frac{1}{2} \left\| \Sigma^2 - I_p \right\|_F^2 = \frac{1}{2} \left\| X^\top X - I_p \right\|_F^2.
$$

Here (i) directly follows from $(\Sigma + 2I_p) (\Sigma - I_p)^2 \preceq (\Sigma + I_p)^2 (\Sigma - I_p)^2$ when $\Sigma \succeq \frac{5}{6} I_p$, and the fact that $\|A^2\|_F \leq \|A\|_F^2$ holds for any symmetric matrix $A$.

Then we can conclude that

$$
h(X) - h(P_{S_{n,p}}(X)) = f \left( X \left( \frac{3}{2} I_p - \frac{1}{2} X^\top X \right) \right) - f(P_{S_{n,p}}(X)) + \beta \left\| X^\top X - I_p \right\|_F^2
$$

$$
\geq - M_1 \left\| X \left( \frac{3}{2} I_p - \frac{1}{2} X^\top X \right) - P_{S_{n,p}}(X) \right\|_F + \frac{\beta}{4} \left\| X^\top X - I_p \right\|_F^2
$$

$$
\geq \left( \frac{\beta}{4} - \frac{M_1}{2} \right) \left\| X^\top X - I_p \right\|_F^2.
$$

Here (ii) follows the Lipschitz continuity of $f$, and (iii) is directly from (2.5).

\[\square\]

3 Properties of ExPen

In this section, we analyze the theoretical properties of ExPen.

3.1 First-order relationship

In this subsection, we study the first-order relationship between OCP and ExPen. The main theoretical results of this subsection can be summarized in Figure 1. Here “A.”, “D.”, “P.”, “T.” are the abbreviations of “Assumption”, “Definition”, “Proposition”, and “Theorem”, respectively.

![Figure 1: Roadmap of the first-order relationship between OCP and ExPen.](image)

The following theorem categorizes the first-order stationary points of ExPen in $\Omega$.

**Theorem 3.1.** Suppose $X^* \in \Omega$ is a first-order stationary point of ExPen, and $\beta \geq \hat{\beta}$, then either $X^*$ is a first-order stationary point of OCP, or $\sigma_{\text{min}}(X^*) \leq \sqrt{\frac{2M_1}{\beta}}$. 

Proof. Suppose $\sigma_{\min}(X^*) > \sqrt{\frac{2M_1}{p}}$, then $\beta X^T X^* - 2M_1 I_p$ is positive definite. Besides, from Lemma 2.10 we achieve
\[
0 = \left\langle \nabla h(X^*), X^*(X^T X^* - I_p) \right\rangle \\
g \geq \left\langle \beta X^*(X^T X^* - I_p), X^*(X^T X^* - I_p) \right\rangle - \left| \left\langle \nabla g(X^*), X^*(X^T X^* - I_p) \right\rangle \right| \\
\geq \left\langle \beta X^*(X^T X^* - I_p), X^*(X^T X^* - I_p) \right\rangle - \frac{3}{2} \left\| X^T g(X^*) \right\|_2^2 \left( (X^T X^* - I_p)^2 \right) \\
g \geq \left\langle \beta X^*(X^T X^* - I_p), X^*(X^T X^* - I_p) \right\rangle - \left\langle \frac{3}{2} \left\| X^* \right\|_2 \left\| G(X^*) \right\|_F \cdot I_p, (X^T X^* - I_p)^2 \right\rangle \\
\geq \left\langle \beta X^*(X^T X^* - 2M_1 I_p), (X^T X^* - I_p)^2 \right\rangle \geq 0,
\]
which illustrates that $X^T X^* = I_p$. Then we can conclude that $0 = \nabla h(X^*) = \text{grad } f(X^*)$ and thus complete the proof.

As illustrated in Theorem 3.1, any first-order stationary point of ExPen in $\Omega$ is either a first-order stationary point of (OCP), or is far from the Stiefel manifold. The following theorem illustrates that any infeasible first-order stationary point of ExPen cannot be a second-order stationary point of $h(X)$.

**Theorem 3.2.** Suppose Assumption 2.6 holds, $\beta \geq \beta^*$, then any infeasible first-order stationary point $\tilde{X}$ of ExPen in $\Omega$ is not a second-order stationary point of ExPen. More specifically, $\lambda_{\min}(\nabla^2 h(\tilde{X})) \leq -\frac{\beta}{24}$.

Proof. Suppose the statement is not true, namely, $\tilde{X}$ is a second-order stationary point of OCP. Since $\beta \geq 12M_1$, it holds that $\sigma_{\min}(\tilde{X}^T \tilde{X}) \leq \frac{1}{6}$ by Proposition 3.1. Let $\tilde{X} = U \Sigma V^T$ be the singular value decomposition of $\tilde{X}$, namely, $U \in \mathbb{R}^{n \times p}$ and $V \in \mathbb{R}^{n \times p}$ are the orthogonal matrices and $\Sigma$ is a diagonal matrix with singular values of $\tilde{X}$ on its diagonal. Without loss of generality, we assume $\sigma_1 \leq \frac{1}{\sqrt{6}}$ which is the first entry of the diagonal matrix $\Sigma$.

Then we denote $D = -u_1 v_1^T$, where $u_1$ and $v_1$ are the first columns of $U$ and $V$, respectively. It holds that
\[
(\tilde{X} + tD)^T (\tilde{X} + tD) = \tilde{X}^T \tilde{X} + 2tD^T \tilde{X} + t^2 D^T D = V^T \Sigma^2 V - 2t \sigma_1 v_1 v_1^T + t^2 v_1 v_1^T.
\]
Due to the first-order stationarity of $\tilde{X}$, it holds $\nabla h(\tilde{X}) = 0$ which implies $D^T \nabla h(\tilde{X}) = 0$. First, we have
\[
\left\| (\tilde{X} + tD)^T (\tilde{X} + tD) - I_p \right\|_F^2 = \left\| \tilde{X}^T \tilde{X} - I_p + 2t \Phi(\tilde{X}^T D) + t^2 D^T D \right\|_F^2 \\
\geq \left\| \tilde{X}^T \tilde{X} - I_p \right\|_F^2 + 4t^2 \left( \Phi(\tilde{X}^T D), \Phi(\tilde{X}^T D) \right) + 2t^2 \left( D^T D, \tilde{X}^T \tilde{X} - I_p \right) + O(t^3) \\
\geq \left\| \tilde{X}^T \tilde{X} - I_p \right\|_F^2 + 4t^2 \sigma_1^2 - 2t^2 (1 - \sigma_1^2) + O(t^3) \geq \left\| \tilde{X}^T \tilde{X} - I_p \right\|_F^2 - t^2 + O(t^3).
\]
As a result,
\[
h(\tilde{X} + tD) \leq h(\tilde{X}) + t \cdot \left\langle D, \nabla h(\tilde{X}) \right\rangle + \frac{t^2}{2} \left\| \nabla^2 h(\tilde{X}) \right\|_F \left\| D \right\|_F^2 \leq \frac{\beta}{24} t^2 + O(t^3)
\]
which contradicts to the second-order optimality of ExPen. Therefore, we can conclude that any infeasible first-order stationary point of ExPen in $\Omega$ is not a second-order stationary point of ExPen, and $\lambda_{\min}(\nabla^2 h(\tilde{X})) \leq -\frac{\beta}{24}$.

Combining Proposition 2.11 with Theorem 3.1, we arrive at the following corollary.

**Corollary 3.3.** Suppose Assumptions 2.5 and 2.6 hold, and $\beta \geq \beta^*$. Let $X^*$ be a first-order stationary point of ExPen, then either $X^*$ is a first-order stationary point of OCP, or is far from the Stiefel manifold and cannot be a second-order stationary point of ExPen.

The proof of this corollary is straightforward and hence omitted.
3.2 Second-order relationship

In this subsection, we study the first-order relationship between OCP and ExPen. The main theoretical results of this subsection can be summarized in Figure 2.

![Figure 2: Roadmap of the second-order relationship between OCP and ExPen under Assumption 2.6.](image)

We first analyze the relationship between Riemannian hessian of the original objective function $f$ and the Euclidean hessian of the penalty function $h$.

**Lemma 3.4.** Suppose $f(X)$ satisfies Assumption 2.6 and $X \in S_{n,p}$ is a first-order stationary point of $h(X)$. Then for any $D_1 \in T_X$ and any $D_2 \in N_X$, we have

\[
\begin{align*}
\langle D_1, \nabla^2 h(X)[D_1] \rangle &= \langle D_1, \nabla^2 f(X)[D_1] - D_1 \Phi(X^\top \nabla f(X)) \rangle ; \\
\langle D_2, \nabla^2 h(X)[D_2] \rangle &\geq (2\beta - M_2) \|D_2\|_F^2 ; \\
\langle D_1, \nabla^2 h(X)[D_2] \rangle &= 0.
\end{align*}
\]  

Proof. Since $D_1 \in T_X$, by the definition of $T_X$ we have $\Phi(D_1^\top X) = 0$. Besides, as $X \in S_{n,p}$ is the first-order stationary point of $h(X)$, Definition 2.1 illustrates that $G(X) = \nabla f(X) = X\Phi(X^\top \nabla f(X))$. Then we can conclude that $\Phi(D_1^\top G(X)) = 0$. Moreover, the definition of $J_X$ indicates that $J_X(D_1) = D_1$. As a result, from Proposition 2.9, we can conclude that

\[
\begin{align*}
\nabla^2 h(X)[D_1] &= \nabla^2 g(X)[D_1] \\
&= J_X(H(X)[J_X(D_1)]) - D_1 \Phi(X^\top \nabla f(X)) - D_1 \Phi(X^\top G(X)) - X\Phi(D_1^\top G(X)) \\
&= J_X(\nabla^2 f(X)[D_1]) - D_1 \Phi(X^\top \nabla f(X)).
\end{align*}
\]

Therefore, for any $D_1 \in T_X$, we have

\[
\langle D_1, \nabla^2 h(X)[D_1] \rangle = \langle D_1, \nabla^2 f(X)[D_1] - D_1 \Phi(X^\top \nabla f(X)) \rangle.
\]

Besides, notice that $D_2 \in N_X$ implies that $\|\Phi(D_2^\top X)\|_F = \|D_2\|_F$. Then by the expression of $\nabla^2 h(X)$ in Proposition 2.9, we can conclude that

\[
\begin{align*}
\langle D_2, \nabla^2 h(X)[D_2] \rangle &= \langle D_2, \nabla^2 g(X)[D_2] \rangle + 2\beta \|\Phi(D_2^\top X)\|_F^2 \geq (2\beta - M_2) \|D_2\|_F^2.
\end{align*}
\]

Moreover, since $D_1 \in T_X$ and $D_2 \in N_X$, we have $J_X(D_2) = 0$, and $\Phi(D_2^\top D_1) = 0$. Then by (3.4),

\[
\begin{align*}
\langle D_2, \nabla^2 h(X)[D_1] \rangle &= \langle D_2, J_X(\nabla^2 f(X)[J_X(D_1)]) - D_1 \Phi(X^\top \nabla f(X)) \rangle \\
&= \langle J_X(D_2), \nabla^2 f(X)[J_X(D_1)] \rangle - \langle D_2, D_1 \Phi(X^\top \nabla f(X)) \rangle \\
&= - \langle \Phi(D_2^\top D_1), \Phi(X^\top \nabla f(X)) \rangle = 0,
\end{align*}
\]

which completes the proof. \qed
Theorem 3.5. Suppose \( f(X) \) satisfies Assumption 2.6, for any first-order stationary point \( X \in S_{n,p} \) of OCP, any eigenvalue of \( \text{hess } f(X) \) is an eigenvalue of \( \nabla^2 h(X) \). In turn, any eigenvalue of \( \nabla^2 h(X) \) is either an eigenvalue of \( \text{hess } f(X) \), or greater than \( 2\beta - M_2 \).

Proof. Let \( \lambda_1 \) be an eigenvalue of \( \text{hess } f(X) \), it follows from Definition 2.2 that there exists an \( \hat{D}_1 \in T_X \) such that
\[
I_X \left( \nabla^2 f(X)[\hat{D}_1] - \hat{D}_1 \Phi(X^T \nabla f(X)) \right) = \sigma D_1.
\]
In addition, equality (3.4) in Lemma 3.4 indicates that
\[
\nabla^2 h(X)[\hat{D}_1] = I_X(\nabla^2 f(X)[\hat{D}_1]) - \hat{D}_1 \Phi(X^T \nabla f(X)) = \sigma D_1.
\]
Therefore, any eigenvalue of \( \text{hess } f(X) \) is an eigenvalue of \( \nabla^2 h(X) \).

On the other hand, Lemma 3.4 verifies that the linear operator \( \nabla^2 h(X) \) maps a vector in \( T_X \) or \( N_X \) to \( T_X \) or \( N_X \), respectively. Then any eigenvector of \( \nabla^2 h(X) \) is either in \( T_X \) or \( N_X \). For any \( D_2 \in N_X \), (3.2) implies that
\[
\left( D_2, \nabla^2 h(X)[D_2] \right) \geq (2\beta - M_2) \| D_2 \|_F^2,
\]
from which we can conclude that any eigenvalue of \( \nabla^2 h(X) \) is either an eigenvalue of \( \text{hess } f(X) \), or greater than \( 2\beta - M_2 \).

Based on Theorem 3.5, we can establish the second-order relationship between OCP and ExPen.

Theorem 3.6. Suppose \( f(X) \) satisfies Assumption 2.6 and \( \beta \geq \hat{\beta} \), then any second-order stationary point of \( h(X) \) in \( \Omega \) is a second-order stationary point of OCP. Moreover, OCP and ExPen have exactly the same second-order stationary points in \( \Omega \).

Proof. Let \( X \in \Omega \) be a second-order stationary point of \( h(X) \), then all eigenvalues of \( \nabla^2 h(X) \) are nonnegative. It follows from Theorems 3.1 and 3.2 that \( X \) is feasible. We can further conclude \( X \) is a first-order stationary point of OCP by Proposition 2.8. In addition, Theorem 3.5 shows that all eigenvalues of \( \text{hess } f(X) \) consist of a subset of the spectra of \( \nabla^2 h(X) \), and thus are nonnegative. Namely, \( X \) is a second-order stationary point of OCP.

In turn, let \( X \in S_{n,p} \) be a second-order stationary point of OCP, naturally, all the eigenvalues of \( \text{hess } f(X) \) are nonnegative. Then we can immediately obtain that all the eigenvalues of \( \nabla^2 h(X) \) are nonnegative resulting from Theorem 3.5 and the fact that \( 2\beta \geq M \). Hence, \( X \) is a second-order stationary point of \( h(X) \).

Based on the second-order relationship between OCP and ExPen in \( \Omega \) illustrated in Theorem 3.6, we can immediately obtain their second-order relationship in \( \mathbb{R}^{n \times p} \) by utilizing Proposition 2.11. We omit the proof, since it is quite straightforward.

Corollary 3.7. Suppose Assumptions 2.5 and 2.6 hold, and \( \beta \geq \hat{\beta} \), then OCP and ExPen share the same second-order stationary points.

Indeed, we can even show that OCP and ExPen share the same local minimizers.

Theorem 3.8. Suppose Assumptions 2.5 and 2.6 hold, and \( \beta \geq \hat{\beta} \), then ExPen and OCP share the same local minimizers.

Proof. By Corollary 3.3 and Corollary 3.7, we can conclude that any local minimizers of ExPen are on Stiefel manifold. Since \( h(X) = f(X) \) holds for any \( X \in S_{n,p} \), then any local minimizers of ExPen are local minimizers of OCP.

On the other hand, let \( X^* \in S_{n,p} \) be a local minimizer of OCP, then there exists \( \gamma \in \left( 0, \frac{1}{12} \right) \) such that \( f(Z) \geq f(X) \) holds for any \( Z \in S_{n,p}, \| Z - X^* \|_F \leq \gamma \). Then for any \( Y \in \mathbb{R}^{n \times p}, \| Y - X^* \|_F \leq \frac{\gamma}{2}, \gamma, Y \in \mathbb{R}_{11\gamma/12} \), we can obtain that
\[
\| P_{S_{n,p}}(Y) - X^* \|_F \leq \| P_{S_{n,p}}(Y) - Y \|_F + \| Y - X^* \|_F \leq \frac{\gamma}{2} + \frac{\gamma}{2} \leq \gamma.
\]
Here the second inequality recalls the relationship (2.4). Then it follows from Proposition 2.14 that
\[ h(Y) - h(X^t) = h(Y) - h(P_{S_n,p}(Y)) + h(P_{S_n,p}(Y)) - h(X^t) \geq \left( \frac{\beta}{4} - \frac{M_1}{2} \right) \|Y^\top Y - I_p\|_F^2 \geq 0, \]
which concludes the proof. \(\square\)

### 3.3 Łojasiewicz gradient inequality

In this section, we study the relationship between the Riemannian Łojasiewicz gradient inequality for \(f(X)\) and the Euclidean Łojasiewicz gradient inequality for \(h(X)\).

**Proposition 3.9.** Suppose \(f(X)\) satisfies the Riemannian Łojasiewicz gradient inequality at \(X \in S_{n,p}\) with Łojasiewicz exponent \(\theta \in \left(0, \frac{1}{2}\right)\), i.e. there exists \(C > 0\) such that
\[ \|\text{grad} f(Y)\|_F \geq C|f(Y) - f(X)|^{1-\theta}, \]
and \(\beta > \max\{8CM_1, 1, \beta\}\). Then \(h(X)\) satisfies the Łojasiewicz gradient inequality at \(X \in S_{n,p}\) with Łojasiewicz exponent \(\theta \in (0, \frac{1}{2})\).

**Proof.** For any \(Y \in \Omega\), we denote \(Z := Y(Y^\top Y)^{-\frac{1}{2}}\). It is clear that \(Z \in S_{n,p}\). By Lemma 2.8 and the Riemannian Łojasiewicz gradient inequality of \(f\), we have
\[ \|\nabla g(Z)\|_F = \|\text{grad} f(Z)\|_F \geq C|f(Z) - f(X)|^{1-\theta} = C|g(Z) - g(X)|^{1-\theta}. \]
Besides, since
\[
\left\| \left( \frac{2}{3} I_p - \frac{1}{2} X^\top X \right)^2 X^\top X - I_p \right\|_F^2 = \left\| X^\top X - I_p + (I_p - X^\top X)X^\top X + \frac{1}{4} X^\top X(X^\top X - I_p) \right\|_F^2
\]
we obtain
\[ |g(Y) - g(Z)| \leq M_1 \left\| Y^\top Y - I_p \right\|_F^2. \quad (3.5) \]
Together with Lemma 2.13, we can conclude that
\[ \|\nabla h(Y)\|_F \geq \frac{1}{2} \|\nabla g(Z)\|_F + \frac{\beta}{4} \left\| Y^\top Y - I_p \right\|_F. \]
In addition, since \(\theta \in \left(0, \frac{1}{2}\right)\), and \(Y \in \Omega\), we have
\[
|h(Y) - h(X)|^{1-\theta} = \left| g(Y) - g(X) + \frac{\beta}{4} \left\| Y^\top Y - I_p \right\|_F \right|^{1-\theta}
\]
\[ \leq |g(Y) - g(X)|^{1-\theta} + \left( \frac{\beta}{4} \left\| Y^\top Y - I_p \right\|_F \right)^{1-\theta} \leq |g(Y) - g(X)|^{1-\theta} + \frac{\beta}{4} \left\| Y^\top Y - I_p \right\|_F. \]
Therefore, we have
\[ \|\nabla h(Y)\|_F \geq \|\nabla g(Z)\|_F + \frac{\beta}{4} \left\| Y^\top Y - I_p \right\|_F \geq C|g(Z) - g(X)|^{1-\theta} + \frac{\beta}{4} \left\| Y^\top Y - I_p \right\|_F \]
\[ \quad \geq C|g(Y) - g(X)|^{1-\theta} - C|g(Z) - g(Y)|^{1-\theta} + \frac{\beta}{4} \left\| Y^\top Y - I_p \right\|_F \]
\[ \quad \geq C|g(Y) - g(X)|^{1-\theta} - CM_1^{1-\theta} \left\| Y^\top Y - I_p \right\|_F^2 + \frac{\beta}{4} \left\| Y^\top Y - I_p \right\|_F \]
\[ \geq C|g(Y) - g(X)|^{1-\theta} + \frac{\beta}{8} \left\| Y^\top Y - I_p \right\|_F \geq \min \left\{ C, \frac{1}{2} \right\} |h(Y) - h(X)|^{1-\theta}. \]
Here inequality (i) uses the fact that $|a|^{1-\theta} + |b|^{1-\theta} \geq (|a| + |b|)^{1-\theta} \geq |a + b|^{1-\theta}$ for any $a, b \in \mathbb{R}$, $\theta \in (0, \frac{1}{2}]$. Besides, inequality (ii) directly follows from (3.5). As a result, we obtain
\[
\| \nabla h(Y) \|_F \geq \min \left\{ \frac{1}{\beta}, \frac{1}{2} \right\} |h(Y) - h(X)|^{1-\theta},
\]
which concludes the proof.

4 Application

The cubic regularization Newton method with momentum proposed by Wang et al. [42] is a recent development in nonconvex unconstrained optimization area. This approach has lots of nice theoretical properties including fast convergence and the ability to escape saddle points, and numerical efficiency if the Hessian of the objective function is easy to access. However, once we want to extend this approach in solving OCP through Riemannian optimization approaches, we are forced to comply with the low efficiency when using the parallel transport or weak inheritance in convergence when using the vector transport.

As shown by the previous two sections, the exact penalty model ExPen can build up a bridge between the unconstrained optimization approaches and the original model OCP. In this section, we use the cubic regularization Newton method with momentum as an instance to demonstrate the power of this “bridge”.

First of all, we illustrate an ExPen version of the cubic regularization Newton method with momentum in Algorithm 1.

Algorithm 1 Cubic regularization Newton method with momentum for solving ExPen.

Require: Input data: objective function $f$, constants $\tau_0 < 1$ and $\rho > 0$.
1: Choose the initial guess $X_0$, set $Y_0 := X_0$ and $k := 0$.
2: while not terminate do
3:   Solve the cubic regularization subproblem:
4:   
5: Compute the trial step:
6:   
7: Denote
\[
\tau_k = \min\{\tau_0, \|\nabla f(Y_{k+1})\|_F, \|Y_{k+1} - X_k\|\}.
\]
8: Compute the momentum step:
9:   
10: Set $X_{k+1} = Y_{k+1}$ when $h(Y_{k+1}) \leq h(V_{k+1})$; otherwise, set $X_{k+1} = V_{k+1}$.
11: Set $k := k + 1$.
12: end while
13: Return $X_k$.

To prove the convergence of Algorithm 1, we first illustrate a nice property of ExPen through the following lemma.

Lemma 4.1. Suppose $\beta \geq 192M_0$. Then $h(Y) < h(Z)$ holds for any $Y \in \overline{\Omega}_{1/12}$ and $Z \in \Omega \setminus \overline{\Omega}_{1/6}$.

Proof. For any $Y \in \overline{\Omega}_{1/12}$ and $Z \in \Omega \setminus \overline{\Omega}_{1/6}$, we have
\[
|h(Y) - h(Z)| < \sup_{W \in \Omega} h(W) - \inf_{W \in \Omega} h(W) + \frac{\beta}{576} - \frac{\beta}{144} \leq M_0 - \frac{\beta}{192} \leq 0.
\]
Lemma 4.1 guarantees that the iterates generated by any nonmonotonic algorithm starting from an initial point \( X_0 \in \overline{\Omega}_{1/12} \) are restricted in the region \( \overline{\Omega}_{1/6} \).

We notice that Step 7 of Algorithm 1 guarantees the monotonic decrease of the function values. Hence, by combining Theorem 1 in [42] and Lemma 2.13, we can easily obtain the global convergence of Algorithm 1. More details are presented in the following theorem.

**Theorem 4.2.** Suppose \( \nabla^2 h(X) \) is Lipschitz continuous in \( \Omega \), and denote

\[
M := \sup_{Y, Z \in \Omega} \frac{\|\nabla^2 g(Y) - \nabla^2 g(Z)\|_F}{\|Y - Z\|_F},
\]

Let \( \beta \geq \max\{192M_0, M, \tilde{B}\} \), \( \rho = \tilde{M} + 7\beta \), \( X_0 \in \overline{\Omega}_{1/12} \) and \( \{X_k\} \) be the sequence generated by Algorithm 1. Then for any given \( \varepsilon > 0 \) and any \( k \) satisfying

\[
k \geq \frac{\tilde{C}}{\varepsilon^{3/2}},
\]

with \( \tilde{C} \) being a constant dependent on \( \beta, M_1, M_2 \) and \( \tilde{M} \), there exists \( k^* \in \{0, 1, ..., k\} \) satisfying

\[
\begin{cases}
\|\nabla h(\mathcal{P}_{S_n,p}(X_{k^*}))\|_F \leq \varepsilon, \\
\lambda_{\min}(\text{hess } f(\mathcal{P}_{S_n,p}(X_{k^*}))) \geq -\varepsilon,
\end{cases}
\]

**Proof.** Due to Step 7 and the fact that \( X_0 \in \overline{\Omega}_{1/12} \), the sequence \( \{X_k\} \) generated by Algorithm 1 satisfies \( h(X_{k+1}) \leq h(X_k) \leq h(X_0) \). Therefore, Lemma 4.1 illustrates that all the iterates are restricted in \( \overline{\Omega}_{1/6} \subset \Omega \), and the Assumption 1 in [42] holds from the compactness of \( \Omega \). As a result, from the expression of \( h(X) \), the Lipschitz constant of \( \nabla^2 h(X) \) in \( \Omega \) is smaller than \( \tilde{M} + 7\beta \). Recall Theorem 1 in [42], there exists a constant \( \tilde{C} > 0 \), for any \( k \geq \frac{\tilde{C}}{\varepsilon^{3/2}} \), there exists \( k^* \in \{0, 1, ..., k\} \) satisfying

\[
\begin{cases}
\|\nabla h(X_{k^*})\|_F \leq \frac{\varepsilon}{2} \\
\lambda_{\min}(\nabla^2 h(X_{k^*})) \geq -\frac{\varepsilon}{2},
\end{cases}
\]

It then follows from Lemma 2.12 that

\[
\begin{cases}
\|\grad f(\mathcal{P}_{S_n,p}(X_{k^*}))\|_F \leq \varepsilon, \\
\|X_{k^*}X_{k^*} - I_p\|_F \leq \frac{2\varepsilon}{\beta},
\end{cases}
\]

Since \( \nabla^2 g \) is \( \tilde{M} \)-Lipschitz continuous, and recall (2.4) in Lemma 2.13, we arrive at

\[
\lambda_{\min}(\text{hess } f(\mathcal{P}_{S_n,p}(X_{k^*}))) = \lambda_{\min}(\nabla^2 g(\mathcal{P}_{S_n,p}(X_{k^*}))) \geq \lambda_{\min}(\nabla^2 g(X_{k^*})) - \tilde{M} \|X_{k^*} - \mathcal{P}_{S_n,p}(X_{k^*})\|_F \\
\geq \lambda_{\min}(\nabla^2 g(X_{k^*})) - \tilde{M} \|X_{k^*} - X_{k^*}\|_F \geq \frac{\varepsilon}{2} - \frac{\tilde{M}^2}{2\beta}\varepsilon \geq -\varepsilon,
\]

which concludes the proof. \( \square \)

5 Conclusion

The optimization over the Stiefel manifold has a close connection with unconstrained optimization. To efficiently extend existing unconstrained optimization approaches to their Stiefel versions and establish the corresponding theoretical analysis, most existing approaches are mainly based on
the frameworks summarized in [3]. These approaches always involve computing the retractions and parallel/vector transports. However, computing retractions or parallel transport on the Stiefel manifold lack efficiency or scalability, while computing the vector transport can hardly inherit nice techniques in theoretical analysis.

In this paper, we present a novel exact smooth penalty function and its corresponding penalty model ExPen for OCP. We show that ExPen is well-defined under mild assumptions and study its theoretical properties. As illustrated in Figure 1 and Figure 2, we have proved the first-order and second-order relationships between OCP and ExPen, respectively. These properties guarantee that ExPen and OCP share first-order or second-order stationary points or local minimizers with a sufficiently large given penalty parameter.

In conclusion, we can directly adopt unconstrained optimization approaches to solve OCP through the bridge built by ExPen. Meanwhile, we can easily inherit the nice convergence properties of those approaches. We use cubic regularized Newton methods with momentum as an instance. We present its ExPen version and establish its global convergence, worst-case complexity and the ability to escaping the saddle point. It is worth mentioning that this ExPen version is performed in Euclidean space and hence avoids computing the retractions or parallel transports on the Stiefel manifold. Our present example highlights that those progress in nonconvex unconstrained optimization will immediately benefit optimization over the Stiefel manifold through ExPen, which further address the great potential of ExPen.

References


