Riemannian optimization using three different metrics for Hermitian PSD fixed-rank constraints

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Abstract

For smooth optimization problems with a Hermitian positive semidefinite fixed-rank constraint, we consider three existing approaches including the simple Burer–Monteiro method, and Riemannian optimization over quotient geometry and the embedded geometry. These three methods can be all represented via quotient geometry with three Riemannian metrics $\boldsymbol{g^i(\cdot,\cdot)}$ $\boldsymbol{(i = 1, 2, 3)}$. By taking the nonlinear conjugate gradient method (CG) as an example, we show that CG in the factor-based Burer–Monteiro approach is equivalent to Riemannian CG on the quotient geometry with the Bures-Wasserstein metric $\boldsymbol{g^1}$. Riemannian CG on the quotient geometry with the metric $\boldsymbol{g^3}$ is equivalent to Riemannian CG on the embedded geometry. For comparing the three approaches, we analyze the condition number of the Riemannian Hessian near a minimizer under the three different metrics. Under certain assumptions, the condition number from the Bures-Wasserstein metric $\boldsymbol{g^1}$ is significantly worse than the other two metrics. Numerical experiments show that the Burer–Monteiro CG method has obviously slower asymptotic convergence rate either when the minimizer has a large condition number or when it is rank deficient, which is consistent with the condition number analysis.

Keywords: Riemannian optimization, Hermitian PSD fixed-rank matrices, embedded manifold, quotient manifold, Burer–Monteiro, conjugate gradient, Riemannian Hessian, Bures-Wasserstein metric

1 Introduction

1.1 The Hermitian PSD low-rank constraints

In this paper, we are interested in algorithms for minimizing a real-valued function f with a Hermitian positive semidefinite (PSD) low-rank constraint

$$\begin{array}{ll} \underset{X}{\text{minimize}} & f(X) \\ \text{subject to} & X \in \mathcal{H}_+^{n,p} \end{array}, \tag{1}$$

where $\mathcal{H}_+^{n,p}$ denotes the set of n-by-n Hermitian PSD matrices of fixed rank $p \ll n$. Even though $X \in \mathcal{H}_+^{n,p}$ is a nonconvex constraint, in practice (1) is often used for approximating solutions to a minimization with a convex PSD constraint:

$$\begin{array}{ll} \underset{X \in \mathbb{C}^{n\times n}}{\text{minimize}} & f(X) \\ \text{subject to} & X \succcurlyeq 0 \end{array}. \tag{2}$$

There are many applications of PSD constraints. They arise in semidefinite programming serving as covariance matrices in statistics and kernels in machine learning, etc. See [1] and [2] for some of these applications. If the solution of (2) is of low rank and $\mathcal{O}(n^2)$ complexity is too large for storage or computation, it is preferable to consider a low-rank representation of PSD matrices. For example, real symmetric PSD fixed-rank matrices were used in [3, 4]. Since $X \in \mathcal{H}_+^{n,p}$ has a low-rank structure, they can be represented in a low-rank compact form on the order of $\mathcal{O}(np)$, which is smaller than the $\mathcal{O}(n^2)$ storage when directly using $X \in \mathbb{C}^{n\times n}$. In many applications, the cost function in (2) takes the form $f(X) = \frac{1}{2}\|\mathcal{A}(X) - b\|_F^2$ where $\mathcal{A}$ is a linear operator and the norm is the Frobenius norm, and $f(X)$ can be evaluated efficiently by $\mathcal{O}(pn\log n)$ flops for $X \in \mathcal{H}_+^{n,p}$, e.g., the PhaseLift problem [5, 6] and the interferometry recovery problem [7, 8]. For some of these problems, solving (1) may lead to a good approximate solution to (2) with compact storage and computational cost.

1.2 The real inner product and induced gradient

Since $f(X)$ is real-valued, $f(X)$ does not have a complex derivative. In this paper, all linear spaces of complex matrices will therefore be regarded as vector spaces over $\mathbb{R}$. For any real vector space $\mathcal{E}$, the inner product on $\mathcal{E}$ is denoted by $\langle\cdot,\cdot\rangle_{\mathcal{E}}$. For $A, B \in \mathbb{R}^{m\times n}$, the Hilbert–Schmidt inner product is $\langle A, B\rangle_{\mathbb{R}^{m\times n}} = \mathrm{tr}(A^T B)$. Let $\Re(A)$ and $\Im(A)$ represent the real and imaginary parts of a complex matrix $A \in \mathbb{C}^{m\times n}$. The real inner product for $\mathbb{C}^{m\times n}$ is

$$\langle A, B\rangle_{\mathbb{C}^{m\times n}} := \Re(\mathrm{tr}(A^* B)), \quad A, B \in \mathbb{C}^{m\times n}, \tag{3}$$

where * is the conjugate transpose. With the real inner product (3) for the real vector space $\mathbb{C}^{m\times n}$, the gradient of $f(X)$ is

$$\nabla f(X) = \frac{\partial f(X)}{\partial \Re(X)} + \mathbb{i}\frac{\partial f(X)}{\partial \Im(X)} \in \mathbb{C}^{m\times n}. \tag{4}$$

See [9] for a derivation of (4). For $f(X) = \frac{1}{2}\|\mathcal{A}(X) - b\|_F^2$ with a linear operator $\mathcal{A}$, (4) becomes $\nabla f(X) = \mathcal{A}^*(\mathcal{A}(X) - b)$, where $\mathcal{A}^*$ is the adjoint operator of $\mathcal{A}$. See [9, Appendix A] for details.

1.3 Three different methodologies

We consider three methods for solving (1). The first approach, often called the Burer–Monteiro method [10, 11], is to solve

$$\min_{Y\in\mathbb{C}^{n\times p}} F(Y) := f(YY^*). \tag{5}$$

As shown in [9, Appendix A], the chain rule gives $\nabla F(Y) = 2\nabla f(YY^*)Y \in \mathbb{C}^{n\times p}$. Thus the gradient descent method simply takes the form of

$$Y_{n+1} = Y_n - \tau\nabla F(Y_n) = Y_n - \tau 2\nabla f(Y_nY_n^*)Y_n,$$

which is one of the simplest low-rank algorithms. The nonlinear conjugate gradient and quasi-Newton type methods, like L-BFGS [7], can also be easily used for (5).

The second approach is to consider a quotient manifold. Notice that $F(Y) = F(YO)$ for any unitary matrix $O \in \mathcal{O}_p = \{O \in \mathbb{C}^{p\times p} : O^*O = OO^* = I\}$. To remove the ambiguity from $\mathcal{O}_p$, it is natural to consider the quotient manifold $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$, see [1, 12–15], where $\mathbb{C}_*^{n\times p} = \{X \in \mathbb{C}^{n\times p} : \mathrm{rank}(X) = p\}$ denotes the noncompact Stiefel manifold.

Another natural approach is to consider Riemannian optimization algorithms on $\mathcal{H}_+^{n,p}$ as an embedded manifold in the Euclidean space $\mathbb{C}^{n\times n}$ [16–18]. We shall regard $\mathcal{H}_+^{n,p} \subset \mathbb{C}^{n\times n}$ as a manifold over $\mathbb{R}$ since $f(X)$ is real-valued.

1.4 Main results: a unified representation and analysis of three methods using quotient geometry

Even though the unconstrained Burer–Monteiro method is quite straightforward to use, its performance is sometimes observed to be inferior to Riemannian optimization on embedded and quotient geometries. To compare these three methods, we will first show that it is possible to equivalently rewrite both the Burer–Monteiro approach and embedded manifold approach as Riemannian optimization over the quotient manifold $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ with suitable metrics, retractions and vector transports.

It is common to explore different metrics in Riemannian optimization [2, 19, 20]. For any $Y \in \mathbb{C}_*^{n\times p}$, $A, B \in \mathbb{C}^{n\times p}$, we consider metrics $g_Y^i(\cdot,\cdot)$ for the total space $\mathbb{C}_*^{n\times p}$:

$$g_Y^1(A, B) = \langle A, B\rangle_{\mathbb{C}^{n\times p}} = \Re(\mathrm{tr}(A^*B))$$

$$g_Y^2(A,B) = \langle AY^*, BY^* \rangle_{\mathbb{C}^{n\times n}} = \Re(\mathrm{tr}((Y^*Y)A^*B))$$
$$g_Y^3(A,B) = \langle YA^* + AY^*, YB^* + BY^* \rangle_{\mathbb{C}^{n\times n}} + \left\langle Y\,\mathrm{Skew}\left((Y^*Y)^{-1}Y^*A\right)Y^*, Y\,\mathrm{Skew}\left((Y^*Y)^{-1}Y^*B\right)Y^* \right\rangle_{\mathbb{C}^{n\times n}},$$

where $\mathrm{Skew}(X) = (X - X^*)/2$. Then the submersion $\mathbb{C}_*^{n\times p} \longrightarrow \mathbb{C}_*^{n\times p}/\mathcal{O}_p$ induces three metrics g^i for the quotient manifold.

The first metric g^1 is also called the Bures-Wasserstein metric [1, 21]. Even though the simple Burer–Monteiro approach does not involve any manifold explicitly, we will prove that the gradient descent and nonlinear conjugate gradient methods for solving the Burer–Monteiro formulation (5) are exactly equivalent to the Riemannian gradient descent and Riemannian conjugate gradient methods on the quotient manifold $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$, with the Bures-Wasserstein metric and a particular retraction and vector transport.

The second metric g^2 is a popular metric for the quotient manifold, see [15].

For the third metric, we will prove that the Riemannian gradient descent and the Riemannian conjugate gradient methods using the embedded geometry of $\mathcal{H}_+^{n,p}$ are equivalent to a Riemannian gradient descent and a Riemannian conjugate gradient algorithms on the quotient manifold $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ with the metric g^3 and a specific vector transport.

It is well known that the condition number of the Hessian of the cost function is closely related to the asymptotic performance of optimization methods, see e.g., [22]. We will analyze and compare the condition numbers of the Riemannian Hessian using these three different metrics by estimating their Rayleigh quotient.

1.5 Related work

The Burer–Monteiro approach for the PSD constraint has been popular in applications due to its simplicity. For instance, an L-BFGS method for (5) was used for solving convex recovery from interferometric measurements in [8]. It is straightforward to verify that (1.3) with $p = 1$ and a suitable step size τ for the PhaseLift problem [5] is precisely the Wirtinger flow algorithm [6]. In [11], it was shown that first-order and second-order optimality conditions of the nonconvex Burer–Monteiro approach are sufficient to find the global minimizer of the convex semidefinite program under certain assumptions.

The quotient geometry of Hermitian PSD matrices of fixed rank for the metric g_Y^2 has been studied in [14, 15]. The quotient geometry with metric g_Y^2 in this paper is exactly the same one as the one in [14, 15]. As we will show in Section 2.3.2, the Bures-Wasserstein metric g^1 for low-rank PSD matrices is consistent with the Bures-Wasserstein metric for Hermitian positive-definite matrices [23–25].

The geometry of real symmetric PSD matrices of fixed rank $\mathcal{S}_+^{n,p}$ has also been studied intensively in the literature. Its embedded geometry was studied in [16] and its quotient geometry was studied in [1, 12, 13]. Riemannian optimization based on the embedded geometry has been well studied in [17] for real matrices of fixed rank, which can be easily extended to real symmetric PSD matrices of fixed rank [16]. As expected, Section 2.2 is its natural extensions to Hermitian PSD matrices of fixed rank. This is not surprising, but it is not a straightforward result either, because such a natural extension holds only when using the real inner product (3) and its associated derivatives.

It is not uncommon to explore different metrics of a manifold for Riemannian optimization [19, 20]. Comparison between embedded geometry and quotient geometry for low-rank matrices was considered in [26]. In [2], a new embedded geometry and complete geodesics for real PSD fixed-rank matrices were, for example, obtained from a special quotient metric.

1.6 Contributions

In this paper, for simplicity, we only focus on the nonlinear conjugate gradient method.

The first major contribution is the equivalence between the CG method for the unconstrained Burer–Monteiro formulation (5) and the CG method on $(\mathbb{C}_*^{n\times p}/\mathcal{O}_p, g^1)$ for solving (1). Thus, the convergence of the simple Burer–Monteiro optimization algorithms can be understood in the context of Riemannian optimization on the quotient manifold with the Bures-Wasserstein metric.

Second, we will show that a Riemannian conjugate gradient method on the embedded manifold $\mathcal{H}_+^{n,p}$ for solving (1) is equivalent to a Riemannian conjugate gradient method on the quotient manifold $(\mathbb{C}_*^{n\times p}/\mathcal{O}_p, g^3)$. This is unnecessary for implementation, but it allows a comparison of metrics for studying the comparison of algorithms using the embedded geometry and algorithms using the quotient geometry.

Finally, for the sake of understanding the differences among the three methodologies, we will analyze the condition number of the Riemannian Hessian on the quotient manifold $(\mathbb{C}_*^{n\times p}/\mathcal{O}_p, g^i)$ near the minimizer, which is another contribution. Our analysis is also consistent with empirical observation of the performance of different methods in numerical tests.

1.7 Organization of the paper

The rest of the paper is organized as follows. In Section 2, we review some known results for embedded and quotient geometries of $\mathcal{H}_+^{n,p}$. In Section 3, we outline the Riemannian Conjugate Gradient (RCG) methods on different geometries and discuss equivalences among them, with implementation details given in Section 3.3. In Section 4, we analyze and compare the Rayleigh quotient bounds of the Riemannian Hessian on $(\mathbb{C}_*^{n\times p}/\mathcal{O}_p, g^i)$ for the three metrics. Numerical tests are given in Section 5. Concluding remarks are given in Section 6.

2 The embedded and quotient geometries of $\mathcal{H}_+^{n,p}$

In this section, we review the embedded and quotient geometries of $\mathcal{H}_+^{n,p}$. All results in this section are natural extensions of well known results for the embedded and quotient geometries of $\mathbb{R}_+^{n,p}$, the manifold of real PSD matrices of fixed rank p. Some of these extensions are not entirely obvious, thus we outline the results in this paper, while all detailed proof can be found in [9].

2.1 Notation

Let $\mathbb{C}^{m\times n}$ denote all complex matrices of size $m \times n$. For a matrix $X \in \mathbb{C}^{m\times n}$, X^* denotes its conjugate transpose and $\overline{X}$ denotes its complex conjugate. If X is real, X^* becomes the matrix transpose and is denoted by X^T. We define

$$\mathrm{Herm}(X) := \frac{X + X^*}{2}, \quad \mathrm{Skew}(X) := \frac{X - X^*}{2}.$$

Let $p \le n$ and define

$$\begin{aligned} \mathbb{C}_*^{n\times p} &= \{X \in \mathbb{C}^{n\times p} : \mathrm{rank}(X) = p\}, \\ \mathcal{H}_+^{n,p} &= \{X \in \mathbb{C}^{n\times n} : X^* = X, X \succcurlyeq 0, \mathrm{rank}(X) = p\}, \\ \mathcal{S}_+^{n,p} &= \{X \in \mathbb{R}^{n\times n} : X^T = X, X \succcurlyeq 0, \mathrm{rank}(X) = p\}, \\ \mathcal{O}_p &= \{O \in \mathbb{C}^{p\times p} : O^*O = OO^* = I\}. \end{aligned}$$

Let $\Re(X)$ and $\Im(X)$ denote the real part and imaginary part of X respectively so that $X = \Re(X) + \mathrm{i}\Im(X)$. Let I_p be the identity matrix of size p-by-p. For any n-by-p matrix Z, $Z_\perp$ denotes the n-by-$(n-p)$ matrix such that $Z_\perp^* Z_\perp = I_{n-p}$ and $Z_\perp^* Z = \mathbf{0}$.

Let $\mathrm{Diag}(m, n)$ be the set of all m-by-n diagonal matrices. Let $\mathrm{diag}(M)$ be the n-by-1 vector that is the diagonal of the n-by-n matrix M. Given a vector v, $\mathrm{Diag}(v)$ is a square matrix with its i-th diagonal entry equal to v_i. Given a matrix A, $\mathrm{tr}(A)$ denotes the trace of A and A_{ij} denotes the (i, j)-th entry of A.

For any $X \in \mathcal{H}_+^{n,p}$, its eigenvalues coincide with its singular values. The compact singular value decomposition (SVD) of X is denoted by $X = U\Sigma U^*$, where $U \in \mathbb{C}^{n\times p}$ satisfies $U^*U = I$ and $\Sigma = \mathrm{Diag}(\sigma)$ with $\sigma = (\sigma_1, \cdots, \sigma_p)^T$ and $\sigma_1 \ge \cdots \ge \sigma_p > 0$. In the rest of the paper, U and Σ are reserved for denoting the compact SVD of $X \in \mathcal{H}_+^{n,p}$.

In this paper, all manifolds of complex matrices are viewed as manifolds over $\mathbb{R}$. Given a Euclidean space $\mathcal{E}$, the inner product on $\mathcal{E}$ is denoted by $\langle ., . \rangle_{\mathcal{E}}$. Specifically, $\langle A, B\rangle_{\mathbb{R}^{m\times n}} = \mathrm{tr}(A^T B)$ for $A, B \in \mathbb{R}^{m\times n}$ and $\langle A, B\rangle_{\mathbb{C}^{m\times n}} = \Re(\mathrm{tr}(A^* B))$ for $A, B \in \mathbb{C}^{m\times n}$ denotes the canonical inner product on $\mathbb{R}^{m\times n}$ and $\mathbb{C}^{m\times n}$, respectively.

2.2 Embedded geometry of $\mathcal{H}_+^{n,p}$

The results in this subsection are natural extensions of results for $\mathcal{S}_+^{n,p}$ in [16]. Such an extension is not entirely obvious since $\mathcal{H}_+^{n,p}$ is treated as a real manifold and the real inner product (3) is not the complex Hilbert–Schmidt inner product. Nonetheless, all proofs can be done following [16]. Useful formulae in this subsection are summarized in Table 1.

2.2.1 Tangent space

We first point out that $\mathcal{H}_+^{n,p}$ is a smooth embedded submanifold of $\mathbb{C}^{n\times n}$.

Theorem 2.1. *Regard $\mathbb{C}^{n\times n}$ as a real vector space over $\mathbb{R}$ of dimension $2n^2$. Then $\mathcal{H}_+^{n,p}$ is a smooth embedded submanifold of $\mathbb{C}^{n\times n}$ of dimension $2np - p^2$.*

Embedded Manifold	$\mathcal{H}_+^{n,p}$
Riemannian metric	$g_X^E(\xi_X,\eta_X)=\Re(\mathrm{tr}(\xi_X^*\eta_X))$
Riemannian gradient	$\mathrm{grad}\, f(X)=P_X^t(\nabla f(X))$
Projection to tangent space	$P_X^t(Z)=[U\ U_\perp]\begin{bmatrix} U^*\frac{Z+Z^*}{2}U & U^*\frac{Z+Z^*}{2}U_\perp \\ U_\perp^*\frac{Z+Z^*}{2}U & 0\end{bmatrix}\begin{bmatrix}U^*\\ U_\perp^*\end{bmatrix}$
Retraction	$R_X(\eta_X)=P_{\mathcal{H}_+^{n,p}}(X+\eta_X)$
Vector transport	$\mathcal{T}_{\eta_X}\xi_X=P^t_{R_X(\eta_X)}\xi_X$
Riemannian Hessian	$\mathrm{Hess}\, f(X)[\xi_X]=P_X^t(\nabla^2 f(X)[\xi_X])$ $+P_X^p\left(\nabla f(X)(X^\dagger\xi_X^p)^*+(\xi_X^pX^\dagger)^*\nabla f(X)\right)$

Table 1 Useful formulae for the embedded manifold $\mathcal{H}_+^{n,p}\subset\mathbb{C}^{n\times n}$.

Proof. The proof can be found in [9, Theorem 3.1]. Similar results for the case of $\mathcal{S}_+^{n,p}$ can be found in See [27, Prop. 2.1] and [28, Chap. 5]. □

The next result characterizes the tangent space.

Theorem 2.2. *Let $X=U\Sigma U^*\in\mathcal{H}_+^{n,p}$. Then the tangent space of $\mathcal{H}_+^{n,p}$ at X is*

$$T_X\mathcal{H}_+^{n,p}=\left\{[U\ U_\perp]\begin{bmatrix}H & K^*\\ K & 0\end{bmatrix}\begin{bmatrix}U^*\\ U_\perp^*\end{bmatrix}\right\},\quad H=H^*\in\mathbb{C}^{p\times p}, K\in\mathbb{C}^{(n-p)\times p}.$$

Proof. The proof follows from the differentiation of a curve in $\mathcal{H}_+^{n,p}$ and a counting on dimensionality, which can be found in [9, Theorem 3.2]. Similar result for the case of fix-rank real matrices can be found in [17, Prop. 2.1]. □

2.2.2 Riemannian gradient

The *Riemannian metric* of the embedded manifold at $X\in\mathcal{H}_+^{n,p}$ is induced from the Euclidean inner product on $\mathbb{C}^{n\times n}$,

$$g_X(\zeta_1,\zeta_2)=\langle\zeta_1,\zeta_2\rangle_{\mathbb{C}^{n\times n}}=\Re(\mathrm{tr}(\zeta_1^*\zeta_2)),\quad \zeta_1,\zeta_2\in T_X\mathcal{H}_+^{n,p}. \tag{6}$$

Let $f(X)$ be a smooth real-valued function for $X\in\mathbb{C}^{n\times n}$ with its gradient $\nabla f(X)$ given in (4). The *Riemannian gradient* of f at $X\in\mathcal{H}_+^{n,p}$, denoted by $\mathrm{grad}\, f(X)$, is the projection of $\nabla f(X)$ onto $T_X\mathcal{H}_+^{n,p}$; see [29, Sect. 3.6.1],

$$\mathrm{grad}\, f(X)=P_X^t(\nabla f(X)),$$

where P_X^t denotes the orthogonal projection onto $T_X\mathcal{H}_+^{n,p}$. In order to get a closed-form expression of P_X^t, we should characterize the *normal space* to $\mathcal{H}_+^{n,p}$ at X, denoted by $(T_X\mathcal{H}_+^{n,p})^\perp$ or $N_X\mathcal{H}_+^{n,p}$, which is the orthogonal complement of $T_X\mathcal{H}_+^{n,p}$ in $\mathbb{C}^{n\times n}$,

$$N_X\mathcal{H}_+^{n,p}:=\{\xi_X\in T_X\mathbb{C}^{n\times n}:\langle\xi_X,\eta_X\rangle_{\mathbb{C}^{n\times n}}=0 \text{ for all } \eta_X\in T_X\mathcal{H}_+^{n,p}\}.$$

Lemma 2.3. *The normal space $N_X\mathcal{H}_+^{n,p}$ at $X = U\Sigma U^* \in \mathcal{H}_+^{n,p}$ is given by*

$$N_X\mathcal{H}_+^{n,p} = \left\{ \begin{bmatrix} U & U_\perp \end{bmatrix} \begin{bmatrix} \Omega & -L^* \\ L & M \end{bmatrix} \begin{bmatrix} U^* \\ U_\perp^* \end{bmatrix} \right\}, \tag{7}$$

where $\Omega = -\Omega^* \in \mathbb{C}^{p\times p}$, $M \in \mathbb{C}^{(n-p)\times(n-p)}$, and $L \in \mathbb{C}^{(n-p)\times p}$.

Proof. It suffices to check that $N_X\mathcal{H}_+^{n,p}$ is indeed perpendicular to $T_X\mathcal{H}_+^{n,p}$ and a counting on dimensionality. The complete proof can be found in [9, Lemma 3.4]. □

The orthogonal projection from $\mathbb{C}^{n\times n}$ onto $T_X\mathcal{H}_+^{n,p}$ is given as follows:

Proposition 2.4. *Let $X = YY^* = U\Sigma U^*$ be the compact SVD for $X \in \mathcal{H}_+^{n,p}$ with $Y \in \mathbb{C}_*^{n\times p}$. Let $Z \in \mathbb{C}^{n\times n}$. Then the operator P_X^t defined below is the orthogonal projection onto $T_X\mathcal{H}_+^{n,p}$:*

$$\begin{aligned} P_X^t(Z) &= \frac{1}{2}\left(P_Y(Z+Z^*)P_Y + P_Y^\perp(Z+Z^*)P_Y + P_Y(Z+Z^*)P_Y^\perp\right) \\ &= \frac{1}{2}\left(P_U(Z+Z^*)P_U + P_U^\perp(Z+Z^*)P_U + P_U(Z+Z^*)P_U^\perp\right) \\ &= \begin{bmatrix} U & U_\perp \end{bmatrix} \begin{bmatrix} U^*\frac{(Z+Z^*)}{2}U & U^*\frac{(Z+Z^*)}{2}U_\perp \\ U_\perp^*\frac{(Z+Z^*)}{2}U & 0 \end{bmatrix} \begin{bmatrix} U^* \\ U_\perp^* \end{bmatrix}, \end{aligned} \tag{8}$$

where $P_Y = Y(Y^*Y)^{-1}Y^*$, $P_Y^\perp = I - P_Y = P_{Y_\perp}$, $P_U = UU^*$ and $P_U^\perp = I - P_U = P_{U_\perp}$.

Proof. It suffices to check that $P_X^t(Z)$ is indeed a tangent vector and $Z - P_X^t(Z)$ is a normal vector. The complete proof can be found in [9, Theorem 3.5]. Similar result for the case of fix-rank real matrices can be found in [17, Eq. 2.5]. □

Remark 2.5. *To facilitate later reference in notation, we write $P_X^t = P_X^s + P_X^p$ as the sum of two operators:*

$$P_X^s : Z \mapsto P_U\frac{Z+Z^*}{2}P_U, \tag{9a}$$

$$P_X^p : Z \mapsto P_{U_\perp}\frac{Z+Z^*}{2}P_U + P_U\frac{Z+Z^*}{2}P_{U_\perp}. \tag{9b}$$

2.2.3 A retraction by projection to the embedded manifold

A retraction is essentially a first-order approximation to the exponential map; see [29, Def. 4.1.1]. By [30, Prop. 3.2 and 3.3], the truncated SVD $R_X(Z) := P_{\mathcal{H}_+^{n,p}}(X+Z) = \sum_{i=1}^p \sigma_i(X+Z)v_iv_i^*$ is a retraction on $\mathcal{H}_+^{n,p}$, where v_i is the singular vector of $X+Z$ corresponding to the i-th largest singular value $\sigma_i(X+Z)$. We remark that such a retraction can be compactly implemented; see Section 3.3 and [9] for implementation details.

2.2.4 Vector transport

The vector transport is a mapping that transports a tangent vector from one tangent space to another tangent space; see [29, Def. 8.1.1]. Let $\xi_X, \eta_X \in T_X\mathcal{H}_+^{n,p}$ and let R be a retraction on $\mathcal{H}_+^{n,p}$. By [29, Sect. 8.1.3], the projection of one tangent vector onto another tangent space is a vector transport,

$$\mathcal{T}_{\eta_X}\xi_X := P^t_{R_X(\eta_X)}\xi_X, \tag{10}$$

where P^t_Z is the projection operator onto $T_Z\mathcal{H}_+^{n,p}$. Namely, we first apply retraction to $X + \eta_X$ to arrive at a new point on the manifold, then we project the old tangent vector ξ_X onto the tangent space at that new point.

2.2.5 Riemannian Hessian operator

For a real-valued function $f(X)$ defined on the Euclidean space $\mathbb{C}^{n\times n}$, the Hessian $\nabla^2 f(X)$ is defined in the sense of the Fréchet derivative; see [9, Appendix A]. The *Riemannian Hessian* $\operatorname{Hess} f(X)$ (see [29, Def. 5.5.1]) is a linear mapping of $T_x\mathcal{M}$ to $T_x\mathcal{M}$ satisfying $\operatorname{Hess} f(x)[\xi_x] = \nabla_{\xi_x}\operatorname{grad} f$ for all ξ_x in $T_x\mathcal{M}$, where ∇ is the Riemannian connection on $\mathcal{M}$. The following proposition shows the connection between Riemannian Hessian and $\nabla^2 f(X)$. The proof follows similar ideas as in [4, Prop. 5.10] and [31, Prop. 2.3] where a second-order retraction based on a simple power expansion is constructed. We will leave the outline of the proof in Appendix A.

Proposition 2.6. *Let $f(X)$ be a real-valued function defined on $\mathcal{H}_+^{n,p}$. Let $X \in \mathcal{H}_+^{n,p}$ and $\xi_X \in T_X\mathcal{H}_+^{n,p}$. Then the Riemannian Hessian operator of f at X is given by*

$$\mathit{Hess}\, f(X)[\xi_X] = P^t_X(\nabla^2 f(X)[\xi_X]) + P^p_X\left(\nabla f(X)(X^\dagger \xi^p_X)^* + (\xi^p_X X^\dagger)^*\nabla f(X)\right)$$

where $\xi^s_X = P^s_X(\xi_X)$ and $\xi^p_X = P^p_X(\xi_X)$ and P^t_X and P^p_X are defined in (9).

2.3 The quotient geometry of $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ using three Riemannian metrics

The manifold $\mathcal{H}_+^{n,p}$ can also be viewed as a quotient set $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ since any $X \in \mathcal{H}_+^{n,p}$ can be written as $X = YY^*$ with $Y \in \mathbb{C}_*^{n\times p}$. We define an equivalence relation on $\mathbb{C}_*^{n\times p}$ through the smooth Lie group action of $\mathcal{O}_p$ on the manifold $\mathbb{C}_*^{n\times p}$:

$$\begin{aligned} \mathbb{C}_*^{n\times p} \times \mathcal{O}_p &\to \quad \mathbb{C}_*^{n\times p} \\ (Y, O) &\mapsto \quad YO. \end{aligned}$$

This action defines an equivalence relation on $\mathbb{C}_*^{n\times p}$ by setting $Y_1 \sim Y_2$ if there exists an $O \in \mathcal{O}_p$ such that $Y_1 = Y_2 O$. Hence we have constructed a quotient space $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ that removes this ambiguity. The set $\mathbb{C}_*^{n\times p}$ is called the *total space* of $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$.

Denote the natural projection as

$$\pi : \mathbb{C}_*^{n\times p} \to \mathbb{C}_*^{n\times p}/\mathcal{O}_p.$$

For any $Y \in \mathbb{C}_*^{n\times p}$, $\pi(Y)$ is an element in $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$. We denote the equivalence class containing Y as

$$[Y] = \pi^{-1}(\pi(Y)) = \{YO | O \in \mathcal{O}_p\}\,.$$

With the one-to-one correspondence between $X = YY^* \in \mathcal{H}_+^{n,p}$ and $\pi(Y) \in \mathbb{C}_*^{n\times p}/\mathcal{O}_p$, define $h(\pi(Y)) = f(YY^*)$, then (1) is equivalent to

$$\begin{array}{ll} \underset{\pi(Y)}{\text{minimize}} & h(\pi(Y)) \\ \text{subject to } \pi(Y) \in \mathbb{C}_*^{n\times p}/\mathcal{O}_p \end{array}. \tag{11}$$

Define

$$\begin{aligned} \beta : \mathbb{C}_*^{n\times p} &\to \mathcal{H}_+^{n,p} \\ Y &\mapsto YY^*. \end{aligned}$$

Then β is invariant under the equivalence relation $\sim$ and induces a unique function $\tilde{\beta}$ on $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$, called the projection of β, such that $\beta = \tilde{\beta} \circ \pi$; see [29, Sect. 3.4.2]. One can easily check that $\tilde{\beta}$ is a bijection. For any real-valued function f defined on $\mathcal{H}_+^{n,p}$, there is a real-valued function F defined on $\mathbb{C}_*^{n\times p}$ that induces f: for any $X = YY^* \in \mathcal{H}_+^{n,p}$, $F(Y) := f \circ \beta(Y) = f(YY^*)$. This is summarized in the diagram below:

$$\begin{array}{ccccc} \mathbb{C}_*^{n\times p} & & & & \\ \downarrow \pi & \overset{\beta:=\tilde{\beta}\circ\pi}{\searrow} & & & \\ \mathbb{C}_*^{n\times p}/\mathcal{O}_p & \overset{\tilde{\beta}}{\longleftrightarrow} & \mathcal{H}_+^{n,p} & \overset{f}{\longrightarrow} & \mathbb{R} \end{array}$$

The next theorem shows that $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ is a smooth manifold, and the proof follows from general results of smooth manifolds; see [32, Corollary 21.6; Theorem 21.10].

Theorem 2.7. *The quotient space $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ is a quotient manifold over $\mathbb{R}$ of dimension $2np - p^2$ and has a unique smooth structure such that the natural projection π is a smooth submersion.*

The next theorem shows that $\mathcal{H}_+^{n,p}$ and $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ are essentially the same in the sense that there is a diffeomorphism between them.

Theorem 2.8. *The quotient manifold $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ is diffeomorphic to $\mathcal{H}_+^{n,p}$ under $\tilde{\beta}$.*

Proof. Similar result of the real case has been shown in [1, Prop. A.7]; and the proof of this theorem follows the same technique therein. The complete proof can be found in [9, Theorem 4.2]. □

We list some useful formulae of quotient manifold in Table 2.

2.3.1 Vertical space, three Riemannian metrics and horizontal space

The equivalence class $[Y]$ is an embedded submanifold of $\mathbb{C}_*^{n\times p}$([29, Prop. 3.4.4]). The tangent space of $[Y]$ at Y is therefore a subspace of $T_Y\mathbb{C}_*^{n\times p}$ called the *vertical space* at Y and is denoted by $\mathcal{V}_Y$. The following proposition characterizes $\mathcal{V}_Y$.

Proposition 2.9. *The vertical space at $Y \in [Y] = \{YO | O \in \mathcal{O}_p\}$, which is the tangent space of $[Y]$ at Y,*

$$\mathcal{V}_Y = \left\{ Y\Omega | \Omega^* = -\Omega, \Omega \in \mathbb{C}^{p\times p} \right\}.$$

Quotient manifold	$\mathbb{C}_*^{n\times p}/\mathcal{O}_p$		
Riemannian Metric $g^i_{\pi(Y)}(\xi_{\pi(Y)}, \eta_{\pi(Y)})$	$g^1 = \Re(\mathrm{tr}(\overline{\xi}_Y^* \overline{\eta}_Y))$ is the Bures-Wasserstein metric	$g^2 = \Re(\mathrm{tr}((Y^*Y)\overline{\xi}_Y^* \overline{\eta}_Y))$	$g^3 = g^E_{YY^*}(Y\overline{\xi}_Y^* + \overline{\xi}_Y Y^*, Y\overline{\eta}_Y^* + \overline{\eta}_Y Y^*)$ corresponds to Embedded Geometry
Horizontal lift of Riemannian gradient $\overline{\mathrm{grad}\, h(\pi(Y))}_Y$	$2\nabla f(YY^*)Y$	$2\nabla f(YY^*)Y(Y^*Y)^{-1}$	$\left(I - \frac{1}{2}Y(Y^*Y)^{-1}Y^*\right) \nabla f(YY^*)Y(Y^*Y)^{-1}$
Projection to horizontal space	$P_Y^{\mathcal{H}^1}(A) = A - Y\Omega,$ where Ω solves $\Omega Y^*Y + Y^*Y\Omega = Y^*A - A^*Y$	$P_Y^{\mathcal{H}^i}(A) = Y\,\mathrm{Herm}\left((Y^*Y)^{-1}Y^*A\right) + Y_\perp Y_\perp^* A$	
Retraction	$R_{\pi(Y)}(\tau\eta_{\pi(Y)}) = \pi(Y + \tau\overline{\eta}_Y)$		
Vector Transport	$\overline{\left(\mathcal{T}_{\eta_{\pi(Y)}}\xi_{\pi(Y)}\right)}_{Y+\overline{\eta}_Y} = P^{\mathcal{H}^i}_{Y+\overline{\eta}_Y}(\overline{\xi}_Y)$		
Riemannian Hessian	See (22)	See (23)	See (24)

Table 2 Some useful formulae for $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$.

Proof. The proof is given in [9, Prop. 4.3]. Similar result for the real case can be found in [21]. □

A *Riemannian metric* g is a smoothly varying inner product defined on the tangent space. That is, $g_Y(\cdot,\cdot)$ is an inner product on $T_Y\mathbb{C}_*^{n\times p}$. Once we choose a Riemannian metric g for $\mathbb{C}_*^{n\times p}$, we can obtain the orthogonal complement in $T_Y\mathbb{C}_*^{n\times p}$ of $\mathcal{V}_Y$ with respect to the metric. In other words, we choose the *horizontal distribution* as orthogonal complement w.r.t. Riemannian metric, see [29, Sect. 3.5.8]. This orthogonal complement to $\mathcal{V}_Y$ is called *horizontal space* at Y and is denoted by $\mathcal{H}_Y$. We thus have

$$T_Y\mathbb{C}_*^{n\times p} = \mathcal{H}_Y \oplus \mathcal{V}_Y. \tag{12}$$

Once we have the horizontal space, there exists a unique vector $\overline{\xi}_Y \in \mathcal{H}_Y$ that satisfies $\mathrm{D}\,\pi(Y)[\overline{\xi}_Y] = \xi_{\pi(Y)}$ for each $\xi_{\pi(Y)} \in T_{\pi(Y)}\mathbb{C}_*^{n\times p}/\mathcal{O}_p$. This $\overline{\xi}_Y$ is called the *horizontal lift* of $\xi_{\pi(Y)}$ at Y. In the rest of the paper, we use bar notation above any tangent bundle ξ on quotient manifold to denote that $\overline{\xi}$ is a horizontal distribution.

There exist more than one choice of Riemannian metric on $\mathbb{C}_*^{n\times p}$. Different Riemannian metrics do not affect the vertical space, but generally result in different horizontal spaces. One of the main focuses of this paper is to examine how three different Riemannian metrics affect the convergence behavior of Riemannian optimization algorithms.

2.3.2 The Bures-Wasserstein metric

The most straightforward choice of a Riemannian metric on $\mathbb{C}_*^{n\times p}$ is the canonical Euclidean inner product on $\mathbb{C}^{n\times p}$ defined by

$$g^1_Y(A,B) := \langle A,B\rangle_{\mathbb{C}^{n\times p}} = \Re(\mathrm{tr}(A^*B)), \quad \forall A,B \in T_Y\mathbb{C}_*^{n\times p} = \mathbb{C}^{n\times p}.$$

The metric g^1 is also called the Bures-Wasserstein metric [21, Sect. 2] for the quotient manifold $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$. On the other hand, the following metric in Definition 2.1 for Hermitian positive-definite matrices $\mathcal{H}_+^{n,n}$ [23–25] is also called the Bures-Wasserstein metric.

Notice that it is not clear whether Definition 2.1 can also apply to a low-rank matrix $X \in \mathcal{H}_+^{n,p}$. In this subsection, we show how the metric g^1 can be used to generalize Definition 2.1 to Definition 2.2, which defines the Bures-Wasserstein metric in the low-rank case $\mathcal{H}_+^{n,p}$. This non-trivial generalization is presented as Theorem 2.10. Although the theorem is not the primary focus of this paper, it is of interest to see how g^1 connects the Bures-Wasserstein metric on the quotient manifold to its counterpart on the embedded manifold.

Definition 2.1 (The Bures-Wasserstein metric for $\mathcal{H}_+^{n,n}$)**.** *Let $X \in \mathcal{H}_+^{n,n}$ and $A, B \in T_X\mathcal{H}_+^{n,n}$. Then*

$$g_X^{BW}(A,B) := \frac{1}{2}\langle \mathcal{L}_X(A), B\rangle,$$

where $\mathcal{L}_X(A) = M$ solves the following Lyapunov equation

$$XM + MX = A \tag{13}$$

which has a unique solution provided X is Hermitian positive-definite.

Definition 2.2 (The Bures-Wasserstein metric on $\mathcal{H}_+^{n,p}$)**.** *Let $A, B \in T_{YY^*}\mathcal{H}_+^{n,p}$, then by the 1-to-1 correspondence between $T_{YY^*}\mathcal{H}_+^{n,p}$ and the horizontal space $\mathcal{H}_Y^1$, there exist unique $\xi_Y, \eta_Y \in \mathcal{H}_Y^1$ such that $A = Y\xi_Y^* + \xi_Y Y^*$ and $B = Y\eta_Y^* + \eta_Y Y^*$. We define the Bures-Wasserstein metric at the low-rank $X = YY^*$ as*

$$g_{YY^*}^{BW}(A,B) := g_Y^1(\xi_Y, \eta_Y).$$

Theorem 2.10 (Equivalence of the two Bures-Wasserstein metrics)**.** *If $p = n$, then the Definition 2.2 reduces to the Definition 2.1.*

Proof. We first claim that for any $A, B \in T_X\mathcal{H}_+^{n,p}$ with $X = YY^*$, there is a unique solution $M \in T_X\mathcal{H}_+^{n,p}$ satisfying both

$$Y^*XMY + Y^*MXY = Y^*AY \tag{14}$$

and

$$g_{YY^*}^{\mathrm{BW}}(A,B) = \frac{1}{2}\langle M, B\rangle_{\mathbb{C}^{n\times n}}. \tag{15}$$

Then for the case $p = n$, Y is invertible, thus (14) is equivalent to the Lyapunov equation (13). Therefore, the Definition 2.2 indeed reduces to the Definition 2.1 when $p = n$.

Now we prove the claim above. Let $\xi_Y = Y(Y^*Y)^{-1}S + Y_\perp K \in \mathcal{H}_Y^1$ with $S^* = S$ be the unique horizontal vector such that $A = Y\xi_Y^* + \xi_Y Y^*$. Let $Y = UR$ where U has size n-by-p with orthonormal columns and R is an p-by-p invertible matrix. Thus (14) is equivalent to

$$RR^*(U^*MU) + (U^*MU)RR^* = RSR^{-1} + (R^*)^{-1}SR^*. \tag{16}$$

Since RR^* is positive definite, (16) has a unique solution in U^*MU; see [1], which can be written explicitly:

$$U^*MU = (R^*)^{-1}SR^{-1}. \tag{17}$$

Thus $M = \begin{bmatrix} U & Y_\perp \end{bmatrix} \begin{bmatrix} (R^*)^{-1}SR^{-1} & K_M^* \\ K_M & 0 \end{bmatrix} \begin{bmatrix} U^* \\ Y_\perp^* \end{bmatrix}$, where K_M is to be determined by the additional equation (15). With $B = Y\eta_Y^* + \eta_Y Y^*$ we have,

$$\frac{1}{2}\langle M, B\rangle_{\mathbb{C}^{n\times n}} = \frac{1}{2}\langle M, Y\eta_Y^*\rangle_{\mathbb{C}^{n\times n}} + \frac{1}{2}\langle M, \eta_Y Y^*\rangle_{\mathbb{C}^{n\times n}} = \langle MY, \eta_Y\rangle_{\mathbb{C}^{n\times p}}.$$

Thus in order for (15) to hold, M needs to satisfy $MY = \xi_Y$. Recall that $\xi_Y = Y(Y^*Y)^{-1}S + Y_\perp K = U(R^*)^{-1}S + Y_\perp K$. Thus K_M needs to satisfy $Y_\perp K_M R = Y_\perp K$, which gives the unique $K_M = KR^{-1}$. □

Proposition 2.11. *Under metric g^1, the horizontal space at Y satisfies*

$$\begin{aligned} \mathcal{H}_Y^1 &= \{Z \in \mathbb{C}^{n\times p} : Y^*Z = Z^*Y\} \\ &= \left\{Y(Y^*Y)^{-1}S + Y_\perp K | S^* = S, S \in \mathbb{C}^{p\times p}, K \in \mathbb{C}^{(n-p)\times p}\right\}, \end{aligned}$$

where $Y_\perp$ has orthonormal columns.

Proof. The result of real case can be found in [21] but the proof was omitted. For completeness, we outline the proof here. $Z \in \mathbb{C}^{n\times p}$ belongs to $\mathcal{H}_Y^1$ if and only if Z is orthogonal to $\mathcal{V}_Y$ under the metric g_Y^1, i.e., $g_Y^1(Z, Y\Omega) = \langle Z, Y\Omega\rangle_{\mathbb{C}^{n\times p}} = \langle Y^*Z, \Omega\rangle_{\mathbb{C}^{n\times p}} = 0, \forall \Omega = -\Omega^*$. This is equivalent to $Y^*Z = Z^*Y$. The second equality can be obtained by writing any $Z \in \mathcal{H}_Y^1$ as $Z = Y(Y^*Y)^{-1}S + Y_\perp K$ as $Y(Y^*Y)^{-1}$ and $Y_\perp$ forms a basis for the column space of $\mathbb{C}^{n\times p}$, and verify that $S = S^*$ □

2.3.3 The second quotient metric

Another Riemannian metric used in [14, 15] is defined by

$$g_Y^2(A, B) := \langle AY^*, BY^*\rangle_{\mathbb{C}^{n\times n}} = \Re(\mathrm{tr}((Y^*Y)A^*B)), \quad \forall A, B \in T_Y\mathbb{C}_*^{n\times p} = \mathbb{C}^{n\times p}.$$

Proposition 2.12. *Under metric g^2, the horizontal space at Y satisfies*

$$\begin{aligned} \mathcal{H}_Y^2 &= \{Z \in \mathbb{C}^{n\times p} : (Y^*Y)^{-1}Y^*Z = Z^*Y(Y^*Y)^{-1}\} \\ &= \left\{YS + Y_\perp K | S^* = S, S \in \mathbb{C}^{p\times p}, K \in \mathbb{C}^{(n-p)\times p}\right\}. \end{aligned}$$

Proof. The same result was given in [15] but the proof was omitted. The proof follows the same idea used in proving Proposition 2.11. □

2.3.4 The third quotient metric

The third Riemannian metric for $\mathbb{C}_*^{n\times p}$ is motivated by the Riemannian metric of $\mathcal{H}_+^{n,p}$ and the diffeomorphism between $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ and $\mathcal{H}_+^{n,p}$. We know that β is a submersion. Every tangent vector of $\mathcal{H}_+^{n,p}$ corresponds to a tangent vector of $\mathbb{C}_*^{n\times p}$. We can use the Riemannian metric of $\mathcal{H}_+^{n,p}$ and the correspondence of tangent vectors between $\mathcal{H}_+^{n,p}$

and $\mathbb{C}_*^{n\times p}$ to define a Riemannian metric for $\mathbb{C}_*^{n\times p}$. A natural first attempt would be to use

$$g_Y(A,B) := \langle \mathrm{D}\,\beta(Y)[A], \mathrm{D}\,\beta(Y)[B]\rangle_{\mathbb{C}^{n\times n}} = \langle YA^* + AY^*, YB^* + BY^*\rangle_{\mathbb{C}^{n\times n}}\,,$$

which is, however, not a Riemannian metric because it is not positive-definite. To see this, notice that $\ker(\mathrm{D}\,\beta(Y)[\cdot]) = \mathcal{V}_Y$. Consider $C \neq 0 \in \mathcal{V}_Y$, then $g_Y^3(C,C) = 0$. To modify this definition for g^3, we can use the Riemannian metric g^2 and the decomposition $T_Y\mathbb{C}_*^{n\times p} = \mathcal{H}_Y^2 \oplus \mathcal{V}_Y$, by which $A \in T_Y\mathbb{C}_*^{n\times p}$ can be uniquely decomposed as

$$A = A^{\mathcal{V}} + A^{\mathcal{H}^2},$$

where $A^{\mathcal{V}} \in \mathcal{V}_Y$ and $A^{\mathcal{H}^2} \in \mathcal{H}_Y^2$. Now define g^3 as

$$\begin{aligned} g_Y^3(A,B) &:= \left\langle \mathrm{D}\,\beta(Y)[A^{\mathcal{H}^2}], \mathrm{D}\,\beta(Y)[B^{\mathcal{H}^2}]\right\rangle_{\mathbb{C}^{n\times n}} + g_Y^2\left(A^{\mathcal{V}}, B^{\mathcal{V}}\right) \\ &= \langle \mathrm{D}\,\beta(Y)[A], \mathrm{D}\,\beta(Y)[B]\rangle_{\mathbb{C}^{n\times n}} + \left\langle P_Y^{\mathcal{V}}(A)Y^*, P_Y^{\mathcal{V}}(B)Y^*\right\rangle_{\mathbb{C}^{n\times n}}\,, \\ &= \langle YA^* + AY^*, YB^* + BY^*\rangle_{\mathbb{C}^{n\times n}} + \left\langle P_Y^{\mathcal{V}}(A)Y^*, P_Y^{\mathcal{V}}(B)Y^*\right\rangle_{\mathbb{C}^{n\times n}} \end{aligned}$$

where $P_Y^{\mathcal{V}}$ is the projection of any tangent vector of $\mathbb{C}_*^{n\times p}$ to the vertical space $\mathcal{V}_Y$. It is straightforward to verify that g^3 defined above is now a Riemannian metric. With the definition (3), the properties $\mathrm{tr}(UV) = tr(VU)$ for two matrices U, V and $\Re(\mathrm{tr}(C + C^*)) = 2\Re(\mathrm{tr}(C))$, we have

$$\forall A, B \in A^{\mathcal{H}^2}, \quad g_Y^3(A,B) = \langle YA^* + AY^*, YB^* + BY^*\rangle_{\mathbb{C}^{n\times n}} = 2\,\langle AY^*Y + YA^*Y, B\rangle_{\mathbb{C}^{n\times p}}\,. \tag{18}$$

Proposition 2.13. *Under metric g^3, the horizontal space at Y is the same set as $\mathcal{H}_Y^2$. That is,*

$$\begin{aligned} \mathcal{H}_Y^3 &= \left\{Z \in \mathbb{C}^{n\times p} : (Y^*Y)^{-1}Y^*Z = Z^*Y(Y^*Y)^{-1}\right\} \\ &= \left\{YS + Y_\perp K | S^* = S, S \in \mathbb{C}^{p\times p}, K \in \mathbb{C}^{(n-p)\times p}\right\}. \end{aligned}$$

Proof. The proof follows the same idea used in proving Proposition 2.11. □

2.3.5 Projections onto vertical space and horizontal space

Due to the direct sum property (12), for our choices of $\mathcal{H}_Y^i$, there exist projection operators for any $A \in T_Y\mathbb{C}_*^{n\times p}$ to $\mathcal{H}_Y^i$ as

$$A = P_Y^{\mathcal{V}}(A) + P_Y^{\mathcal{H}^i}(A).$$

It is straightforward to verify the following formulae for projection operators $P_Y^{\mathcal{V}}$ and $P_Y^{\mathcal{H}^i}$. Similar results can be found in [1, 15] with proof omitted. To verify these formulae, we can rewrite them as $P_Y^{\mathcal{V}}(A) = Y\Omega$ and $P_Y^{\mathcal{H}^i}(A) = A - Y\Omega$, and then solve for Ω by the definition of $\mathcal{H}_Y^i$.

Proposition 2.14. *If we use g^1 as our Riemannian metric on $\mathbb{C}_*^{n\times p}$, then the orthogonal projections of any $A \in \mathbb{C}^{n\times p}$ to $\mathcal{V}_Y$ and $\mathcal{H}_Y^1$ are*

$$P_Y^{\mathcal{V}}(A) = Y\Omega, \quad P_Y^{\mathcal{H}^1}(A) = A - Y\Omega,$$

where Ω is the skew-symmetric matrix that solves the Lyapunov equation

$$\Omega Y^*Y + Y^*Y\Omega = Y^*A - A^*Y.$$

Proposition 2.15. *If we use g^2 as our Riemannian metric on $\mathbb{C}_*^{n\times p}$, then the orthogonal projection of any $A \in \mathbb{C}^{n\times p}$ to vertical space $\mathcal{V}_Y$ satisfies*

$$P_Y^{\mathcal{V}}(A) = Y\left(\frac{(Y^*Y)^{-1}Y^*A - A^*Y(Y^*Y)^{-1}}{2}\right) = Y\,\mathrm{Skew}\left((Y^*Y)^{-1}Y^*A\right),$$

and the orthogonal projection of any $A \in \mathbb{C}^{n\times p}$ to the horizontal space $\mathcal{H}_Y^2$ is

$$\begin{aligned} P_Y^{\mathcal{H}^2}(A) &= A - P_Y^{\mathcal{V}}(A) \\ &= Y\left(\frac{(Y^*Y)^{-1}Y^*A + A^*Y(Y^*Y)^{-1}}{2}\right) + Y_\perp Y_\perp^* A \\ &= Y\,\mathrm{Herm}\left((Y^*Y)^{-1}Y^*A\right) + Y_\perp Y_\perp^* A. \end{aligned}$$

Proposition 2.16. *If we use g^3 as our Riemannian metric on $\mathbb{C}_*^{n\times p}$, then the orthogonal projection of any $A \in \mathbb{C}^{n\times p}$ to vertical space $\mathcal{V}_Y$ satifies*

$$P_Y^{\mathcal{V}}(A) = Y\left(\frac{(Y^*Y)^{-1}Y^*A - A^*Y(Y^*Y)^{-1}}{2}\right) = Y\,\mathrm{Skew}((Y^*Y)^{-1}Y^*A),$$

and the orthogonal projection of any $A \in \mathbb{C}^{n\times p}$ to the horizontal space $\mathcal{H}_Y^3$ is

$$\begin{aligned} P_Y^{\mathcal{H}^3}(A) &= A - P_Y^{\mathcal{V}}(A) \\ &= Y\left(\frac{(Y^*Y)^{-1}Y^*A + A^*Y(Y^*Y)^{-1}}{2}\right) + Y_\perp Y_\perp^* A \\ &= Y\,\mathrm{Herm}\left((Y^*Y)^{-1}Y^*A\right) + Y_\perp Y_\perp^* A. \end{aligned}$$

2.3.6 $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ as Riemannian quotient manifold

First we show in the following lemma the relationship between the horizontal lifts of the quotient tangent vector $\xi_{\pi(Y)}$ lifted at different representatives in $[Y]$.

Lemma 2.17. *Let η be a vector field on $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$, and let $\bar{\eta}$ be the horizontal lift of η. Then for each $Y \in \mathbb{C}_*^{n\times p}$, we have*

$$\bar{\eta}_{YO} = \bar{\eta}_Y O$$

for all $O \in \mathcal{O}_p$.

Proof. [1, Prop. A.8] gives a proof based on metric g^1 but it is for real case; and [15, Lemma 5.1] proves the result for metric g^2. The proof for complex case with all three metrics g^i can be found in [9, Lemma 4.13]. □

Recall from [29, Sect. 3.6.2] that if the expression $g_Y(\bar{\xi}_Y, \bar{\zeta}_Y)$ does not depend on the choice of $Y \in [Y]$ for every $\pi(Y) \in \mathbb{C}_*^{n\times p}/\mathcal{O}_p$ and every $\xi_{\pi(Y)}, \zeta_{\pi(Y)} \in T_{\pi(Y)}\mathbb{C}_*^{n\times p}/\mathcal{O}_p$, then

$$g_{\pi(Y)}(\xi_{\pi(Y)}, \zeta_{\pi(Y)}) := g_Y(\bar{\xi}_Y, \bar{\zeta}_Y) \tag{19}$$

defines a Riemannian metric on the quotient manifold $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$. By Lemma 2.17, it is straightforward to verify that each Riemannian metric g^i on $\mathbb{C}_*^{n\times p}$ induces a Riemannian metric on $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$. The quotient manifold $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ endowed with a Riemannian metric defined in (19) is called a *Riemannian quotient manifold*. By abuse of notation, we use g^i for denoting Riemannian metrics on both total space $\mathbb{C}_*^{n\times p}$ and quotient space $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$.

2.3.7 Riemannian gradient

Given a smooth real-valued function f on $\mathcal{H}_+^{n,p}$, recall that a corresponding cost function h is defined on $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ satisfying (11). The next theorem shows that the horizontal lift of $\operatorname{grad} h(\pi(Y))$ can be obtained from the Riemannian gradient of F. Its proof can be found in [29, Sect. 3.6.2].

Theorem 2.18. *The horizontal lift of the Riemannian gradient of h at $\pi(Y)$ is the Riemannian gradient of F at Y. That is,*

$$\overline{\operatorname{grad} h(\pi(Y))}_Y = \operatorname{grad} F(Y).$$

Therefore, $\operatorname{grad} F(Y)$ is always in $\mathcal{H}_Y$.

The next proposition summarizes the expression of $\operatorname{grad} F(Y)$ under different metrics. The proof is by simple calculation and definition of each metric, which can be found in [9].

Proposition 2.19. *Let f be a smooth real-valued function defined on $\mathcal{H}_+^{n,p}$ and let $F : \mathbb{C}_*^{n\times p} \to \mathbb{R} : Y \mapsto f(YY^*)$. Assume $YY^* = X$. Then*

$$\operatorname{grad} F(Y) = \begin{cases} 2\nabla f(YY^*)Y, & \text{if using metric } g^1 \\ 2\nabla f(YY^*)Y(Y^*Y)^{-1}, & \text{if using metric } g^2 \\ \left(I - \frac{1}{2}Y(Y^*Y)^{-1}Y^*\right)\nabla f(YY^*)Y(Y^*Y)^{-1} & \text{if using metric } g^3 \end{cases}$$

where ∇f denotes the gradient (4).

2.3.8 Retraction

The retraction on the quotient manifold $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ can be defined using the retraction on the total space $\mathbb{C}_*^{n\times p}$. For any $A \in T_Y\mathbb{C}_*^{n\times p}$ and a step size $\tau > 0$,

$$\overline{R}_Y(\tau A) := Y + \tau A,$$

is a retraction on $\mathbb{C}_*^{n\times p}$ if $Y+\tau A$ remains full rank, which is ensured for small enough τ. Then Lemma 2.17 indicates that $\overline{R}$ satisfies the conditions of [29, Prop. 4.1.3], which implies that

$$R_{\pi(Y)}(\tau\eta_{\pi(Y)}) := \pi(\overline{R}_Y(\tau\overline{\eta}_Y)) = \pi(Y+\tau\overline{\eta}_Y) \tag{20}$$

defines a retraction on the quotient manifold $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ for a small enough step size $\tau > 0$.

2.3.9 Vector transport

A vector transport on $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ is projection to horizontal space; see [29, Sect. 8.1.2]:

$$\overline{\left(\mathcal{T}_{\eta_{\pi(Y)}}\xi_{\pi(Y)}\right)}_{Y+\overline{\eta}_Y} := P^{\mathcal{H}}_{Y+\overline{\eta}_Y}(\overline{\xi}_Y). \tag{21}$$

It can be shown that this vector transport is actually the differential of the retraction R defined in (20). Denote $Y_2 = Y_1 + \overline{\eta}_{Y_1}$. Based on the projection formulae in Section 2.3.5, the explicit formula of (21) using different Riemannian metrics is then

$$\overline{\left(\mathcal{T}_{\eta_{\pi(Y_1)}}\xi_{\pi(Y_1)}\right)}_{Y_1+\overline{\eta}_{Y_1}} = \begin{cases} \overline{\xi}_{Y_1} - Y_2\Omega, \text{ with } \Omega \text{ defined in Prop. 2.14}, & \text{for } g^1, \\ Y_2\,\mathrm{Herm}((Y_2^*Y_2)^{-1}Y_2^*\overline{\xi}_{Y_1}) + Y_{2\perp}Y_{2\perp}^*\overline{\xi}_{Y_1}, & \text{for } g^2 \text{ or } g^3. \end{cases}$$

2.3.10 Riemannian Hessian operator

In this section, we summarize the Riemannian Hessian of the cost function h under the three different metrics g^i. The proofs are tedious calculations and are given in Appendix B.

Proposition 2.20. *Using g^1, the Riemannian Hessian of h is given by*

$$\overline{\left(\mathit{Hess}\, h(\pi(Y))[\xi_{\pi(Y)}]\right)}_Y = P_Y^{\mathcal{H}^1}\left(2\nabla^2 f(YY^*)[Y\overline{\xi}_Y^* + \overline{\xi}_Y Y^*]Y + 2\nabla f(YY^*)\overline{\xi}_Y\right). \tag{22}$$

Using g^2, the Riemannian Hessian of h is given by

$$\begin{aligned}\overline{\left(\mathit{Hess}\, h(\pi(Y))[\xi_{\pi(Y)}]\right)}_Y = & P_Y^{\mathcal{H}^2}\Big\{2\nabla^2 f(YY^*)[Y\overline{\xi}_Y^* + \overline{\xi}_Y Y^*]Y(Y^*Y)^{-1} \\ & + \nabla f(YY^*)P_Y^\perp\overline{\xi}_Y(Y^*Y)^{-1} + P_Y^\perp\nabla f(YY^*)\overline{\xi}_Y(Y^*Y)^{-1} \\ & + 2\,\mathrm{Skew}(\overline{\xi}_Y Y^*)\nabla f(YY^*)Y(Y^*Y)^{-2} \\ & + 2\,\mathrm{Skew}\{\overline{\xi}_Y(Y^*Y)^{-1}Y^*\nabla f(YY^*)\}Y(Y^*Y)^{-1}\Big\}.\end{aligned} \tag{23}$$

Using g^3, the Riemannian Hessian of h is given by

$$\begin{aligned}\overline{\left(\mathit{Hess}\, h(\pi(Y))[\xi_{\pi(Y)}]\right)}_Y = & \left(I - \frac{1}{2}P_Y\right)\nabla^2 f(YY^*)[Y\overline{\xi}_Y^* + \overline{\xi}_Y Y^*]Y(Y^*Y)^{-1} \\ & + (I-P_Y)\nabla f(YY^*)(I-P_Y)\overline{\xi}_Y(Y^*Y)^{-1}.\end{aligned} \tag{24}$$

3 The Riemannian conjugate gradient method

For simplicity, in this paper we only consider the Riemannian conjugate gradient (RCG) method described as Algorithm 1 in [17] with the geometric variant of Polak–Ribiére (PR+) for computing the conjugate direction. It is possible to explore other methods such as the limited-memory version of the Riemannian BFGS method (LRBFGS) as in [33]. However, RCG performs very well on a wide variety of problems and is easier to implement for our numerical examples.

In this section, we focus on establishing two equivalences in algorithms. First, we show that the Burer–Monteiro CG method, which is simply applying the CG method for the unconstrained problem (5), is equivalent to RCG on the Riemannian quotient manifold $(\mathbb{C}_*^{n\times p}/\mathcal{O}_p, g^1)$ with our retraction and vector transport defined in the previous sections. Second, we show that RCG on the embedded manifold $\mathcal{H}_+^{n,p}$ is equivalent to RCG on the quotient manifold $(\mathbb{C}_*^{n\times p}/\mathcal{O}_p, g^3)$ with a specific retraction and vector transport.

We first summarize two Riemannian CG algorithms in Algorithm 1 and Algorithm 2 below. Algorithm 1 is the RCG on the embedded manifold for solving (1) and Algorithm 2 is the RCG on the quotient manifold $(\mathbb{C}_*^{n\times p}/\mathcal{O}_p, g^i)$ for solving (11). We remark that the explicit constants 0.0001 and 0.5 in the Armijo backtracking are chosen for convenience.

Algorithm 1 Riemannian Conjugate Gradient on the embedded manifold $\mathcal{H}_+^{n,p}$

Require: initial iterate $X_0 \in \mathcal{H}_+^{n,p}$, initial gradient $\xi_0 = \operatorname{grad} f(X_0)$, initial conjugate direction $\eta_0 = -\operatorname{grad} f(X_0)$, tolerance $\varepsilon > 0$

1: **for** $k = 1, 2, \ldots$ **do**

2: Compute an initial step t_k. For special cost functions, it is possible to compute: $t_k = \arg\min_t f(X_{k-1} + t\eta_{k-1})$

3: Perform Armijo backtracking to find the smallest integer $m \geq 0$ such that

$$f(X_{k-1}) - f(R_{X_{k-1}}(0.5^m t_k \eta_{k-1})) \geq -0.0001 \times 0.5^m t_k g_{X_{k-1}}(\xi_{k-1}, \eta_{k-1})$$

$$\zeta_k := 0.5^m t_k \eta_{k-1}$$

4: Obtain the new iterate by retraction $X_k = R_{X_{k-1}}(\zeta_k)$ ▷ See Algorithm 6

5: Compute gradient $\xi_k := \operatorname{grad} f(X_k)$ ▷ See Algorithm 3

6: Check convergence if $\|\xi_k\| := \sqrt{g_{X_k}(\xi_k, \xi_k)} < \varepsilon$ or $f(X_k) < \varepsilon$, then break

7: Compute a conjugate direction by PR_+ and vector transport $\eta_k = -\xi_k + \beta_k \mathcal{T}_{\zeta_k}(\eta_{k-1})$, ▷ See Algorithm 4, 5

$$\text{with } \beta_k := \frac{g_{X_k}(\xi_k, \xi_k - \mathcal{T}_{\zeta_k}(\xi_{k-1}))}{g_{X_{k-1}}(\xi_{k-1}, \xi_{k-1})}.$$

8: **end for**

Algorithm 2 Riemannian Conjugate Gradient on the quotient manifold $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ with metric g^i

Require: initial iterate $Y_0 \in \pi^{-1}(\pi(Y_0))$, initial horizontal lift of gradient $\overline{\xi}_0 = \operatorname{grad} F(Y_0)$, initial conjugate direction $\overline{\eta}_0 = -\overline{\xi}_0$, tolerance $\varepsilon > 0$

1: **for** $k = 1, 2, \dots$ **do**

2: Compute an initial step t_k. For special cost functions, it is possible to compute: $t_k = \arg\min_t F(Y_{k-1} + t\overline{\eta}_{k-1})$

3: Perform Armijo backtracking to find the smallest integer $m \geq 0$ such that

$$F(Y_{k-1}) - F(\overline{R}_{Y_{k-1}}(0.5^m t_k \overline{\eta}_{k-1})) \geq -0.0001 \times 0.5^m t_k g^i_{Y_{k-1}}(\overline{\xi}_{k-1}, \overline{\eta}_{k-1})$$

$$\overline{\zeta}_k := 0.5^m t_k \overline{\eta}_k$$

4: Obtain the new iterate by retraction $Y_k = \overline{R}_{Y_{k-1}}(\overline{\zeta}_k)$

5: Compute the horizontal lift of gradient $\overline{\xi}_k := \overline{(\operatorname{grad} h(\pi(Y_k)))}_{Y_k} = \operatorname{grad} F(Y_k)$ ▷ See Algorithm 7

6: Check convergence if $\|\overline{\xi}_k\| := \sqrt{g^i_{Y_k}(\overline{\xi}_k, \overline{\xi}_k)} < \varepsilon$ or $F(Y_k) < \varepsilon$, then break

7: Compute a conjugate direction by PR_+ and vector transport $\overline{\eta}_k = -\overline{\xi}_k + \beta_k \overline{(\mathcal{T}_{\zeta_k}\eta_{k-1})}_{Y_k}$, ▷ See Algorithm 8

$$\text{with } \beta_k := \frac{g^i_{Y_k}\left(\operatorname{grad} F(Y_k), \operatorname{grad} F(Y_k) - \overline{(\mathcal{T}_{\zeta_k}\xi_{k-1})}_{Y_k}\right)}{g^i_{Y_{k-1}}\left(\operatorname{grad} F(Y_{k-1}), \operatorname{grad} F(Y_{k-1})\right)}.$$

8: **end for**

3.1 Equivalence between Burer–Monteiro CG and RCG on the Riemannian quotient manifold with the Bures-Wasserstein metric $(\mathbb{C}_*^{n\times p}/\mathcal{O}_p, g^1)$

Theorem 3.1. *Using retraction (20), vector transport (21) and the Bures-Wasserstein metric g^1, Algorithm 2 is equivalent to the conjugate gradient method solving (5) in the sense that they produce exactly the same iterates if started from the same initial point.*

Proof. First of all, for g^1, the Riemannian gradient of F at Y is $\operatorname{grad} F(Y) = 2\nabla f(YY^*)Y$, which is equal to the gradient of $F(Y) = f(YY^*)$ at Y. Since vector transport is the orthogonal projection to the horizontal space, the β_k of PR_+ used in Riemannian CG becomes

$$\beta_k = \frac{g^1_{Y_k}\left(\operatorname{grad} F(Y_k), \operatorname{grad} F(Y_k) - P^{\mathcal{H}^1}_{Y_k}(\operatorname{grad} F(Y_{k-1}))\right)}{g^1_{Y_{k-1}}\left(\operatorname{grad} F(Y_{k-1}), \operatorname{grad} F(Y_{k-1})\right)}. \tag{25}$$

Now observe that

$$P_{Y_k}^{\mathcal{H}^1}(\operatorname{grad} F(Y_{k-1})) = \operatorname{grad} F(Y_{k-1}) - P_{Y_k}^{\mathcal{V}}(\operatorname{grad} F(Y_{k-1}))$$

and g^1 is equivalent to the classical inner product for $\mathbb{C}^{n\times p}$. Hence β_k computed by (25) is equal to β_k of PR_+ in conjugate gradient for (5).

Since $\overline{\eta}_0 = -\operatorname{grad} F(Y_0) = -\nabla F(Y_0)$, Burer–Monteiro CG coincides with RCG for the first iteration. It remains to show that $\overline{\eta}_k$ generated in Riemannian CG by

$$\overline{\eta}_k = -\overline{\xi}_k + \beta_k P_{Y_k}^{\mathcal{H}^1}(\overline{\eta}_{k-1})$$

is equal to η_k generated in Burer–Monteiro CG for each $k \geq 1$. It suffices to show

$$P_{Y_k}^{\mathcal{H}^1}(\overline{\eta}_{k-1}) = \overline{\eta}_{k-1}, \quad \forall k \geq 1.$$

Equivalently we need to show that for all $k \geq 1$, the Lyapunov equation

$$(Y_k^* Y_k)\Omega + \Omega(Y_k^* Y_k) = Y_k^* \overline{\eta}_{k-1} - \overline{\eta}_{k-1}^* Y_k \tag{26}$$

only has trivial solution $\Omega = 0$. By the invertibility of the equation, this means that we only need to show the right hand side is zero. We prove it by induction. For $k = 1$, $\overline{\eta}_{k-1} = \overline{\eta}_0 = -\overline{\xi}_0 = -\operatorname{grad} F(Y_0)$. The following shows that the RHS of (26) satisfies

$$\begin{aligned} Y_1^* \overline{\eta}_0 - \overline{\eta}_0^* Y_1 &= -Y_1^* \overline{\xi}_0 + \overline{\xi}_0^* Y_1 = -(Y_0 - c\overline{\xi}_0)^* \overline{\xi}_0 + \overline{\xi}_0^* (Y_0 - c\overline{\xi}_0) = \overline{\xi}_0^* Y_0 - Y_0^* \overline{\xi}_0 \\ &= Y_0^*(2\nabla f(Y_0 Y_0^*))Y_0 - Y_0^*(2\nabla f(Y_0 Y_0^*))Y_0 = 0. \end{aligned}$$

Hence $\Omega = 0$ and $P_{Y_k}^{\mathcal{H}^1}(\eta_{k-1}) = \eta_{k-1}$ for $k = 1$.

Now suppose for $k \geq 1$, the RHS of (26) is 0 and hence $P_{Y_k}^{\mathcal{H}^1}(\overline{\eta}_{k-1}) = \overline{\eta}_{k-1}$ holds. Then the RHS of the Lyapunov equation of step $k+1$ is

$$\begin{aligned} & Y_{k+1}^* \overline{\eta}_k - \overline{\eta}_k^* Y_{k+1} = (Y_k + c\overline{\eta}_k)^* \overline{\eta}_k - \overline{\eta}_k^* (Y_k + c\overline{\eta}_k) = Y_k^* \overline{\eta}_k - \overline{\eta}_k^* Y_k \\ &= Y_k^* \left(-\overline{\xi}_k + \beta_k P_{Y_k}^{\mathcal{H}^1}(\overline{\eta}_{k-1})\right) - \left(-\overline{\xi}_k + \beta_k P_{Y_k}^{\mathcal{H}^1}(\eta_{k-1})\right)^* Y_k \\ &= Y_k^*(-\overline{\xi}_k + \beta_k \overline{\eta}_{k-1}) - (-\overline{\xi}_k + \beta_k \overline{\eta}_{k-1})^* Y_k \\ &= -Y_k^* \overline{\xi}_k + \overline{\xi}_k^* Y_k = -Y_k^*(2\nabla f(Y_k Y_k^*))Y_k + Y_k^*(2\nabla f(Y_k Y_k^*))Y_k = 0. \end{aligned}$$

So $P_{Y_{k+1}}^{\mathcal{H}^1}(\overline{\eta}_k) = \overline{\eta}_k$ also holds, thus RCG is equivalent to Burer–Monteiro CG. □

Since the gradient descent corresponds to $\beta_k \equiv 0$, the same discussion also implies the following

Corollary 3.2. *Using retraction (20) and metric g^1, the Riemannian gradient descent on the quotient manifold is equivalent to the Burer–Monteiro gradient descent method with suitable step size (1.3) in the sense that they produce exactly the same iterates.*

3.2 Equivalence between RCG on embedded manifold and RCG on the quotient manifold $(\mathbb{C}_*^{n\times p}/\mathcal{O}_p, g^3)$

In this subsection we show that Algorithm 1 is equivalent to Algorithm 2 with Riemannian metric g^3, a specific initial step in step 2, a specific retraction (27) and a specific vector transport (28). The idea is to take the advantage of the diffeomorphism $\tilde{\beta}$ between $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ and $\mathcal{H}_+^{n,p}$, as well as the fact that the metric g^3 of $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ is induced from the metric of $\mathcal{H}_+^{n,p}$.

Since $\tilde{\beta} : \pi(Y) \mapsto YY^*$ is a diffeomorphism between $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ and $\mathcal{H}_+^{n,p}$, thus, $D\tilde{\beta}(\pi(Y))[\cdot]$ defines an isomorphism between the tangent spaces. We denote this isomorphism by $L_{\pi(Y)} : T_{\pi(Y)}\mathbb{C}_*^{n\times p}/\mathcal{O}_p \to T_{YY^*}\mathcal{H}_+^{n,p}$. The following lemma can be verified by straightforward computation; see [9].

Lemma 3.3. *For $(\mathbb{C}_*^{n\times p}/\mathcal{O}_p, g^3)$, the Riemannian gradient of f and h is related by $(D\tilde{\beta})(\pi(Y))[\mathrm{grad}\, h(\pi(Y))] = \mathrm{grad}\, f(YY^*)$ and*

$$L_{\pi(Y)}(\mathrm{grad}\, h(\pi(Y))) = \mathrm{grad}\, f(\tilde{\beta}(\pi(Y))).$$

In Algorithm 1, we have a retraction R^E and a vector transport $\mathcal{T}^E$ on the embedded manifold $\mathcal{H}_+^{n,p}$, (with the superscript E for *Embedded*), such that R^E is the retraction associated with $\mathcal{T}^E$. Then we claim in the following theorem that there is a retraction R^Q and a vector transport $\mathcal{T}^Q$, (with the superscript Q denoting *Quotient*), on the Riemannian quotient manifold $(\mathbb{C}_*^{n\times p}/\mathcal{O}_p, g^3)$, such that Algorithm 2 is equivalent to Algorithm 1. The idea is again to use the diffeomorphism $\tilde{\beta}$ and the isomorphism $L_{\pi(Y)}$. We give the desired expression of R^Q and $\mathcal{T}^Q$ as follows.

Theorem 3.4. *Let R^E and $\mathcal{T}^E$ denote any retraction and vector transport used in Algorithm 1 on the embedded manifold $\mathcal{H}_+^{n,p}$. Using the diffeomorphism $\tilde{\beta}$ between $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ and $\mathcal{H}_+^{n,p}$ and isomorphism $L_{\pi(Y)}$ between $T_{\pi(Y)}\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ and $T_{YY^*}\mathcal{H}_+^{n,p}$, define the retraction R^Q and vector transport $\mathcal{T}^Q$ on the quotient manifold $(\mathbb{C}_*^{n\times p}/\mathcal{O}_p, g^3)$ as*

$$R^Q_{\pi(Y)}(\xi_{\pi(Y)}) := \tilde{\beta}^{-1}\left(R^E_{\tilde{\beta}(\pi(Y))}\left(L(\xi_{\pi(Y)})\right)\right), \tag{27}$$

$$\mathcal{T}^Q_{\eta_{\pi(Y)}}(\xi_{\pi(Y)}) := L^{-1}_{\pi(Y_2)}\left(\mathcal{T}^E_{L(\eta_{\pi(Y)})}\left(L(\xi_{\pi(Y)})\right)\right), \tag{28}$$

where $\pi(Y_2)$ is in $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ such that $\tilde{\beta}(\pi(Y_2))$ denotes the foot of the tangent vector $\mathcal{T}^E_{L(\eta_{\pi(Y)})}\left(L(\xi_{\pi(Y)})\right)$. Using R^Q and $\mathcal{T}^Q$ as the retraction and vector transport in Algorithm 2 and assume the initial step t_k in Algorithm 1 and 2 is be chosen to be the same, then Algorithm 2 is equivalent to Algorithm 1 in the sense that if they produce exactly the same iterates if started from the same initial point.

Proof. It suffices to show that the newly defined R^Q and $\mathcal{T}^Q$ are indeed retraction and vector transport. This will be shown in the following Lemma 3.5 and Lemma 3.6. □

Lemma 3.5. *R^Q defined in (27) is a retraction.*

Proof. First it is easy to see that $R^Q_{\pi(Y)}(0_{\pi(Y)}) = \pi(Y)$. Then we also have for all $v_{\pi(Y)} \in T_{\pi(Y)}\mathbb{C}^{n\times p}_*/\mathcal{O}_p$, $\mathrm{D}\, R^Q_{\pi(Y)}(0_{\pi(Y)})[\cdot]$ is an identity map because

$$\begin{aligned} &\mathrm{D}\, R^Q_{\pi(Y)}(0_{\pi(Y)})[v_{\pi(Y)}] = (\mathrm{D}\,\tilde{\beta}^{-1})(\tilde{\beta}(\pi(Y)) \left[\mathrm{D}\, R^E_{\tilde{\beta}(\pi(Y))}(0) \left[\mathrm{D}\, L(0) \left[v_{\pi(Y)}\right]\right]\right] \\ &= (\mathrm{D}\,\tilde{\beta}^{-1})(\tilde{\beta}(\pi(Y)) \left[\mathrm{D}\, R^E_{\tilde{\beta}(\pi(Y))}(0) \left[L(v_{\pi(Y)})\right]\right] \\ &= (\mathrm{D}\,\tilde{\beta}^{-1})(\tilde{\beta}(\pi(Y)) \left[L(v_{\pi(Y)})\right] = \left(\mathrm{D}\,\tilde{\beta}(\pi(Y))\right)^{-1} \left[L(v_{\pi(Y)})\right] = L^{-1}(L(v_{\pi(Y)})) = v_{\pi(Y)} \end{aligned}$$

□

Lemma 3.6. *$\mathcal{T}^Q$ defined in (28) is a vector transport and R^Q is the retraction associated with $\mathcal{T}^Q$.*

Proof. Consistency and linearity are straightforward. It thus suffices to verify that the foot of $\mathcal{T}^Q_{\eta_{\pi(Y)}}(\xi_{\pi(Y)})$ is equal to $R^Q_{\pi(Y)}(\eta_{\pi(Y)})$. Since R^E is the associated retraction with $\mathcal{T}^E$, the foot of $\mathcal{T}^E_{L(\eta_{\pi(Y)})}(L(\xi_{\pi(Y)}))$ is equal to $R^E_{\tilde{\beta}(\pi(Y))}\left(L(\eta_{\pi(Y)})\right)$, which we denote by $\tilde{\beta}(\pi(Y_2))$ for some $\pi(Y_2)$. Hence $R^Q_{\pi(Y)}(\eta_{\pi(Y)}) = \tilde{\beta}^{-1}\left(R^E_{\tilde{\beta}(\pi(Y))}\left(L(\eta_{\pi(Y)})\right)\right) = \pi(Y_2)$.

Furthermore, we have that $\mathcal{T}^Q_{\eta_{\pi(Y)}}(\xi_{\pi(Y)}) = L^{-1}_{\pi(Y_2)}\left(\mathcal{T}^E_{L(\eta_{\pi(Y)})}\left(L(\xi_{\pi(Y)})\right)\right)$ is a tangent vector in $T_{\pi(Y_2)}\mathbb{C}^{n\times p}_*/\mathcal{O}_p$. Hence, the foot of $\mathcal{T}^Q_{\eta_{\pi(Y)}}(\xi_{\pi(Y)})$ is also $\pi(Y_2)$. □

Remark 3.7. *To reach an equivalence, we also need the initial step size to match the one in step 2 of Algorithm 1. We simply replace the original initial step size t_k by*

$$t_k = \arg\min_t f(Y_kY_k^* + t(Y_k\overline{\eta}_k^* + \overline{\eta}_kY_k^*)).$$

This value of t_k now is equivalent to the initial step size in step 5 of Algorithm 1.

3.3 Implementation details

The algorithms in this paper can be applied for minimizing any smooth function $f(X)$ in (1). For problems with large n, however, it is advisable to avoid constructing and storing the derivative $\nabla f(X) \in \mathbb{C}^{n\times n}$ explicitly. Instead, one directly computes the matrix-vector multiplications $\nabla f(X)U$. In the PhaseLift problem [5], for example, these matrix-vector multiplications can be implemented via the FFT at a cost of $\mathcal{O}(pn\log n)$ when $U \in \mathbb{C}^{n\times p}$; see [15]. To store a tangent vector $\zeta_X \in T_X\mathcal{M}$, there is no need to compute and store $U_\perp \in \mathbb{C}^{n\times(n-p)}$. By Theorem 2.2, it suffices to only store U, H and $U_p := U_\perp K \in \mathbb{C}^{n\times p}$.

Below, we detail the calculations needed in Algorithms 1 and 2. When giving flop counts, we assume that $\nabla f(X)U \in \mathbb{C}^{n\times p}$ can be computed in $spn\log n$ flops with s small. For g^2 and g^3 in Algorithms 7 and 8, we use forward slash "/" and backslash "\" in Matlab command to compute the inverse of Y^*Y.

3.3.1 Embedded manifold

Algorithm 3 Calculate the Riemannian gradient $\operatorname{grad} f(X)$

Require: $X = U\Sigma U^* \in \mathcal{H}_+^{n,p}$
Ensure: $\operatorname{grad} f(X) = UHU^* + U_pU^* + UU_p^* \in T_X\mathcal{H}_+^{n,p}$

$T \leftarrow \nabla f(X)U$ $\triangleright$ # $spn\log n$ flops
$H \leftarrow U^*T$ $\triangleright$ # $p^2(2n-1)$ flops
$U_p \leftarrow T - UH$ $\triangleright$ # $np + np(2p-1)$ flops

Algorithm 4 Calculate the vector transport by projection to tangent space $P_{X_2}^t(\nu)$

Require: $X_1 = U_1\Sigma_1U_1^*$, $X_2 = U_2\Sigma_2U_2^*$ and tangent vector $\nu = U_1H_1U_1^* + U_{p1}U_1^* + U_1U_{p1}^* \in T_{X_1}\mathcal{H}_+^{n,p}$.
Ensure: $P_{X_2}^t(\nu) = U_2H_2U_2^* + U_{p2}U_2^* + U_2U_{p2}^*$

$A \leftarrow U_1^*U_2$ $\triangleright$ # $p^2(2n-1)$ flops
$H_2^{(1)} \leftarrow A^*H_1A, \quad U_p^{(1)} \leftarrow U_1(H_1A)$ $\triangleright$ # $3p^2(2p-1) + np(2p-1)$ flops
$H_2^{(2)} \leftarrow U_2^*U_{p1}A, \quad U_p^{(2)} \leftarrow U_{p1}A$ $\triangleright$ # $p^2(2n-1) + 2np(2p-1)$ flops
$H_2^{(3)} \leftarrow {H_2^{(2)}}^*, \quad U_p^{(3)} \leftarrow U_1(U_{1p}^*U_2)$ $\triangleright$ # $np(2p-1) + p^2(2n-1)$ flops
$H_2 \leftarrow H_2^{(1)} + H_2^{(2)} + H_2^{(3)}$ $\triangleright$ # $2p^2$ flops
$U_{p2} \leftarrow U_p^{(1)} + U_p^{(2)} + U_p^{(3)}, \quad U_{p2} \leftarrow U_{p2} - U_2(U_2^*U_{p2})$ $\triangleright$ # $3np + np(2p-1) + p^2(2n-1)$ flops

In implementation, we observe a vector transport that has better numerical performance if we only keep the first term in the above sum of H_2 and the second term of U_{2p} in Algorithm 4, which is outlined in Algorithm 5.

Algorithm 5 Calculate the simpler form of vector transport used in implementation that has a better performance $P_{X_2}^t(\nu)$

Require: $X_1 = U_1\Sigma_1U_1^*$, $X_2 = U_2\Sigma_2U_2^*$ and tangent vector $\nu = U_1H_1U_1^* + U_{p1}U_1^* + U_1U_{p1}^* \in T_{X_1}\mathcal{H}_+^{n,p}$.
Ensure: $P_{X_2}^t(\nu) = U_2H_2U_2^* + U_{p2}U_2^* + U_2U_{p2}^*$

$A \leftarrow U_1^*U_2$ $\triangleright$ # $p^2(2n-1)$ flops
$H_2 \leftarrow A^*H_1A$ $\triangleright$ # $2p^2(2p-1)$ flops
$U_p \leftarrow U_{p1}A$ $\triangleright$ # $np(2p-1)$ flops
$U_{p2} \leftarrow U_p - U_2(U_2^*U_p)$ $\triangleright$ # $np + p^2(2n-1) + np(2p-1)$ flops

Algorithm 6 Calculate the retraction $R_X(Z) = P_{\mathcal{H}_+^{n,p}}(X+Z)$

Require: $X = U\Sigma U^* \in \mathcal{H}_+^{n,p}$, tangent vector $Z = UHU^* + U_pU^* + UU_p^*$.
Ensure: $P_{\mathcal{H}_+^{n,p}}(X+Z) = U_+\Sigma_+U_+^*$.

$(Q,R) \leftarrow \mathrm{qr}(U_p, 0) \quad M \leftarrow \begin{bmatrix} \Sigma + H & R^* \\ R & 0 \end{bmatrix}$ ▷ # $20np^2$ flops
$[V,S] \leftarrow \mathrm{eig}(M)$ ▷ $O(p^3)$ flops
$\Sigma+ \leftarrow S(1:p,1:p), \quad U_+ \leftarrow \begin{bmatrix} U & Q \end{bmatrix} V(:,1:p)$ ▷ # $np(4p-1)$ flops

3.3.2 Quotient manifold

Algorithm 7 Calculate the Riemannian gradient $\mathrm{grad}\, F(Y)$

Require: $Y \in \mathbb{C}_*^{n\times p}$
Ensure: $T = \mathrm{grad}\, F(Y)$

if metric is g^1 **then**
  $T \leftarrow 2\nabla f(YY^*)Y.$ ▷ # $2spn\log n$ flops
else if metric is g^2 **then**
  $Z \leftarrow Y(Y^*Y)^{-1}$ ▷ # $np(2p-1) + p^2(2n-1) + O(p^3)$ flops
  $T \leftarrow 2\nabla f(YY^*)Z$ ▷ # $2spn\log n$ flops
else if metric is g^3 **then**
  $Z \leftarrow Y(Y^*Y)^{-1}$ ▷ # $np(2p-1) + p^2(2n-1) + O(p^3)$ flops
  $T \leftarrow 2\nabla f(YY^*)Z$ ▷ # $2spn\log n$ flops
  $M \leftarrow Y^*T, \quad T \leftarrow T - \frac{1}{2}ZM$ ▷ # $p^2(2n-1) + np + 2np^2$ flops
end if

Algorithm 8 Calculate the quotient vector transport $P_{Y_2}^{\mathcal{H}}(h_1)$

Require: $Y_1 \in \mathbb{C}_*^{n\times p}$, $Y_2 \in \mathbb{C}_*^{n\times p}$ and horizontal vector $h_1 \in \mathcal{H}_{Y_1}$.
Ensure: $h_2 = P_{Y_2}^{\mathcal{H}}(h_1) \in \mathcal{H}_{Y_2}$.

if metric is g^1 **then**
  $E \leftarrow Y_2^*Y_2$ ▷ # $p^2(2n-1)$ flops
  $(Q,S) \leftarrow \mathrm{eig}(E), \quad d \leftarrow \mathrm{diag}(S)$ ▷ # $O(p^3)$ flops
  $\lambda \leftarrow d\begin{bmatrix}1,1,\cdots,1\end{bmatrix} + \begin{bmatrix}1,1,\cdots,1\end{bmatrix}^T d^T$ ▷ # $2p^2$ flops
  $A \leftarrow Q^*(Y_2^*h_1 - h_1^*Y_2)Q$ ▷ # $p^2(2n-1) + np + 2p^2(2p-1)$ flops
  $\Omega \leftarrow Q(A./\lambda)Q^*$ ▷ # $p^2 + 2p^2(2p-1)$ flops
  $h_2 \leftarrow h_1 - Y_2\Omega$ ▷ # $np + np(2p-1)$ flops
else if metric is g^2 or g^3 **then**
  $\tilde{\Omega} \leftarrow (Y^*Y)^{-1}(Y_2^*h_1)$ ▷ # $2p^2(2p-1) + p^2(2n-1) + O(p^3)$ flops
  $\Omega \leftarrow \frac{1}{2}(\tilde{\Omega} - \tilde{\Omega}^*)$ ▷ # $2p^2$ flops
  $h_2 \leftarrow h_1 - Y_2\Omega$ ▷ # $np + np(2p-1)$ flops
end if

3.3.3 Initial guess for the line search

The initial guess for the line search generally depends on the expression of the cost function $f(X)$. For the important case of $f(X) = \frac{1}{2}\|\mathcal{A}(X) - b\|_F^2$ where $\mathcal{A}$ is a linear operator and b is a matrix, the initial guess for embedded CG requires solving a linear equation and for quotient CG it requires solving a cubic equation. Below this calculation is detailed for b of size mn for some m and assuming that $\mathcal{A}(X), \mathcal{A}(T)$ and $\mathcal{A}(Y\eta^*)$ can be evaluated in $sp^\alpha n \log n$ flops for $X \in \mathcal{H}_+^{n,p}$, $T \in T_X\mathcal{H}_+^{n,p}$ and $Y, \eta \in \mathbb{C}_*^{n\times p}$.

Algorithm 9 Calculate the initial guess $t_* = \arg\min_t f(X + tT)$

Require: $X \in \mathcal{H}_+^{n,p}$ and a descend direction $T \in T_X\mathcal{H}_+^{n,p}$

Ensure: $t_* = \arg\min_t f(X + tT) = \arg\min_t \frac{1}{2}\|\mathcal{A}(X + tT) - b\|_F^2$

$R \leftarrow \mathcal{A}(X) - b$ $\quad\triangleright$ # $sp^\alpha n \log n + mn$ flops

$S \leftarrow \mathcal{A}(T)$ $\quad\triangleright$ # $sp^\alpha n \log n$ flops

$t_* \leftarrow -\frac{\langle R,S\rangle}{\langle S,S\rangle}$ $\quad\triangleright$ # $4mn - 1$ flops

---

Algorithm 10 Calculate the initial guess $t_* = \arg\min_t F(Y + t\eta)$

Require: $Y \in \mathbb{C}_*^{n\times p}$, a descend direction $\eta \in \mathcal{H}_Y$,

Ensure: $t_* = \arg\min_t F(Y + t\eta) = \arg\min_t \frac{1}{2}\|\mathcal{A}((Y + t\eta)(Y + t\eta)^*) - b\|_F^2$

$c_0 \leftarrow \mathcal{A}(YY^*) - b$ $\quad\triangleright$ # $sp^\alpha n \log n + mn$ flops

$c_1^{(1)} \leftarrow \mathcal{A}(Y\eta^*)$, $\quad c_1^{(2)} \leftarrow \mathcal{A}(\eta Y^*)$, $\quad c_1 \leftarrow c_1^{(1)} + c_1^{(2)}$ $\triangleright$ # $2sp^\alpha n \log n + mn$ flops

$c_2 \leftarrow \mathcal{A}(\eta\eta^*)$ $\quad\triangleright$ # $sp^\alpha n \log n$ flops

$d_4 \leftarrow \langle c_2, c_2\rangle$, $\quad d_3 \leftarrow 2\langle c_2, c_1\rangle$ $\quad\triangleright$ # $4mn - 1$ flops

$d_2 \leftarrow 2\langle c_2, c_0\rangle + \langle c_1, c_1\rangle$, $\quad d_1 \leftarrow 2\langle c_1, c_0\rangle$ $\quad\triangleright$ # $6mn - 1$ flops

$C \leftarrow \begin{bmatrix} 4d_4 & 3d_3 & 2d_2 & d_1 \end{bmatrix}$

$S \leftarrow roots(C)$, $\quad t_* \leftarrow$ the smallest real positive root in S

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4 Estimates of Rayleigh quotient for Riemannian Hessians

In many applications, (1) or (11) is often used for solving (2). Even if the global minimizer of (2) has a known rank r, one might consider solving (1) or (11) for Hermitian PSD matrices with fixed rank $p \geq r$. For instance, in PhaseLift [5] and interferometry recovery [8], the minimizer to (2) is rank one, but in practice, optimization over the set of PSD Hermitian matrices of rank p with $p \geq 2$ is often used because of a larger basin of attraction [8, 15]. If $p > r$, then an algorithm that solves (1) or (11) can generate a sequence that goes to the boundary of the manifold. Numerically, the smallest $p - r$ singular values of the iterates X_k will become very small as $k \to \infty$.

In this section, we analyze the eigenvalues of the Riemannian Hessian near the global minimizer. We will obtain upper and lower bounds of the Rayleigh quotient at $X = YY^*$ (or $\pi(Y)$) that is close to the global minimizer $\hat{X} = \hat{Y}\hat{Y}^*$ (or $\pi(\hat{Y})$).

Definition 4.1. *The Rayleigh quotient of the Riemannian Hessian of f on $(\mathcal{H}_+^{n,p}, g)$ is defined by*

$$\rho^E(X, \zeta_X) = \frac{g_X(\mathrm{Hess}\, f(X)[\zeta_X], \zeta_X)}{g_X(\zeta_X, \zeta_X)}, \forall \zeta_X \in T_X\mathcal{H}_+^{n,p}.$$

The Rayleigh quotient of the Riemannian Hessian of h on $(\mathbb{C}_*^{n\times p}/\mathcal{O}_p, g^i)$ is defined by

$$\rho^i(\pi(Y), \xi_{\pi(Y)}) = \frac{g^i_{\pi(Y)}\left(\mathrm{Hess}\, h(\pi(Y))[\xi_{\pi(Y)}], \xi_{\pi(Y)}\right)}{g^i_{\pi(Y)}(\xi_{\pi(Y)}, \xi_{\pi(Y)})}, \quad \forall \xi_{\pi(Y)} \in T_{\pi(Y)}\mathbb{C}_*^{n\times p}/\mathcal{O}_p.$$

If the Rayleigh quotient has a lower bound μ and an upper bound L, then we define $\frac{L}{\mu}$ as an upper bound on the condition number of the Riemannian Hessian.

4.1 The Rayleigh quotient estimates

We assume that the Hessian $\nabla^2 f$ is well conditioned on the tangent space near the global minimizer $\hat{X}$:

Assumption 4.1. *Let $\hat{X}$ be the global minimizer of f. For a fixed $\epsilon > 0$, there exist constants $A > 0$ and $B > 0$ such that for all X with $\left\|X - \hat{X}\right\|_F < \epsilon$, the following inequality holds,*

$$A \left\|\zeta_X\right\|_F^2 \leq \left\langle \nabla^2 f(X)[\zeta_X], \zeta_X \right\rangle_{\mathbb{C}^{n\times n}} \leq B \left\|\zeta_X\right\|_F^2, \quad \forall \zeta_X \in T_X\mathcal{H}_+^{n,p}.$$

Observe that the Assumption 4.1 is always satisfied for sufficiently small ϵ when f is smooth and $\hat{X}$ is a nondegenerate minimizer of f. However, the condition number B/A might be large in general. An important case for which this assumption holds is $f(X) = \frac{1}{2}\left\|X - H\right\|_F^2$ with H being a given Hermitian PSD matrix. In this case, $\nabla^2 f(X)$ is the identity operator thus $A = B = 1$.

Our main result is given in the following theorem.

Theorem 4.1. *Let $\hat{X} = \hat{Y}\hat{Y}^*$ be the global minimizer of (2) with rank $r \leq p$. For $X = YY^* = U\Sigma U^*$ with singular values σ_i, $Y \in \mathbb{C}_*^{n\times p}$, and X near $\hat{X}$, under the Assumption 4.1, for any arbitrary tangent vectors ζ_X and $\xi_{\pi(Y)}$, the following hold:*

1. $A - \frac{2}{\sigma_p}\left\|\nabla f(X)\right\| \leq \rho^E(X, \zeta_X) \leq B + \frac{2}{\sigma_p}\left\|\nabla f(X)\right\|,$
2. $2A\sigma_p - 2\left\|\nabla f(YY^*)\right\| \leq \rho^1(\pi(Y), \xi_{\pi(Y)}) \leq B \cdot D^1_{\pi(Y)} + 2\left\|\nabla f(YY^*)\right\|,$
3. $2A - \frac{4(\sqrt{p}+1)}{\sigma_p}\left\|\nabla f(YY^*)\right\| \leq \rho^2(\pi(Y), \xi_{\pi(Y)}) \leq 4B + \frac{4(\sqrt{p}+1)}{\sigma_p}\left\|\nabla f(YY^*)\right\|,$
4. $A - \frac{1}{\sigma_p}\left\|\nabla f(YY^*)\right\| \leq \rho^3(\pi(Y), \xi_{\pi(Y)}) \leq B + \frac{1}{\sigma_p}\left\|\nabla f(YY^*)\right\|,$

where $D^1_{\pi(Y)}$ *satisfies* $2\sigma_1 \leq D^1_{\pi(Y)} \leq 2\left(\frac{\sigma_1^2}{\sigma_p} + \sigma_1\right)$*. In particular, if* $\hat{X} = \hat{Y}\hat{Y}^*$ *has rank* p*, we have the following limits, where* $X \to \hat{X}$ *and* $\pi(Y) \to \pi(\hat{Y})$ *are taken in the sense of* $\left\|X - \hat{X}\right\|_F \to 0$ *and* $\left\|YY^* - \hat{Y}\hat{Y}^*\right\|_F \to 0$*:*

1. $A - \frac{2}{\hat{\sigma}_p}\left\|\nabla f(\hat{X})\right\| \leq \lim_{X\to\hat{X}} \rho^E(X, \xi_X) \leq B + \frac{2}{\hat{\sigma}_p}\left\|\nabla f(\hat{X})\right\|,$
2. $2A\hat{\sigma}_p - 2\left\|\nabla f(\hat{X})\right\| \leq \lim_{\pi(Y)\to\pi(\hat{Y})} \rho^1(\pi(Y), \xi_{\pi(Y)}) \leq B \cdot D^1_{\pi(\hat{Y})} + 2\left\|\nabla f(\hat{X})\right\|,$
3. $2A - \frac{4(\sqrt{p}+1)}{\hat{\sigma}_p}\left\|\nabla f(\hat{X})\right\| \leq \lim_{\pi(Y)\to\pi(\hat{Y})} \rho^2(\pi(Y), \xi_{\pi(Y)}) \leq 4B + \frac{4(\sqrt{p}+1)}{\hat{\sigma}_p}\left\|\nabla f(\hat{X})\right\|,$
4. $A - \frac{1}{\hat{\sigma}_p}\left\|\nabla f(\hat{X})\right\| \leq \lim_{\pi(Y)\to\pi(\hat{Y})} \rho^3(\pi(Y), \xi_{\pi(Y)}) \leq B + \frac{1}{\hat{\sigma}_p}\left\|\nabla f(\hat{X})\right\|,$

where $D^1_{\pi(\hat{Y})}$ *satisfies* $2\hat{\sigma}_1 \leq D^1_{\pi(\hat{Y})} \leq 2\left(\frac{\hat{\sigma}_1^2}{\hat{\sigma}_p} + \hat{\sigma}_1\right)$.

Before we present the proof of Theorem 4.1, we give two remarks on this theorem:

Remark 4.2. *If we also assume* $\nabla f(\hat{X}) = 0$*, then the limits above can be further simplified. Though* $\nabla f(\hat{X}) = 0$ *may not be true in general, it holds for all numerical examples considered in this paper, where the cost function takes the form* $f(X) = \frac{1}{2}\|\mathcal{A}(X) - b\|_F^2$ *, and the minimizer* $\hat{X}$ *for* (1) *or* (2) *satisfies* $f(\hat{X}) = 0$*. Thus* $\hat{X}$ *is also the minimizer for minimizing* $f(X)$ *over all* $X \in \mathbb{C}$*, which implies* $\nabla f(\hat{X}) = 0$*.*

Remark 4.3. *Under the assumption* $\nabla f(\hat{X}) = 0$*, the limit of the condition number for the Bures-Wasserstein metric* g^1 *depends on the condition number of the minimizer* $\hat{X}$*. This reflects a significant difference between* g^1 *and the other two metrics. For certain problems, the minimizer* $\hat{X}$ *may have a huge condition number, and the methods using metric* g^1 *indeed shows much slower asymptotic convergence rate, e.g., see the numerical example shown in Figure 2 in the next Section.*

The rest of this subsection is the proof of Theorem 4.1. By the expressions of Riemannian Hessian, we have

$$\rho^E(X, \zeta_X) = \frac{\left\langle \nabla^2 f(X)[\zeta_X], \zeta_X \right\rangle_{\mathbb{C}^{n\times n}}}{g_X(\zeta_X, \zeta_X)} + \frac{g_X\left(P_X^p\left(\nabla f(X)(X^\dagger \zeta_X^p)^* + (\zeta_X^p X^\dagger)^* \nabla f(X)\right), \zeta_X\right)}{g_X(\zeta_X, \zeta_X)}.$$

$$\rho^1(\pi(Y), \xi_{\pi(Y)}) = \frac{\left\langle \nabla^2 f(YY^*)[Y\overline{\xi}_Y^* + \overline{\xi}_Y Y^*], Y\overline{\xi}_Y^* + \overline{\xi}_Y Y^* \right\rangle_{\mathbb{C}^{n\times n}}}{g_Y^1(\overline{\xi}_Y, \overline{\xi}_Y)} + \frac{g_Y^1(2\nabla f(YY^*)\overline{\xi}_Y, \overline{\xi}_Y)}{g_Y^1(\overline{\xi}_Y, \overline{\xi}_Y)}.$$

$$\begin{aligned}\rho^2(\pi(Y), \xi_{\pi(Y)}) = {} & \frac{\left\langle \nabla^2 f(YY^*)[Y\overline{\xi}_Y^* + \overline{\xi}_Y Y^*], Y\overline{\xi}_Y^* + \overline{\xi}_Y Y^* \right\rangle_{\mathbb{C}^{n\times n}}}{g_Y^2(\overline{\xi}_Y, \overline{\xi}_Y)} + \frac{\left\langle \nabla f(YY^*) P_Y^\perp \overline{\xi}_Y, \overline{\xi}_Y \right\rangle_{\mathbb{C}^{n\times p}}}{g_Y^2(\overline{\xi}_Y, \overline{\xi}_Y)} \\ & + \frac{\left\langle P_Y^\perp \nabla f(YY^*)\overline{\xi}_Y, \overline{\xi}_Y \right\rangle_{\mathbb{C}^{n\times p}}}{g_Y^2(\overline{\xi}_Y, \overline{\xi}_Y)} + \frac{\left\langle Y\overline{\xi}_Y^*\overline{\xi}_Y, 2\nabla f(YY^*)Y(Y^*Y)^{-1} \right\rangle_{\mathbb{C}^{n\times p}}}{g_Y^2(\overline{\xi}_Y, \overline{\xi}_Y)} - \frac{\left\langle \overline{\xi}_Y Y^*\overline{\xi}_Y, 2\nabla f(YY^*)Y(Y^*Y)^{-1} \right\rangle_{\mathbb{C}^{n\times p}}}{g_Y^2(\overline{\xi}_Y, \overline{\xi}_Y)}.\end{aligned}$$

$$\rho^3(\pi(Y), \xi_{\pi(Y)}) = \frac{\left\langle \nabla^2 f(YY^*)[Y\overline{\xi}_Y^* + \overline{\xi}_Y Y^*], Y\overline{\xi}_Y^* + \overline{\xi}_Y Y^* \right\rangle_{\mathbb{C}^{n\times n}}}{g_Y^3(\overline{\xi}_Y, \overline{\xi}_Y)} + \frac{g_Y^3((I-P_Y)\nabla f(YY^*)(I-P_Y)\overline{\xi}_Y(Y^*Y)^{-1}, \overline{\xi}_Y)}{g_Y^3(\overline{\xi}_Y, \overline{\xi}_Y)}.$$

Observe that the leading terms in the above Rayleigh quotients take similar forms: the numerator involves the Hessian $\nabla^2 f$, and the denominator is the induced norm of the tangent vector from the respective Riemannian metric. We call the leading term *second order term* (SOT) as it involves the Hessian of f as the second-order information of f, and we call the other terms that follow the leading term *first order terms* (FOTs) as they only contain the first-order gradient.

Under Assumption 4.1, we get bounds of the SOT in $\rho^E(X, \zeta_X)$ as:

$$A = A\frac{\|\zeta_X\|_F^2}{g_X(\zeta_X, \zeta_X)} \leq \frac{\left\langle \nabla^2 f(X)[\zeta_X], \zeta_X \right\rangle_{\mathbb{C}^{n\times n}}}{g_X(\zeta_X, \zeta_X)} \leq B\frac{\|\zeta_X\|_F^2}{g_X(\zeta_X, \zeta_X)} = B.$$

For quotient manifold, since $Y\bar{\xi}_Y^* + \bar{\xi}_Y Y^* \in T_{YY^*}\mathcal{H}_+^{n,p}$, under Assumption 4.1, we get

$$A\frac{\left\|Y\bar{\xi}_Y^* + \bar{\xi}_Y Y^*\right\|_F^2}{g_Y^i\left(\bar{\xi}_Y, \bar{\xi}_Y\right)} \leq \frac{\left\langle \nabla^2 f(YY^*)[Y\bar{\xi}_Y^* + \bar{\xi}_Y Y^*], Y\bar{\xi}_Y^* + \bar{\xi}_Y Y^* \right\rangle_{\mathbb{C}^{n\times n}}}{g_Y^i(\bar{\xi}_Y, \bar{\xi}_Y)} \leq B\frac{\left\|Y\bar{\xi}_Y^* + \bar{\xi}_Y Y^*\right\|_F^2}{g_Y^i\left(\bar{\xi}_Y, \bar{\xi}_Y\right)}.$$

So the estimates of SOT for quotient manifold reduces to analyzing $\frac{\left\|Y\bar{\xi}_Y^* + \bar{\xi}_Y Y^*\right\|_F^2}{g_Y^i\left(\bar{\xi}_Y, \bar{\xi}_Y\right)}$. We denote its infimum and supremum by

$$C_{\pi(Y)}^i := \inf_{\xi_{\pi(Y)} \in T_{\pi(Y)}\mathbb{C}_*^{n\times p}/\mathcal{O}_p} \frac{\left\|Y\bar{\xi}_Y^* + \bar{\xi}_Y Y^*\right\|_F^2}{g_Y^i(\bar{\xi}_Y, \bar{\xi}_Y)}, D_{\pi(Y)}^i := \sup_{\xi_{\pi(Y)} \in T_{\pi(Y)}\mathbb{C}_*^{n\times p}/\mathcal{O}_p} \frac{\left\|Y\bar{\xi}_Y^* + \bar{\xi}_Y Y^*\right\|_F^2}{g_Y^i(\bar{\xi}_Y, \bar{\xi}_Y)}.$$

The subscript is used to emphasize that the infimum and supremum are dependent on $\pi(Y)$. The next lemma characterizes these infimum and supremum.

Lemma 4.4. *Let $YY^* = U\Sigma U^*$ denote the compact SVD of YY^* and denote the i-th diagonal entry of Σ by σ_i with $\sigma_1 \geq \cdots \geq \sigma_p > 0$. Then the following estimates for the infimum $C_{\pi(Y)}^i$ and the supremum $D_{\pi(Y)}^i$ of $\frac{\left\|Y\bar{\xi}_Y^* + \bar{\xi}_Y Y^*\right\|_F^2}{g_Y^i\left(\bar{\xi}_Y, \bar{\xi}_Y\right)}$ hold: $C_{\pi(Y)}^1 = 2\sigma_p, 2\sigma_1 \leq D_{\pi(Y)}^1 \leq 2\left(\frac{\sigma_1^2}{\sigma_p} + \sigma_1\right)$; $C_{\pi(Y)}^2 = 2, D_{\pi(Y)}^2 = 4$; and $C_{\pi(Y)}^3 = D_{\pi(Y)}^3 = 1$.*

Next we estimate the FOTs in Rayleigh quotient.

Lemma 4.5. *Let $X = YY^*$ for any $Y \in \pi^{-1}(\pi(Y))$ with $X \in \mathcal{H}_+^{n,p}$ and $\pi(Y) \in \mathbb{C}_*^{n\times p}/\mathcal{O}_p$. Let $U\Sigma U^*$ be the compact SVD of X and denote the i-th diagonal entry of Σ with $\sigma_1 \geq \cdots \geq \sigma_p > 0$.*

1. *For the embedded manifold we have $|FOT| \leq \frac{2}{\sigma_p}\|\nabla f(X)\|$.*
2. *For the quotient manifold with metric g^1 we have $|FOT| \leq 2\|\nabla f(YY^*)\|$.*
3. *For the quotient manifold with g^2 we have $|FOTs| \leq \frac{4(\sqrt{p}+1)}{\sigma_p}\|\nabla f(YY^*)\|$.*
4. *For the quotient manifold with g^3 we have $|FOTs| \leq \frac{1}{\sigma_p}\|\nabla f(YY^*)\|$.*

The proofs for Lemma 4.5 and Lemma 4.4 are given in Appendix C. With Lemma 4.5 and Lemma 4.4, the proof of Theorem 4.1 is concluded.

4.2 The Rayleigh quotient for a rank-deficient minimizer

Next, we consider the rank deficient case $p > r$ where r is the rank of the minimizer $\hat{X}$, i.e., the minimizer $\hat{X}$ lies on the boundary of the constraint manifold. Under the Assumption $\nabla f(\hat{X}) = 0$, any convergent algorithm that solves (1) or (11) will generate a sequence such that both $\sigma_{r+1}, \cdots, \sigma_p$ and $\nabla f(X)$ will vanish as $X \to \hat{X}$. We make one more assumption for a simpler quantification of the lower and upper bounds of Rayleigh quotient near the minimizer.

Assumption 4.2. *For a sequence* $\{X_k\}$ *with* $X_k \in \mathcal{H}_+^{n,p}$ *(or* $\pi(Y_k) \in \mathbb{C}_*^{n\times p}/\mathcal{O}_p$ *) that converges to the minimizer* $\hat{X}$ *(or* $\pi(\hat{Y})$*), let* $(\sigma_p)_k$ *be the smallest nonzero singular value of* $X_k = Y_k Y_k^*$*, assume the following limits hold.*

1. *For the embedded manifold,* $\lim_{k\to\infty} \frac{2}{(\sigma_p)_k} \|\nabla f(X_k)\| \le \frac{A}{2}$.
2. *For the quotient manifold with metric* g^1, $\lim_{k\to\infty} \frac{1}{(\sigma_p)_k} \|\nabla f(Y_k Y_k^*)\| \le \frac{A}{2}$.
3. *For the quotient manifold with metric* g^2, $\lim_{k\to\infty} \frac{4(\sqrt{p}+1)}{(\sigma_p)_k} \|\nabla f(Y_k Y_k^*)\| \le A$.
4. *For the quotient manifold with metric* g^3, $\lim_{k\to\infty} \frac{1}{(\sigma_p)_k} \|\nabla f(Y_k Y_k^*)\| \le \frac{A}{2}$.

We remark that Assumption 4.2 may not always hold. In the next section, we will give some numerical evaluation of this assumption for four examples listed in Figure 3 (eigenvalue problem), Figure 5 (matrix completion), Figure 7 (phase retrieval), and Figure 9 (interferometry recovery). Assumption 4.2 holds numerically in most of these tests.

If $\hat{X}$ has rank $r < p$ and $\{X_k\}$ is a sequence that satisfies Assumption 4.2, then Theorem 4.1 implies

1. For the embedded manifold we have $\frac{A}{2} \le \lim_{k\to\infty} \rho^E(X_k, \xi_{X_k}) \le B + \frac{A}{2}$.
2. $A \le \lim_{k\to\infty} \frac{\rho^1(\pi(Y_k), \xi_{\pi(Y_k)})}{(\sigma_p)_k} \le B \lim_{k\to\infty} \frac{D^1_{\pi(Y_k)}}{(\sigma_p)_k} + 2A$,
3. $A \le \lim_{k\to\infty} \rho^2(\pi(Y_k), \xi_{\pi(Y_k)}) \le 4B + A$,
4. $\frac{A}{2} \le \lim_{k\to\infty} \rho^3(\pi(Y_k), \xi_{\pi(Y_k)}) \le B + \frac{A}{2}$,

where $\lim\limits_{k\to\infty} \frac{D^1_{\pi(Y_k)}}{(\sigma_p)_k} \ge \lim\limits_{k\to\infty} \frac{2(\sigma_1)_k}{(\sigma_p)_k} = +\infty$ since $\sigma_p \to \hat{\sigma}_p = 0$.

Notice that the condition number in the Bures-Wasserstein metric g^1 is fundamentally different from the other ones since it is the only metric where the condition number may blow up.

5 Numerical experiments

In this section, we report on the numerical performance of the Riemannian conjugate gradient methods on four kinds of cost functions of $f(X)$: eigenvalue problem, matrix completion, phase-retrieval, and interferometry. In particular, we implement and compare the following five algorithms:

1. Burer–Monteiro L-BFGS method, that is, using the L-BFGS method directly applied to (5). This method was used in [8].
2. Riemannian CG on the quotient manifold $(\mathbb{C}_*^{n\times p}/\mathcal{O}_p, g^1)$, i.e., Algorithm 2 with metric g^1. **This algorithm is equivalent to CG applied directly to Burer–Monteiro formulation (5).**
3. Riemannian CG on the quotient manifold $(\mathbb{C}_*^{n\times p}/\mathcal{O}_p, g^2)$, i.e., Algorithm 2 with metric g^2. The same metric g^2 was used in [15].
4. Riemannian CG on the quotient manifold $(\mathbb{C}_*^{n\times p}/\mathcal{O}_p, g^3)$, i.e., Algorithm 2 with metric g^3.

5. Riemannian CG on the embedded manifold, i.e., Algorithm 1, which is equivalent to Riemannian CG on the quotient manifold $(\mathbb{C}_*^{n\times p}/\mathcal{O}_p, g^3)$, i.e., Algorithm 2 with metric g^3 using a specific retraction, vector transport and initial step as described in Section 3.2.

5.1 Eigenvalue problem

For any n-by-n Hermitian PSD matrix A, its top p eigenvalues and associated eigenvectors can be found by solving (1) with $f(X) = \frac{1}{2}\|X - A\|_F^2$ or equivalently (11) with $h(\pi(Y)) = \frac{1}{2}\|YY^* - A\|_F^2$. It is easy to verify that

$$\nabla f(X) = X - A, \quad \nabla^2 f(X)[\zeta_X] = \zeta_X, \quad \zeta_X \in \mathbb{C}^{n\times n}.$$

In practice we only need A as an operator $A : v \mapsto Av$. We consider a numerical test for a random Hermitian PSD matrix A of size 50 000-by-50 000 with rank 10. We solve the minimization problem above with $p = 15$. Obviously, the minimizer is rank-10 thus rank deficient for $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ with $p = 15$. This corresponds to a scenario of finding the eigenvalue decomposition of a low rank Hermitian PSD matrix A with estimated rank at most 15. The results are shown in Figure 1. The initial guess is the same random initial matrix for all four algorithms. We see that the simpler Burer–Monteiro approach, including the L-BFGS method and the CG method with metric g^1, is significantly slower.

In the second test of Figure 2, the minimizer has rank $r = 15$, and the fixed rank for the manifold is also set to $p = 15$; i.e., there is no rank deficiency. But the condition number of the minimizer A causes a difference in the asymptotic convergence rate for the CG method with metric g^1. In Figure 2(a), the condition number of A is large and we observe a slower asymptotic convergence rate for the CG method with metric g^1; while in Figure 2(b), the condition number of A is smaller and the asymptotic convergence rate becomes much faster. This is consistent with Theorem 4.1. In the third test of Figure 3, we show the ratio term $\frac{\|\nabla f(Y_k Y_k^*)\|}{(\sigma_p)_k}$ in Assumption 4.2 versus the iteration number k. This ratio does not blow up as $\pi(Y_k)$ converges to $\pi(\hat{Y})$.

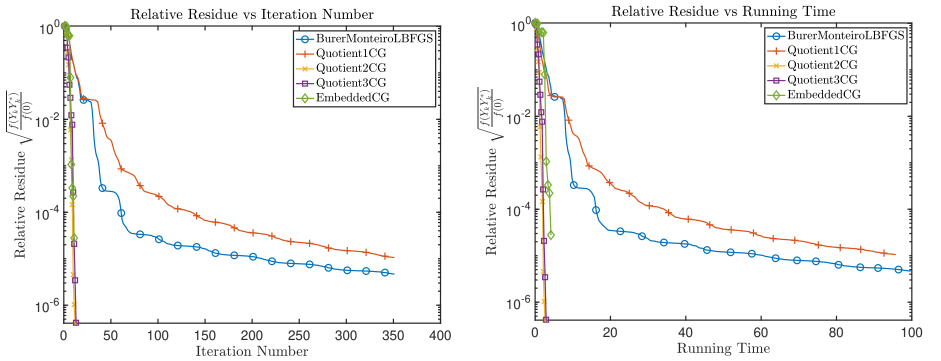
5.2 Matrix completion

Let Ω be a subset of of the complete set $\{1, \cdots, n\} \times \{1, \cdots, n\}$. Then the projection operator onto Ω is a sampling operator defined as

$$P_\Omega : \mathbb{C}^{n\times n} \to \mathbb{C}^{n\times n} : X_{i,j} \mapsto \begin{cases} X_{i,j} & \text{if } (i,j) \in \Omega, \\ 0 & \text{if } (i,j) \notin \Omega. \end{cases}$$

We consider a matrix completion problem under Hermitian constraint by solving (1) with $f(X) = \frac{1}{2}\|P_\Omega(X - A)\|_F^2$ or equivalently (11) with $h(\pi(Y)) = \frac{1}{2}\|P_\Omega(YY^* - A)\|_F^2$. Straightforward calculation shows

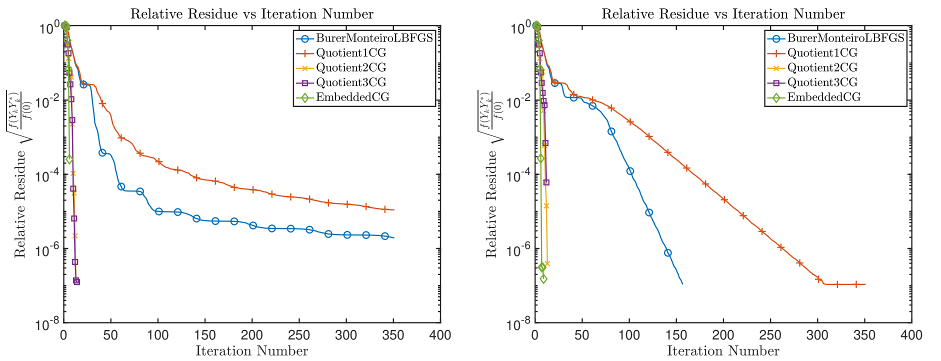
$$\nabla f(X) = P_\Omega(X - A), \quad \nabla^2 f(X)[\zeta_X] = P_\Omega(\zeta_X), \quad \zeta_X \in \mathbb{C}^{n\times n}.$$



(a) Relative Residue vs Iteration Number

(b) Relative Residue vs Running Time (CPU Time in seconds)

Fig. 1 Eigenvalue problem of a random 50 000-by-50 000 PSD matrix of rank 10 solved on the rank 15 manifold: a comparison of relative residue $\frac{\|Y_k Y_k^* - A\|_F}{\|A\|_F}$ decrease versus iteration number k and running time when using L-BFGS approach, quotient CG method with metric $g^i, i = 1, 2, 3$ and embedded CG method.



(a) $\frac{\hat{\sigma}_1}{\hat{\sigma}_p} = 10^7$

(b) $\frac{\hat{\sigma}_1}{\hat{\sigma}_p} = 10^2$

Fig. 2 Numerical justification of Theorem 4.1 for the eigenvalue problem of a random 50 000-by-50 000 PSD matrix of rank 15 on the rank 15 manifold. Effect of condition number of A on the convergence speed of relative residue $\frac{\|Y_k Y_k^* - A\|_F}{\|A\|_F}$ versus iteration number k. (a): when the condition number of A is large, Burer-Monteiro LBFGS and CG with metric g^1 is slower; (b): when the condition number of A is smaller, CG with metric g^1 becomes faster.

We consider a Hermitian PSD matrix $A \in \mathbb{C}^{n\times n}$ with $n = 10\,000$ and P_Ω a random 60% sampling operator. In the first test of Figure 4(a), the minimizer has rank $r = 25$, and the fixed rank for the manifold is set to $p = 30$. In the second test of Figure 4(b), the minimizer has rank $r = 25$, and the fixed rank for the manifold is set to $p = 25$. The initial guess is the same random matrix for all four algorithms. For both cases, we see that the simpler Burer–Monteiro approach, including the L-BFGS method and the CG method with metric g^1, is significantly slower.

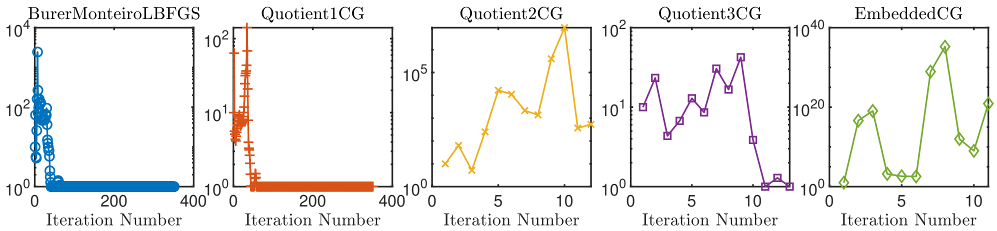
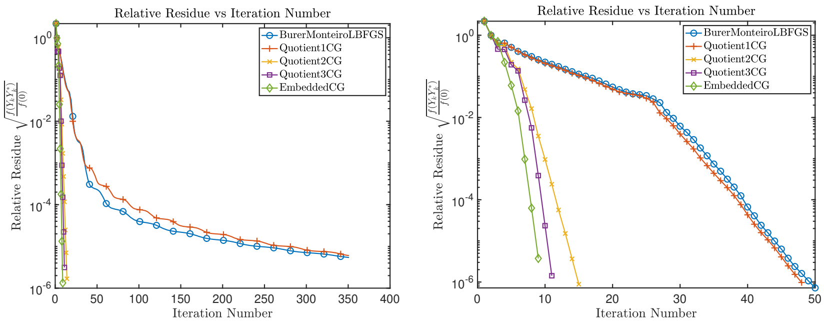


Fig. 3 Numerical examination of Assumption 4.2 for the eigenvalue problem of a random 50 000-by-50 000 PSD matrix of rank 10 on the rank 15 manifold, same setup as the numerical test shown in Fig 1. Plots show the ratio term $\frac{\|\nabla f(Y_k Y_k^*)\|_F}{(\sigma_p)_k}$ in Assumption 4.2 versus the iteration number k for L-BFGS approach, quotient CG method with metric $g^i, i = 1, 2, 3$ and embedded CG method.

In the third test of Figure 5, we show that the ratio term $\frac{\|\nabla f(Y_k Y_k^*)\|}{(\sigma_p)_k}$ in Assumption 4.2 versus the iteration number k does not blow up as $\pi(Y_k)$ converges to $\pi(\hat{Y})$.



(a) The algorithms are solved on the rank 30 manifold

(b) The algorithms are solved on the rank 25 manifold

Fig. 4 Matrix completion of a random 10 000-by-10 000 PSD matrix of rank 25 observed at random 60% entries. A comparison of decrease in relative residue $\frac{\|P_\Omega(Y_k Y_k^* - A)\|_F}{\|P_\Omega(A)\|_F}$ versus iteration number k when using L-BFGS approach, quotient CG method with metric $g^i, i = 1, 2, 3$ and embedded CG method. When the minimizer is rank deficient (the case in (a)), L-BFGS approach and CG method with metric g^1 is significantly slower.

5.3 The phase retrieval problem

We now solve the phase retrieval problem as described in [5]. Take an image $x \in \mathbb{C}^{n\times 1}$ and by lifting $X := xx^*$, the cost function can be written as

$$f(X) = \frac{1}{2} \|\mathcal{A}(X) - b\|^2 ,$$

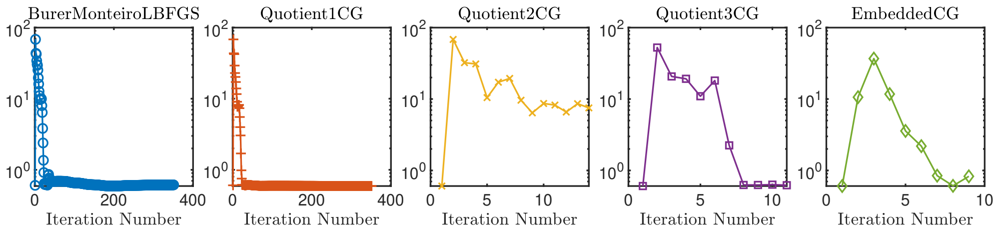


Fig. 5 Numerical examination of Assumption 4.2 for the matrix completion problem of a random 10 000-by-10 000 PSD matrix of rank 25 observed at random 60% entries solved on the rank 30 manifold (same setup as the numerical test shown in Fig 4(a)). Plots show the ratio term $\frac{\|\nabla f(Y_k Y_k^*)\|_F}{(\sigma_p)_k}$ in the Assumption 4.2 versus the iteration number k for L-BFGS approach, quotient CG method with metric $g^i, i = 1, 2, 3$ and embedded CG method.

where $\mathcal{A} : \mathbb{C}^{n\times n} \to \mathbb{R}^{mn\times 1}, \quad X \mapsto [\mathrm{diag}(Z^1 X Z^{1*}), \cdots, \mathrm{diag}(Z^m X Z^{m*})]^T$ with given $Z^i \in \mathbb{C}^{n\times n}$. See [9] for the complete definition of $\mathcal{A}$. The conjugate of operator $\mathcal{A}$, denoted by $\mathcal{A}^*$ can be shown to be

$$A^*(b) = \begin{cases} \displaystyle\sum_{i=1}^{m}\sum_{j=1}^{n} b_j^i z_j^i {z_j^i}^* = \sum_{i=1}^{m} {Z^i}^* \,\mathrm{Diag}(b^i) Z^i, & \text{if domain of } \mathcal{A} \text{ is } \mathbb{C}^{n\times n} \\ \Re\left(\displaystyle\sum_{i=1}^{m}\sum_{j=1}^{n} b_j^i z_j^i {z_j^i}^*\right) = \Re\left(\sum_{i=1}^{m} {Z^i}^* \,\mathrm{Diag}(b^i) Z^i\right), & \text{if domain of } \mathcal{A} \text{ is } \mathbb{R}^{n\times n}. \end{cases}$$

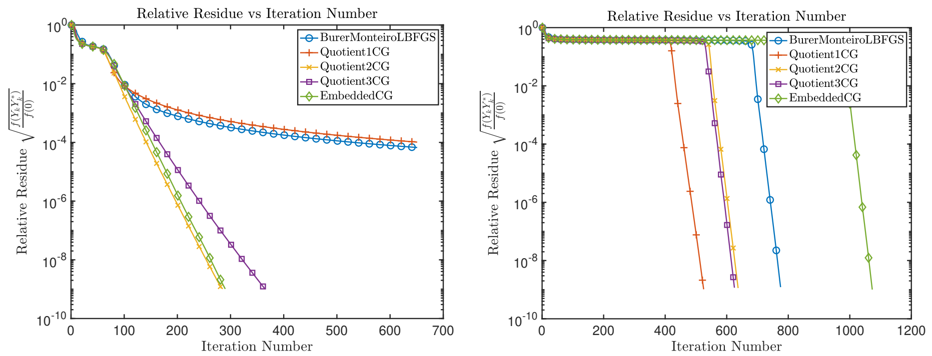
Straightforward calculation shows

$$\nabla f(X) = \mathcal{A}^*(\mathcal{A}(X) - b), \quad \nabla^2 f(X)[\zeta_X] = \mathcal{A}^*(\mathcal{A}(\zeta_X)) \quad \text{for all } \zeta_X \in \mathbb{C}^{n\times n}.$$

For the numerical experiments, we take the phase retrieval problem for a complex gold ball image of size 256×256 as in [15]. Thus $n = 256^2 = 65,536$ in (2) or (1). We consider the operator $\mathcal{A}$ that corresponds to 6 Gaussian random masks. Hence, the size of b is $6n = 393,216$. Remark that problem is easier to solve with more masks.

We first test the algorithms on the rank 3 manifold, and then on the rank 1 manifolds. The results are visible in Figure 6. The initial guess is randomly generated. First, we observe that solving the PhaseLift problem on the rank p manifold with $p > 1$ can accelerate the convergence, compared to solving it on the rank 1 manifold. Second, when $p = r = 1$, the asymptotic convergence rates of all algorithms are essentially the same, though the algorithms differ in the length of their convergence "plateaus". When $p = 3 > r = 1$, we can see that the Burer–Monteiro approach has slower asymptotic convergence rates.

In the second test of Figure 7, we show that the ratio term $\frac{\|\nabla f(Y_k Y_k^*)\|}{(\sigma_p)_k}$ in Assumption 4.2 versus the iteration number k does not blow up as $\pi(Y_k)$ converges to $\pi(\hat{Y})$.



(a) The algorithms are solved on the rank 3 manifold

(b) The algorithms are solved on the rank 1 manifold

Fig. 6 Phase retrieval of a 256-by-256 image with 6 Gaussian masks. A comparison of relative residue $\frac{\|\mathcal{A}(Y_k Y_k^*)-b\|}{\|b\|}$ versus iteration number k when using L-BFGS approach, quotient CG method with metric $g^i, i = 1, 2, 3$ and embedded CG method. When the minimizer is rank deficient (the case in 6(a)), L-BFGS approach and CG method with metric g^1 is significantly slower.

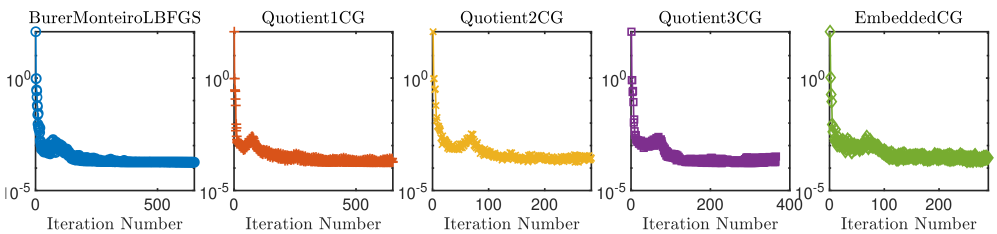


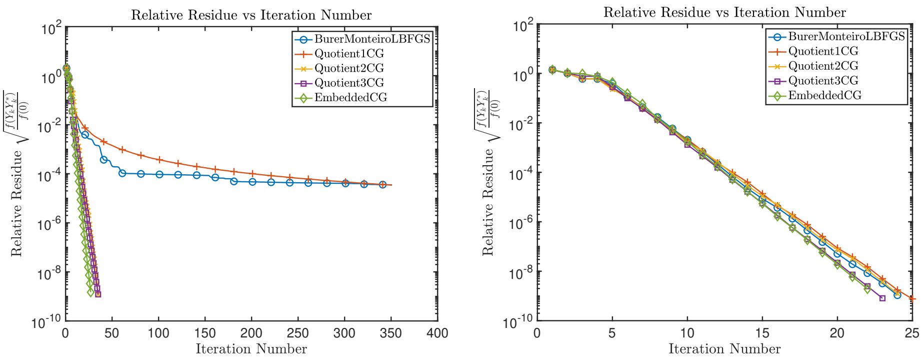
Fig. 7 Numerical examination of Assumption 4.2 for the phase retrieval problem of a 256-by-256 image with 6 Gaussian masks solved on the rank 3 manifold (same setup as the numerical test shown in Fig 6(a)). Plots show the ratio term $\frac{\|\nabla f(Y_k Y_k^*)\|_F}{(\sigma_p)_k}$ in the Assumption 4.2 versus the iteration number k for L-BFGS approach, quotient CG method with metric $g^i, i = 1, 2, 3$ and embedded CG method.

5.4 Interferometry recovery problem

As the last example, we consider solving the interferometry recovery problem described in [8]. Consider solving the linear system $Fx = d$ where $F \in \mathbb{C}_*^{m\times n}$ with $m > n$ and $x \in \mathbb{C}^{n\times 1}$. For the sake of robustness, the interferometry recovery [8] requires solving the lifted problem (1) with $f(X) = \frac{1}{2}\|P_\Omega(FXF^* - dd^*)\|_F^2$ or equivalently (11) with $h(\pi(Y)) = \frac{1}{2}\|P_\Omega(FYY^*F^* - dd^*)\|_F^2$, Ω is a sparse and symmetric sampling index that includes all of the diagonals. Straightforward calculation again shows

$$\nabla f(X) = F^* P_\Omega(FXF^* - dd^*)F, \quad \nabla^2 f(X)[\zeta_X] = F^* P_\Omega(F\zeta_X F^*)F \quad \text{for all } \zeta_X \in \mathbb{C}^{n\times n}.$$

We solve an interferometry problem with a randomly generated $F \in \mathbb{C}^{10\,000\times 1000}$, with $n = 1000$ in (2) or (1). The sampling operator Ω is also randomly generated, with 1% density. In Figure 8(a), for $p = 3$ and $r = 1$, we can see that the Burer–Monteiro approach has slower asymptotic convergence rates. In Figure 8(b), for $p = r = 1$, we can see that all algorithms have more or less the same asymptotic convergence rates. In Figure 9, we show that the ratio term $\frac{\|\nabla f(Y_k Y_k^*)\|}{(\sigma_p)_k}$ in Assumption 4.2 does not blow up as $\pi(Y_k)$ converges to $\pi(\hat{Y})$.



(a) The algorithms are solved on the rank 3 manifold

(b) The algorithms are solved on the rank 1 manifold

Fig. 8 Interferometry recovery of a random 10 000-by-1000 F with 1% sampling. A comparison of relative residue $\frac{\|P_\Omega(FY_kY_k^*F^* - dd^*)\|_F}{\|P_\Omega(dd^*)\|_F}$ versus iteration number k when using L-BFGS approach, quotient CG method with metric $g^i, i = 1, 2, 3$ and embedded CG method. When the minimizer is rank deficient (the case in (a)), L-BFGS approach and CG method with metric g^1 is significantly slower.

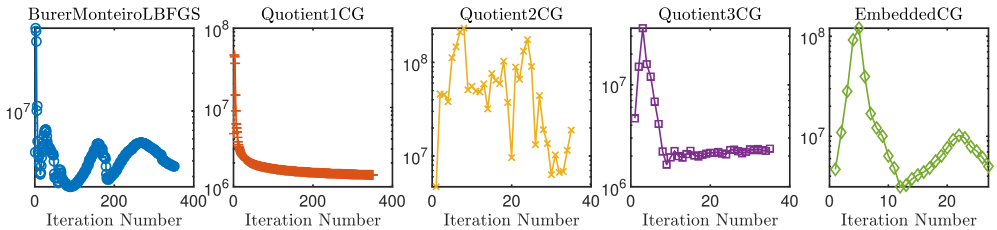


Fig. 9 Numerical examination of Assumption 4.2 for the interferometry recovery problem of a random 10 000-by-1000 F with 1% sampling solved on a rank 3 manifold. (same setup as the numerical test shown in Fig 8(a)). Plots show the ratio term $\frac{\|\nabla f(Y_kY_k^*)\|_F}{(\sigma_p)_k}$ in the Assumption 4.2 versus the iteration number k for L-BFGS approach, quotient CG method with metric $g^i, i = 1, 2, 3$ and embedded CG method.

6 Concluding remarks

We have shown that the CG method on the Burer–Monteiro formulation for Hermitian PSD fixed-rank constraints is equivalent to a Riemannian CG method on a quotient manifold with the Bures-Wasserstein metric g^1. We have also shown that the Riemannian conjugate gradient method on the embedded geometry of $\mathcal{H}_+^{n,p}$ is equivalent to a Riemannian conjugate gradient method on a quotient manifold $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ with a metric g^3. We have analyzed the condition numbers of the Riemannian Hessians on $(\mathbb{C}_*^{n\times p}/\mathcal{O}_p, g^i)$ for three metrics. We have shown that when the rank p of the optimization manifold is larger than the rank of the minimizer to the original PSD constrained minimization, the condition number of the Riemannian Hessian on $(\mathbb{C}_*^{n\times p}/\mathcal{O}_p, g^1)$ can be unbounded, which is consistent with the observation that the Burer–Monteiro approach or Bures-Wasserstein metric often has a slower asymptotic convergence rate in numerical tests.

Acknowledgments

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Declarations

All authors declare that they have no conflict of interest.

Data Availability

The code and the data that support the findings of this study are available from the corresponding author upon request.

Appendix A Calculation for Riemannian Hessian of Embedded manifold $\mathcal{H}_+^{n,p}$

Let f be a smooth real-valued function on $\mathcal{H}_+^{n,p}$. In this section we derive the Riemannian Hessian operator of f.

By [30, Sect. 4] we know that the retraction R by projection is a second-order retraction. [29, Prop. 5.5.5] states that if R is a second-order retraction, then the Riemannian Hessian of f can be computed by $\operatorname{Hess} f(X) = \operatorname{Hess}(f \circ R_X)(0_X)$. Thus $g_X(\operatorname{Hess} f(X)[\xi_X], \xi_X) = \frac{d^2}{dt^2} f(R_X(t\xi_X))\Big|_{t=0}$.

In [4] and [17], a method was proposed to compute $\operatorname{Hess} f(X)$ by constructing a second-order retraction $R^{(2)}$ that has a second-order series expansion which makes it simple to derive a series expansion of $f \circ R_X^{(2)}$ up to second order and thus obtain the Hessian of f. Following [4, Prop. 5.10], we have

Lemma A.1. *$\forall X \in \mathcal{H}_+^{n,p}$, the mapping $R_X^{(2)} : T_X\mathcal{H}_+^{n,p} \to \mathcal{H}_+^{n,p}$*

$$\xi_X \mapsto wX^\dagger w^*, \text{ with } w = X + \frac{1}{2}\xi_X^s + \xi_X^p - \frac{1}{8}\xi_X^s X^\dagger \xi_X^s - \frac{1}{2}\xi_X^p X^\dagger \xi_X^s,$$

is a second-order retraction on $\mathcal{H}_+^{n,p}$, where $X^\dagger$ is the pseudoinverse, $\xi_X^s = P_X^s(\xi_X)$ and $\xi_X^p = P_X^p(\xi_X)$ as defined in (9). Moreover, we have

$$R_X^{(2)}(\xi_X) = X + \xi_X + \xi_X^p X^\dagger \xi_X^p + O(\|\xi_X\|^3).$$

From this the Riemannian Hessian operator of f can be computed in essentially the same way as in [31, Sect. A.2] but applied to the general cost function $f(X)$ instead of a least square cost function. Consider the Taylor expansion of $\hat{f}_X^{(2)} := f \circ R_X^{(2)}$, which is a real-valued function on a vector space. We get

$$\begin{aligned}
&\hat{f}_X^{(2)}(\xi_X) = f(R_X^{(2)}(\xi_X)) = f\left(X + \xi_X + \xi_X^p X^\dagger \xi_X^p + O(\|\xi_X\|^3)\right) \\
&= f(X) + \langle \nabla f(X), \xi_X + \xi_X^p X^\dagger \xi_X^p \rangle_{\mathbb{C}^{n\times n}} + \tfrac{1}{2}\langle \nabla^2 f(X)[\xi_X + \xi_X^p X^\dagger \xi_X^p], \xi_X + \xi_X^p X^\dagger \xi_X^p \rangle_{\mathbb{C}^{n\times n}} + O(\|\xi_X\|^3) \\
&= f(X) + \langle \nabla f(X), \xi_X \rangle_{\mathbb{C}^{n\times n}} + \langle \nabla f(X), \xi_X^p X^\dagger \xi_X^p \rangle_{\mathbb{C}^{n\times n}} + \tfrac{1}{2}\langle \nabla^2 f(X)[\xi_X], \xi_X \rangle_{\mathbb{C}^{n\times n}} + O(\|\xi_X\|^3).
\end{aligned}$$

We can immediately recognize the first-order term and the second-order term that contribute to the Riemannian gradient and Hessian, respectively. That is,

$$\begin{aligned}
&g_X(\operatorname{grad} f(X), \xi_X) = \langle \nabla f(X), \xi_X \rangle_{\mathbb{C}^{n\times n}} \Rightarrow \operatorname{grad} f(X) = P_X^t(\nabla f(X)), \\
&g_X(\operatorname{Hess} f(X)[\xi_X], \xi_X) = \underbrace{2\langle \nabla f(X), \xi_X^p X^\dagger \xi_X^p \rangle_{\mathbb{C}^{n\times n}}}_{f_1 := \langle \mathcal{H}_1(\xi_X), \xi_X \rangle_{\mathbb{C}^{n\times n}}} + \underbrace{\langle \nabla^2 f(X)[\xi_X], \xi_X \rangle_{\mathbb{C}^{n\times n}}}_{f_2 := \langle \mathcal{H}_2(\xi_X), \xi_X \rangle_{\mathbb{C}^{n\times n}}}.
\end{aligned}$$

Since ξ_X is already separated in f_2, the contribution to Riemannian Hessian from $\mathcal{H}_2$ is readily given by $\mathcal{H}_2(\xi_X) = P_X^t(\nabla^2 f(X)[\xi_X])$.

Now, we still need to separate ξ_X in f_1 to see the contribution to Riemannian Hessian from $\mathcal{H}_1$. Since we can choose to bring over $\xi_X^p X^\dagger$ or $X^\dagger \xi_X^p$ to the first position of $\langle .,. \rangle_{\mathbb{C}^{n\times n}}$, we write $\mathcal{H}_1(\xi_X)$ as the linear combination of both:

$$f_1 = 2c \left\langle \nabla f(X)(X^\dagger \xi_X^p)^*, \xi_X^p \right\rangle_{\mathbb{C}^{n\times n}} + 2(1-c) \left\langle (\xi_X^p X^\dagger)^* \nabla f(X), \xi_X^p \right\rangle_{\mathbb{C}^{n\times n}}.$$

Operator $\mathcal{H}_1$ is clearly linear. Since $\mathcal{H}_1$ is symmetric, we must have $\langle \mathcal{H}_1(\xi_X), \nu_X \rangle_{\mathbb{C}^{n\times n}} = \langle \nu_X, \mathcal{H}_1(\xi_X) \rangle_{\mathbb{C}^{n\times n}}$ for all tangent vector ν_X. Hence we must have $c = \frac{1}{2}$ and we obtain

$$\mathcal{H}_1(\xi_X) = P_X^p \left(\nabla f(X)(X^\dagger \xi_X^p)^* + (\xi_X^p X^\dagger)^* \nabla f(X) \right).$$

$$\operatorname{Hess} f(X)[\xi_X] = P_X^t(\nabla^2 f(X)[\xi_X]) + P_X^p \left(\nabla f(X)(X^\dagger \xi_X^p)^* + (\xi_X^p X^\dagger)^* \nabla f(X) \right).$$

Appendix B Calculations for Riemannian Hessian of Quotient manifold $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$

In this section, we outline the computations of the Riemannian Hessian operators of the cost function h defined on $\mathbb{C}_*^{n\times p}/\mathcal{O}_p$ under the three different metrics g^i.

Definition B.1. *[29, Def. 5.5.1] Given a real-valued function f on a Riemannian manifold $\mathcal{M}$, the Riemannian Hessian of f at a point x in $\mathcal{M}$ is the linear mapping Hess $f(x)$ of $T_x\mathcal{M}$ into itself defined by Hess $f(x)[\xi_x] = \nabla_{\xi_x} \operatorname{grad} f(x)$. for all ξ_x in $T_x\mathcal{M}$, where ∇ is the Riemannian connection on $\mathcal{M}$.*

Lemma B.1. *The Riemannian Hessian of $h : \mathbb{C}_*^{n\times p}/\mathcal{O}_p \mapsto \mathbb{R}$ is related to the Riemannian Hessian of $F : \mathbb{C}_*^{n\times p} \mapsto \mathbb{R}$ in the following way: $\overline{\left(\operatorname{Hess} h(\pi(Y))[\xi_{\pi(Y)}]\right)}_Y = P_Y^{\mathcal{H}} \left(\operatorname{Hess} F(Y)[\overline{\xi}_Y]\right)$, where $\overline{\xi}_Y$ is the horizontal lift of $\xi_{\pi(Y)}$ at Y.*

Proof. The result follows from [29, Prop. 5.3.3] and the definition of the Riemannian Hessian. □

B.1 Riemannian Hessian for the metric g^1

Using the Riemannian metric g^1, $\mathbb{C}_*^{n\times p}$ is a Riemannian submanifold of a Euclidean space. By [29, Prop. 5.3.2], the Riemannian connection on $\mathbb{C}_*^{n\times p}$ is the classical directional derivative $\nabla_{\eta_Y} \xi = \mathrm{D}\, \xi(Y)[\eta_Y]$. Recall that for g^1, $\operatorname{grad} F(Y) = 2\nabla f(YY^*)Y$. Thus

$$\operatorname{Hess} F(Y)[\xi_Y] = \nabla_{\xi_Y} \operatorname{grad} F = \mathrm{D} \operatorname{grad} F(Y)[\xi_Y] = 2\nabla^2 f(YY^*)[Y\xi_Y^* + \xi_Y Y^*]Y + 2\nabla f(YY^*)\xi_Y.$$

Therefore we obtain by B.1 that

$$\overline{\left(\operatorname{Hess} h(\pi(Y))[\xi_{\pi(Y)}]\right)}_Y = P_Y^{\mathcal{H}^1} \left(2\nabla^2 f(YY^*)[Y\overline{\xi}_Y^* + \overline{\xi}_Y Y^*]Y + 2\nabla f(YY^*)\overline{\xi}_Y \right).$$

B.2 Riemannian Hessian under metric g^2

First, for any Riemannian metric g, g satisfies the Koszul formula

$$2g_x(\nabla_{\xi_x}\lambda, \eta_x) = \xi_x g(\lambda,\eta) + \lambda_x g(\eta,\xi) - \eta_x g(\xi,\lambda) - g_x(\xi_x, [\lambda,\eta]_x) + g_x(\lambda_x, [\eta,\xi]_x) + g_x(\eta, [\xi,\lambda]_x)$$

$$= \mathrm{D}\, g(\lambda,\eta)(x)[\xi_x] + \mathrm{D}\, g(\eta,\xi)(x)[\lambda_x] - \mathrm{D}\, g(\xi,\lambda)(x)[\eta_x] - g_x(\xi_x,[\lambda,\eta]_x) + g_x(\lambda_x,[\eta,\xi]_x) + g_x(\eta,[\xi,\lambda]_x),$$

where $[\cdot,\cdot]$ is the *Lie bracket*. In particular, for g^2 the Koszul formula turns into

$$2g^2_Y(\nabla_{\xi_Y}\lambda,\eta_Y) = \mathrm{D}\, g^2(\lambda,\eta)(Y)[\xi_Y] + \mathrm{D}\, g^2(\eta,\xi)(Y)[\lambda_Y] - \mathrm{D}\, g^2(\xi,\lambda)(Y)[\eta_Y] - g^2_Y(\xi_Y,[\lambda,\eta]_Y) + g^2_Y(\lambda_Y,[\eta,\xi]_Y) + g^2_Y(\eta,[\xi,\lambda]_Y).$$

Recall that $g^2(\lambda,\eta)(Y) = \Re(\mathrm{tr}(Y^*Y\lambda_Y^*\eta_Y))$. The first term equals

$$\mathrm{D}\, g^2(\lambda,\eta)(Y)[\xi_Y] = g^2_Y(\mathrm{D}\,\lambda(Y)[\xi_Y],\eta_Y) + g^2_Y(\lambda_Y,\mathrm{D}\,\eta(Y)[\xi_Y]) + \Re(\mathrm{tr}(\xi_Y^*Y\lambda_Y^*\eta_Y)) + \Re(\mathrm{tr}(Y^*\xi_Y\lambda_Y^*\eta_Y)).$$

Following [29, Sect. 5.3.4], since $\mathbb{C}^{n\times p}_*$ is an open subset of $\mathbb{C}^{n\times p}$, we also have $[\lambda,\eta]_Y = \mathrm{D}\,\eta(Y)[\lambda_Y] - \mathrm{D}\,\lambda(Y)[\eta_Y]$. Thus we get

$$\begin{aligned}
&2g^2_Y(\nabla_{\xi_Y}\lambda,\eta_Y) = \mathrm{D}\, g^2(\lambda,\eta)(Y)[\xi_Y] + \mathrm{D}\, g^2(\eta,\xi)(Y)[\lambda_Y] - \mathrm{D}\, g^2(\xi,\lambda)(Y)[\eta_Y]\\
&\quad -g^2(\xi_Y,\mathrm{D}\,\eta(Y)[\lambda_Y] - \mathrm{D}\,\lambda(Y)[\eta_Y]) + g^2(\lambda_Y,\mathrm{D}\,\xi(Y)[\eta_Y] - \mathrm{D}\,\eta(Y)[\xi_Y]) + g^2(\eta_Y,\mathrm{D}\,\lambda(Y)[\xi_Y] - \mathrm{D}\,\xi(Y)[\lambda_Y])\\
&= 2g^2_Y(\eta_Y,\mathrm{D}\,\lambda(Y)[\xi_Y]) + \Re(\mathrm{tr}(\eta_Y^*(\lambda_Y(\xi_Y^*Y + Y^*\xi_Y) + \xi_Y(Y^*\lambda_Y + \lambda_Y^*Y) - Y\lambda_Y^*\xi_Y - Y\xi_Y^*\lambda_Y)))\\
&= 2g^2_Y(\eta_Y,\mathrm{D}\,\lambda(Y)[\xi_Y]) + g^2_Y(\eta_Y,(\lambda_Y(\xi_Y^*Y + Y^*\xi_Y) + \xi_Y(Y^*\lambda_Y + \lambda_Y^*Y) - Y\lambda_Y^*\xi_Y - Y\xi_Y^*\lambda_Y)(Y^*Y)^{-1}).
\end{aligned}$$

We therefore obtain a closed-form expression for Riemannian connection on $\mathbb{C}^{n\times p}_*$:

$$\nabla_{\xi_Y}\lambda = \mathrm{D}\,\lambda(Y)[\xi_Y] + \tfrac{1}{2}\left(\lambda_Y(\xi_Y^*Y + Y^*\xi_Y) + \xi_Y(Y^*\lambda_Y + \lambda_Y^*Y) - Y\lambda_Y^*\xi_Y - Y\xi_Y^*\lambda_Y\right)(Y^*Y)^{-1}.$$

Thus we have

$$\begin{aligned}
&\mathrm{Hess}\, F(Y)[\xi_Y] = \nabla_{\xi_Y}\mathrm{grad}\, F = \mathrm{D}\,{}_Y\mathrm{grad}\, F(Y)[\xi_Y]\\
&\quad +\tfrac{1}{2}\{\mathrm{grad}\, F(Y)(\xi_Y^*Y + Y^*\xi_Y) + \xi_Y(Y^*\mathrm{grad}\, F(Y) + \mathrm{grad}\, F(Y)^*Y) - Y\mathrm{grad}\, F(Y)^*\xi_Y - Y\xi_Y^*\mathrm{grad}\, F(Y)\}(Y^*Y)^{-1}\\
&= 2\nabla^2 f(YY^*)[Y\xi_Y^* + \xi_YY^*]Y(Y^*Y)^{-1} + 2\nabla f(YY^*)\xi_Y(Y^*Y)^{-1} - \nabla f(YY^*)Y(Y^*Y)^{-1}(Y^*\xi_Y + \xi_Y^*Y)(Y^*Y)^{-1}\\
&\quad +\xi_Y\{Y^*\nabla f(YY^*)Y(Y^*Y)^{-1} + (Y^*Y)^{-1}Y^*\nabla f(YY^*)Y\}(Y^*Y)^{-1} - \{Y(Y^*Y)^{-1}Y^*\nabla f(YY^*)\xi_Y + Y\xi_Y^*\nabla f(YY^*)Y(Y^*Y)^{-1}\}(Y^*Y)^{-1}\\
&= 2\nabla^2 f(YY^*)[Y\xi_Y^* + \xi_YY^*]Y(Y^*Y)^{-1} + \nabla f(YY^*)P_Y^{\perp}\xi_Y(Y^*Y)^{-1} + P_Y^{\perp}\nabla f(YY^*)\xi_Y(Y^*Y)^{-1}\\
&\quad +2\,\mathrm{Skew}(\xi_YY^*)\nabla f(YY^*)Y(Y^*Y)^{-2} + 2\,\mathrm{Skew}\{\xi_Y(Y^*Y)^{-1}Y^*\nabla f(YY^*)\}Y(Y^*Y)^{-1}.
\end{aligned}$$

B.2.1 Riemannian Hessian under metric g^3

Denote

$$\tilde{g}_Y(\xi_Y,\eta_Y) = \langle Y\xi_Y^* + \xi_YY^*, Y\eta_Y^* + \eta_YY^*\rangle_{\mathbb{C}^{n\times n}}.$$

Recall that the Riemannian metric g^3 on $\mathbb{C}^{n\times p}_*$ satisfies $g^3_Y(\xi_Y,\eta_Y) = \tilde{g}_Y(\xi_Y,\eta_Y) + g^2_Y(P_Y^{\mathcal{V}}(\xi_Y), P_Y^{\mathcal{V}}(\eta_Y))$. Hence $\mathrm{D}\, g^3(\lambda,\eta)(Y)[\xi_Y] =$

$$\begin{aligned}
&\tilde{g}_Y(\mathrm{D}\,\lambda(Y)[\xi_Y],\eta_Y) + \tilde{g}(\lambda_Y, D\eta(Y)[\xi_Y]) + 2\Re(\mathrm{tr}(\xi_Y^*\lambda_YY^*\eta_Y + Y^*\lambda_Y\xi_Y^*\eta_Y + \xi_Y^*Y\lambda_Y^*\eta_Y + Y^*\xi_Y\lambda_Y^*\eta_Y))\\
+\ & g^2_Y(P_Y^{\mathcal{V}}(\lambda_Y), DP_Y^{\mathcal{V}}(\eta_Y)[\xi_Y]) + g^2(\mathrm{D}\, P_Y^{\mathcal{V}}(\lambda_Y)[\xi_Y], P_Y^{\mathcal{V}}(\eta_Y)) + \Re(\mathrm{tr}(\xi_YP_Y^{\mathcal{V}}(\lambda_Y)^*P_Y^{\mathcal{V}}(\eta_Y)Y^* + YP_Y^{\mathcal{V}}(\lambda_Y)^*P_Y^{\mathcal{V}}(\eta_Y)\xi_Y^*)).
\end{aligned}$$

If λ,η and ξ are horizontal vector fields, many terms in the above equation vanish:

$$\mathrm{D}\, g^3(\lambda,\eta)(Y)[\xi_Y] = \tilde{g}_Y(\mathrm{D}\,\lambda(Y)[\xi_Y],\eta_Y) + \tilde{g}_Y(\lambda_Y,\mathrm{D}\,\eta_Y[\xi_Y])$$

$$+2\Re(\mathrm{tr}(\xi_Y^* \lambda_Y Y^* \eta_Y + Y^* \lambda_Y \xi_Y^* \eta_Y + \xi_Y^* Y \lambda_Y^* \eta_Y + Y^* \xi_Y \lambda_Y^* \eta_Y)).$$

Combining it with the Koszul formula with ξ, η, λ horizontal vector fields, we obtain

$$\begin{aligned}
&2g_Y^3(\nabla_{\xi_Y}\lambda, \eta_Y) = \mathrm{D}\, g^3(\lambda,\eta)(Y)[\xi_Y] + \mathrm{D}\, g^3(\eta,\xi)(Y)[\lambda_Y] - \mathrm{D}\, g^3(\xi,\lambda)(Y)[\eta_Y] \\
&-g_Y^3(\xi_Y, \mathrm{D}\,\eta(Y)[\lambda_Y] - \mathrm{D}\,\lambda(Y)[\eta_Y]) + g_Y^3(\lambda_Y, \mathrm{D}\,\xi(Y)[\eta_Y] - \mathrm{D}\,\eta(Y)[\xi_Y]) + g_Y^3(\eta_Y, \mathrm{D}\,\lambda(Y)[\xi_Y] - \mathrm{D}\,\xi(Y)[\lambda_Y]) \\
&= 2\tilde{g}_Y(\mathrm{D}\,\lambda(Y)[\xi_Y], \eta_Y) + 4\Re(\mathrm{tr}(Y^*\xi_Y\lambda_Y^*\eta_Y + Y^*\lambda_Y\xi_Y^*\eta_Y)).
\end{aligned}$$

$$g_Y^3(\nabla_{\xi_Y}\lambda, \eta_Y) = \tilde{g}_Y(\mathrm{D}\,\lambda(Y)[\xi_Y], \eta_Y) + 2\Re(\mathrm{tr}(Y^*\xi_Y\lambda_Y^*\eta_Y + Y^*\lambda_Y\xi^*\eta_Y)).$$

Recall $\mathrm{Hess}\, F(Y)[\xi_Y] = \nabla_{\xi_Y}\mathrm{grad}\, F$. For ξ_Y being a horizontal vector we have

$$\begin{aligned}
&g_Y^3(\mathrm{Hess}\, F(Y)[\xi_Y], \eta_Y) = g_Y^3(\nabla_{\xi_Y}\mathrm{grad}\, F, \eta_Y) \\
&= \tilde{g}(\eta_Y, \mathrm{D}\,\mathrm{grad}\, F(Y)[\xi_Y]) + 2\Re(\mathrm{tr}(Y^*\xi_Y \mathrm{grad}\, F(Y)^*\eta_Y + Y^*\mathrm{grad}\, F(Y)\xi_Y^*\eta_Y)) \\
&= \tilde{g}(\eta_Y, \mathrm{D}\,\mathrm{grad}\, F(Y)[\xi_Y]) + \Re(\mathrm{tr}((Y\eta_Y^* + \eta_Y Y^*)(\mathrm{grad}\, F(Y)\xi_Y^* + \xi_Y \mathrm{grad}\, F(Y)^*))) \\
&= \tilde{g}(\eta_Y, \mathrm{D}\,\mathrm{grad}\, F(Y)[\xi_Y]) + \tilde{g}\left(\eta_Y, \left(I - \tfrac{1}{2}P_Y\right)(\mathrm{grad}\, F(Y)\xi_Y^* + \xi_Y \mathrm{grad}\, F(Y)^*)Y(Y^*Y)^{-1}\right).
\end{aligned}$$

$$\begin{aligned}
&\mathrm{D}\,\mathrm{grad}\, F(Y)[\xi_Y] = \left(I - \frac{1}{2}P_Y\right)\nabla^2 f(YY^*)[Y\xi_Y^* + \xi_Y Y^*]Y(Y^*Y)^{-1} \\
&-\tfrac{1}{2}(\mathrm{D}\,(P_Y)[\xi_Y])\nabla f(YY^*)Y(Y^*Y)^{-1} + \left(I - \tfrac{1}{2}P_Y\right)\nabla f(YY^*)\mathrm{D}\,(Y(Y^*Y)^{-1})[\xi_Y],
\end{aligned}$$

where we have

$$\begin{aligned}
\mathrm{D}\,(P_Y)[\xi_Y] &= \mathrm{D}\,(Y(Y^*Y)^{-1}Y^*)[\xi_Y] \\
&= \xi_Y(Y^*Y)^{-1}Y^* - Y(Y^*Y)^{-1}(\xi_Y^*Y + Y^*\xi_Y)(Y^*Y)^{-1}Y^* + Y(Y^*Y)^{-1}\xi_Y^*,
\end{aligned}$$

$$\mathrm{D}\,(Y(Y^*Y)^{-1})[\xi_Y] = \xi_Y(Y^*Y)^{-1} - Y(Y^*Y)^{-1}(\xi_Y^*Y + Y^*\xi_Y)(Y^*Y)^{-1}.$$

Combining these equations we have

$$\begin{aligned}
&g_Y^3(\mathrm{Hess}\, F(Y)[\xi_Y], \eta_Y) = \tilde{g}\left(\eta_Y, \left(I - \tfrac{1}{2}P_Y\right)\nabla^2 f(YY^*)[Y\xi_Y^* + \xi_Y Y^*]Y(Y^*Y)^{-1}\right) \\
&-\tilde{g}\left(\eta_Y, \tfrac{1}{2}(\xi_Y(Y^*Y)^{-1}Y^* - Y(Y^*Y)^{-1}(\xi_Y^*Y + Y^*\xi_Y)(Y^*Y)^{-1}Y^* + Y(Y^*Y)^{-1}\xi_Y^*)\nabla f(YY^*)Y(Y^*Y)^{-1}\right) \\
&+\tilde{g}\left(\eta_Y, \left(I - \tfrac{1}{2}P_Y\right)\nabla f(YY^*)\left(\xi_Y(Y^*Y)^{-1} - Y(Y^*Y)^{-1}(\xi_Y^*Y + Y^*\xi_Y)(Y^*Y)^{-1}\right)\right) \\
&+\tilde{g}\left(\eta_Y, \left(I - \tfrac{1}{2}P_Y\right)\left(\left(I - \tfrac{1}{2}P_Y\right)\nabla f(YY^*)Y(Y^*Y)^{-1}\xi_Y^* + \xi_Y(Y^*Y)^{-1}Y^*\nabla f(YY^*)\left(I - \tfrac{1}{2}P_Y\right)\right)Y(Y^*Y)^{-1}\right) \\
&= \tilde{g}\left(\eta_Y, \left(I - \tfrac{1}{2}P_Y\right)\nabla^2 f(YY^*)[Y\xi_Y^* + \xi_Y Y^*]Y(Y^*Y)^{-1}\right) - \tilde{g}\left(\eta_Y, \tfrac{1}{2}\xi_Y(Y^*Y)^{-1}Y^*\nabla f(YY^*)Y(Y^*Y)^{-1}\right) \\
&-\tilde{g}\left(\eta_Y, \tfrac{1}{2}Y(Y^*Y)^{-1}\xi_Y^*\nabla f(YY^*)Y(Y^*Y)^{-1}\right) + \tilde{g}\left(\eta_Y, \tfrac{1}{2}Y(Y^*Y)^{-1}\xi_Y^* P_Y\nabla f(YY^*)Y(Y^*Y)^{-1}\right) \\
&+\tilde{g}\left(\eta_Y, \tfrac{1}{2}P_Y\xi_Y(Y^*Y)^{-1}Y^*\nabla f(YY^*)Y(Y^*Y)^{-1}\right) + \tilde{g}\left(\eta_Y, \left(I - \tfrac{1}{2}P_Y\right)\nabla f(YY^*)\left((I - P_Y)\xi_Y(Y^*Y)^{-1} - Y(Y^*Y)^{-1}\xi_Y^*Y(Y^*Y)^{-1}\right)\right) \\
&+\tilde{g}\left(\eta_Y, \left(I - \tfrac{1}{2}P_Y\right)\nabla f(YY^*)Y(Y^*Y)^{-1}\xi_Y^*Y(Y^*Y)^{-1} - \tfrac{1}{4}P_Y\nabla f(YY^*)Y(Y^*Y)^{-1}\xi_Y^*Y(Y^*Y)^{-1}\right) \\
&+\tilde{g}\left(\eta_Y, \tfrac{1}{2}(I - P_Y)\xi_Y Y(Y^*Y)^{-1}Y^*\nabla f(YY^*)Y(Y^*Y)^{-1} + \tfrac{1}{4}P_Y\xi_Y(Y^*Y)^{-1}Y^*\nabla f(YY^*)Y(Y^*Y)^{-1}\right) \\
&= \tilde{g}\left(\eta_Y, \left(I - \tfrac{1}{2}P_Y\right)\nabla^2 f(YY^*)[Y\xi_Y^* + \xi_Y Y^*]Y(Y^*Y)^{-1}\right) + \tilde{g}\left(\eta_Y, (I - P_Y)\nabla f(YY^*)(I - P_Y)\xi_Y(Y^*Y)^{-1}\right)
\end{aligned}$$

$$
\begin{aligned}
&+\tilde{g}\left(\eta_Y, \tfrac{1}{2}Y \operatorname{Skew}\left((Y^*Y)^{-1}Y\xi_Y(Y^*Y)^{-1}Y^*\nabla f(YY^*)Y(Y^*Y)^{-1}\right)\right) + \tilde{g}\left(\eta_Y, Y \operatorname{Skew}\left((Y^*Y)^{-1}Y^*\nabla f(YY^*)(I-P_Y)\xi_Y(Y^*Y)^{-1}\right)\right) \\
= \ & \tilde{g}\left(\eta_Y, \left(I - \tfrac{1}{2}P_Y\right)\nabla^2 f(YY^*)[Y\xi_Y^* + \xi_Y Y^*]Y(Y^*Y)^{-1}\right) + \tilde{g}\left(\eta_Y, (I-P_Y)\nabla f(YY^*)(I-P_Y)\xi_Y(Y^*Y)^{-1}\right) \\
= \ & g_Y^3\left(\eta_Y, \left(I - \tfrac{1}{2}P_Y\right)\nabla^2 f(YY^*)[Y\xi_Y^* + \xi_Y Y^*]Y(Y^*Y)^{-1} + (I-P_Y)\nabla f(YY^*)(I-P_Y)\xi_Y(Y^*Y)^{-1}\right).
\end{aligned}
$$

Hence for $\xi_Y \in \mathcal{H}_Y$, we have

$$
\operatorname{Hess} F(Y)[\xi_Y] = \left(I - \tfrac{1}{2}P_Y\right)\nabla^2 f(YY^*)[Y\xi_Y^* + \xi_Y Y^*]Y(Y^*Y)^{-1} + (I-P_Y)\nabla f(YY^*)(I-P_Y)\xi_Y(Y^*Y)^{-1}.
$$

Appendix C Proof of lemmas

C.1 Proof of Lemma 4.4

Proof. It is straightforward to see $C^3_{\pi(Y)} = D^3_{\pi(Y)} = 1$ by the definition of g^3. For g^2, write $\overline{\xi}_Y = YS + Y_\perp K$ for some $S = S^* \in \mathbb{C}^{p\times p}$ and $K \in \mathbb{C}^{n\times p}$. We have

$$
\frac{\left\|Y\overline{\xi}_Y^* + \overline{\xi}_Y Y^*\right\|_F^2}{g_Y^2(\overline{\xi}_Y, \overline{\xi}_Y)} = 2 + \frac{2\left\|YSY^*\right\|_F^2}{\left\|YSY^*\right\|_F^2 + \left\|KY^*\right\|_F^2}.
$$

Hence it is easy to see $C^2_{\pi(Y)} = 2$ when S is zero matrix and $D^2_{\pi(Y)} = 4$ when YSY^* is nonzero and K is zero matrix. For g^1, by its horizontal space, we can write $\overline{\xi}_Y = Y(Y^*Y)^{-1}S + Y_\perp K$ for some $S = S^* \in \mathbb{C}^{p\times p}$ and $K \in \mathbb{C}^{n\times p}$. Notice that the SVD of Y can be given as $Y = U\Sigma^{\frac{1}{2}}V^*$ where V is unitary. Let $\bar{S} = V^*SV$ and $\bar{K} = KV$, and $\bar{K}_i$ be the i-th column of $\bar{K}$, then

$$
\begin{aligned}
&\frac{\left\|Y\overline{\xi}_Y^* + \overline{\xi}_Y Y^*\right\|_F^2}{g_Y^1(\overline{\xi}_Y, \overline{\xi}_Y)} = \frac{\left\|Y((Y^*Y)^{-1}S + S(Y^*Y)^{-1})Y^*\right\|_F^2 + 2\left\|KY^*\right\|_F^2}{\left\|Y(Y^*Y)^{-1}S\right\|_F^2 + \left\|K\right\|_F^2} = \frac{\left\|\Sigma^{-\frac{1}{2}}\bar{S}\Sigma^{\frac{1}{2}} + \Sigma^{\frac{1}{2}}\bar{S}\Sigma^{-\frac{1}{2}}\right\|_F^2 + 2\left\|\bar{K}\Sigma^{\frac{1}{2}}\right\|_F^2}{\left\|\Sigma^{-\frac{1}{2}}\bar{S}\right\|_F^2 + \left\|\bar{K}\right\|_F^2} \\
=\ & \frac{\sum_{i,j=1}^{p}\left(\frac{\sigma_i}{\sigma_j} + \frac{\sigma_j}{\sigma_i} + 2\right)\left|\bar{S}_{ij}\right|^2 + 2\sum_{i=1}^{p}\sigma_i\left\|\bar{K}_i\right\|_F^2}{\sum_{i,j=1}^{p}\frac{\left|\bar{S}_{ij}\right|^2}{\sigma_i} + \sum_{i=1}^{p}\left\|\bar{K}_i\right\|_F^2} = \frac{2\sum_{i,j=1}^{p}\frac{\sigma_j}{\sigma_i}\left|\bar{S}_{ij}\right|^2 + 2\sum_{i,j=1}^{p}\left|\bar{S}_{ij}\right|^2 + 2\sum_{i=1}^{p}\sigma_i\left\|K_i\right\|_F^2}{\sum_{i,j=1}^{p}\frac{\left|\bar{S}_{ij}\right|^2}{\sigma_i} + \sum_{i=1}^{p}\left\|\bar{K}_i\right\|_F^2},
\end{aligned}
\tag{C1}
$$

where symmetry $\bar{S}^* = \bar{S}$ is used in the last step. The lower bound is given by

$$
\frac{2\sum_{i,j=1}^{p}\frac{\sigma_j}{\sigma_i}\left|\bar{S}_{ij}\right|^2 + 2\sum_{i,j=1}^{p}\left|\bar{S}_{ij}\right|^2 + 2\sum_{i=1}^{p}\sigma_i\left\|\bar{K}_i\right\|_F^2}{\sum_{i,j=1}^{p}\frac{\left|\bar{S}_{ij}\right|^2}{\sigma_i} + \sum_{i=1}^{p}\left\|\bar{K}_i\right\|_F^2} \geq \frac{2\left(\frac{\sigma_p}{\sigma_1} + 1\right)\sum_{i,j=1}^{p}\left|\bar{S}_{ij}\right|^2 + 2\sigma_p\sum_{i=1}^{p}\left\|\bar{K}_i\right\|_F^2}{\frac{1}{\sigma_p}\sum_{i,j=1}^{p}\left|\bar{S}_{ij}\right|^2 + \sum_{i=1}^{p}\left\|\bar{K}_i\right\|_F^2} = \frac{2\left(\frac{\sigma_p^2}{\sigma_1} + \sigma_p\right)\sum_{i,j=1}^{p}\left|\bar{S}_{ij}\right|^2 + 2\sigma_p^2\sum_{i=1}^{p}\left\|\bar{K}_i\right\|_F^2}{\sum_{i,j=1}^{p}\left|\bar{S}_{ij}\right|^2 + \sigma_p\sum_{i=1}^{p}\left\|\bar{K}_i\right\|_F^2} \geq 2\sigma_p.
$$

This lower bound is sharp as one can choose $S = 0$ and K with $\left\|\bar{K}_p\right\|_F = 1$ and $\left\|\bar{K}_i\right\|_F = 0$ for $i < p$. We have the upper bound as follows.

$$
\frac{2\sum_{i,j=1}^{p}\frac{\sigma_j}{\sigma_i}\left|\bar{S}_{ij}\right|^2 + 2\sum_{i,j=1}^{p}\left|\bar{S}_{ij}\right|^2 + 2\sum_{i=1}^{p}\sigma_i\left\|\bar{K}_i\right\|_F^2}{\sum_{i,j=1}^{p}\frac{\left|\bar{S}_{ij}\right|^2}{\sigma_i} + \sum_{i=1}^{p}\left\|\bar{K}_i\right\|_F^2} \leq \frac{2\left(\frac{\sigma_1}{\sigma_p} + 1\right)\sum_{i,j=1}^{p}\left|\bar{S}_{ij}\right|^2 + 2\sigma_1\sum_{i=1}^{p}\left\|\bar{K}_i\right\|_F^2}{\frac{1}{\sigma_1}\sum_{i,j=1}^{p}\left|\bar{S}_{ij}\right|^2 + \sum_{i=1}^{p}\left\|\bar{K}_i\right\|_F^2}
$$

$$= \frac{2\left(\frac{\sigma_1^2}{\sigma_p}+\sigma_1\right)\sum_{i,j=1}^{p}\left|\bar{S}_{ij}\right|^2 + 2\sigma_1^2\sum_{i=1}^{p}\left\|\bar{K}_i\right\|_F^2}{\sum_{i,j=1}^{p}\left|\bar{S}_{ij}\right|^2 + \sigma_1\sum_{i=1}^{p}\left\|\bar{K}_i\right\|_F^2} \leq 2\left(\frac{\sigma_1^2}{\sigma_p}+\sigma_1\right),$$

where the last inequality is obtained by the range of the rational function $f(x,y) = \frac{ax+by}{x+dy}$ with $a = 2\left(\frac{\sigma_1^2}{\sigma_p}+\sigma_1\right), b = 2\sigma_1^2$ and $d = \sigma_1$ on $\{(x,y)|x \geq 0, y \geq 0, xy \neq 0\}$.

This upper bound $2\left(\frac{\sigma_1^2}{\sigma_p}+\sigma_1\right)$ may not be the supremum as the inequalities are not sharp. However, we can show that $D^1_{\pi(Y)} \geq 2\sigma_1$. To see this, choose $\bar{S} = 0$ and K with $\left\|\bar{K}_1\right\|_F = 1$ and $\left\|\bar{K}_i\right\|_F = 0$ for $i > 1$. Then (C1) reaches the value $2\sigma_1$. Hence the supremum must be at least $2\sigma_1$. So we have

$$2\sigma_1 \leq D^1_{\pi(Y)} \leq 2\left(\frac{\sigma_1^2}{\sigma_p}+\sigma_1\right). \tag{C2}$$

□

C.2 Proof of Lemma 4.5

Proof. We will use the inequality $\|B^*A^*\|_F = \|AB\|_F \leq \|A\|\|B\|_F \leq \|A\|_F\|B\|_F$ for two matrices where $\|A\|$ is the spectral norm. If X is Hermitian, $\|AX\|_F = \|XA^*\|_F \leq \|X\|\|A^*\|_F = \|X\|\|A\|_F$.

For the embedded manifold, recall that $\xi^s_X = P^s_X(\xi_X)$ and $\xi^p_X = P^p_X(\xi_X)$ and P^t_X and P^p_X are defined in (9), and the bound for the FOT is given by

$$\frac{\left|g_X\left(P^p_X\left(\nabla f(X)(X^\dagger\zeta^p_X)^*+(\zeta^p_X X^\dagger)^*\nabla f(X)\right),\zeta_X\right)\right|}{g_X(\zeta_X,\zeta_X)} = \frac{\left|\left\langle P^p_X\left(\nabla f(X)\zeta^p_X X^\dagger+X^\dagger\zeta^p_X\nabla f(X)\right),\zeta_X\right\rangle_{\mathbb{C}^{n\times n}}\right|}{\langle\zeta_X,\zeta_X\rangle_{\mathbb{C}^{n\times n}}}$$
$$\leq \frac{\left|\left\langle P^p_X\left(\nabla f(X)\zeta^p_X X^\dagger\right),\zeta_X\right\rangle_{\mathbb{C}^{n\times n}}\right|}{\langle\zeta_X,\zeta_X\rangle_{\mathbb{C}^{n\times n}}} + \frac{\left|\left\langle P^p_X\left(X^\dagger\zeta^p_X\nabla f(X)\right),\zeta_X\right\rangle_{\mathbb{C}^{n\times n}}\right|}{\langle\zeta_X,\zeta_X\rangle_{\mathbb{C}^{n\times n}}}$$
$$\leq 2\frac{\|\nabla f(X)\zeta^p_X X^\dagger\|_F\|\zeta_X\|_F}{\langle\zeta_X,\zeta_X\rangle_{\mathbb{C}^{n\times n}}} \leq 2\frac{\|\nabla f(X)\|\|\zeta^p_X X^\dagger\|_F\|\zeta_X\|_F}{\langle\zeta_X,\zeta_X\rangle_{\mathbb{C}^{n\times n}}} \leq 2\frac{\|\nabla f(X)\|\|X^\dagger\|\|\zeta^p_X\|_F\|\zeta_X\|_F}{\langle\zeta_X,\zeta_X\rangle_{\mathbb{C}^{n\times n}}}$$
$$\leq \frac{2\|\nabla f(X)\|\left\|X^\dagger\right\|\|\zeta_X\|_F^2}{\langle\zeta_X,\zeta_X\rangle_{\mathbb{C}^{n\times n}}} = 2\|\nabla f(X)\|\left\|X^\dagger\right\| = \frac{2}{\sigma_p}\|\nabla f(X)\|.$$

For the quotient manifold with g^1, the FOT is bounded by

$$\frac{\left|g^1_Y(2\nabla f(YY^*)\bar{\xi}_Y,\bar{\xi}_Y)\right|}{g^1_Y(\bar{\xi}_Y,\bar{\xi}_Y)} = \frac{\left|\left\langle 2\nabla f(YY^*)\bar{\xi}_Y,\bar{\xi}_Y\right\rangle_{\mathbb{C}^{n\times p}}\right|}{\left\langle\bar{\xi}_Y,\bar{\xi}_Y\right\rangle_{\mathbb{C}^{n\times p}}} \leq \frac{2\left\|\nabla f(YY^*)\bar{\xi}_Y\right\|_F\left\|\bar{\xi}_Y\right\|_F}{\left\langle\bar{\xi}_Y,\bar{\xi}_Y\right\rangle_{\mathbb{C}^{n\times p}}} \leq \frac{2\|\nabla f(YY^*)\|\left\|\bar{\xi}_Y\right\|_F^2}{\left\langle\bar{\xi}_Y,\bar{\xi}_Y\right\rangle_{\mathbb{C}^{n\times p}}} = 2\|\nabla f(YY^*)\|.$$

For the quotient manifold with g^2, the FOTs contains four terms and we estimate each term separately. Notice that the SVD of Y can be given as $Y = U\Sigma^{\frac{1}{2}}V^*$ where V is unitary. Let $\bar{S} = V^*SV$ and $\bar{K} = KV$, and $\bar{K}_i$ be the i-th column of $\bar{K}$. For the first summand we have

$$\frac{\left|\left\langle \nabla f(YY^*)P_Y^{\perp}\bar{\xi}_Y, \bar{\xi}_Y\right\rangle_{\mathbb{C}^{n\times p}}\right|}{g_Y^2(\bar{\xi}_Y,\bar{\xi}_Y)} = \frac{\left|\left\langle \nabla f(YY^*)P_Y^{\perp}\bar{\xi}_Y, \bar{\xi}_Y\right\rangle_{\mathbb{C}^{n\times p}}\right|}{\left\langle \bar{\xi}_Y Y^*, \bar{\xi}_Y Y^*\right\rangle_{\mathbb{C}^{n\times n}}} \leq \frac{\|\nabla f(YY^*)\| \left\|\bar{\xi}_Y\right\|_F^2}{\left\langle \bar{\xi}_Y Y^*, \bar{\xi}_Y Y^*\right\rangle_{\mathbb{C}^{n\times n}}}.$$

$$= \frac{\|YS\|_F^2 + \|K\|_F^2}{\|YSY^*\|_F^2 + \|KY^*\|_F^2} \|\nabla f(YY^*)\| \leq \left(\frac{\|YS\|_F^2}{\|YSY^*\|_F^2} + \frac{\|K\|_F^2}{\|KY^*\|_F^2}\right) \|\nabla f(YY^*)\|$$

$$= \left(\frac{\left\|\sqrt{\Sigma}\bar{S}\right\|_F^2}{\left\|\sqrt{\Sigma}\bar{S}\sqrt{\Sigma}\right\|_F^2} + \frac{\|\bar{K}\|_F^2}{\left\|\bar{K}\sqrt{\Sigma}\right\|_F^2}\right) \|\nabla f(YY^*)\| \leq \frac{2}{\sigma_p} \|\nabla f(YY^*)\|.$$

Similarly we have the second term: $\frac{\left|\left\langle P_Y^{\perp}\nabla f(YY^*)\bar{\xi}_Y,\bar{\xi}_Y\right\rangle_{\mathbb{C}^{n\times p}}\right|}{g_Y^2(\bar{\xi}_Y,\bar{\xi}_Y)} \leq \frac{2}{\sigma_p} \|\nabla f(YY^*)\|$.

For the third term, with the fact $\|A^*A\|_F = \|A\|_F^2$, we have

$$\frac{\left|\left\langle Y\bar{\xi}_Y^*\bar{\xi}_Y, 2\nabla f(YY^*)Y(Y^*Y)^{-1}\right\rangle_{\mathbb{C}^{n\times p}}\right|}{g_Y^2(\bar{\xi}_Y,\bar{\xi}_Y)} = \frac{\left|\left\langle Y\bar{\xi}_Y^*\bar{\xi}_Y Y^*, 2\nabla f(YY^*)Y(Y^*Y)^{-2}Y^*\right\rangle_{\mathbb{C}^{n\times n}}\right|}{g_Y^2(\bar{\xi}_Y,\bar{\xi}_Y)} \leq \frac{\left\|Y\bar{\xi}_Y^*\bar{\xi}_Y Y^*\right\|_F \left\|2\nabla f(YY^*)Y(Y^*Y)^{-2}Y^*\right\|_F}{g_Y^2(\bar{\xi}_Y,\bar{\xi}_Y)}$$

$$\leq \frac{\left\|\bar{\xi}_Y Y^*\right\|_F^2 \|2\nabla f(YY^*)\| \left\|Y(Y^*Y)^{-2}Y^*\right\|_F}{g_Y^2(\bar{\xi}_Y,\bar{\xi}_Y)} = 2\left\|Y(Y^*Y)^{-2}Y^*\right\|_F \|\nabla f(YY^*)\| \leq \frac{2\sqrt{p}}{\sigma_p} \|\nabla f(YY^*)\|.$$

Similarly we can bound the fourth term: $\frac{\left|\left\langle \bar{\xi}_Y Y^*\bar{\xi}_Y, 2\nabla f(YY^*)Y(Y^*Y)^{-1}\right\rangle\right|_{\mathbb{C}^{n\times p}}}{g_Y^2(\bar{\xi}_Y,\bar{\xi}_Y)} \leq \frac{2\sqrt{p}}{\sigma_p} \|\nabla f(YY^*)\|$.

Thus, for the quotient manifold with g^2 we have $|\mathrm{FOTs}| \leq \frac{4(\sqrt{p}+1)}{\sigma_p} \|\nabla f(YY^*)\|$.

For g^3, recall that $P_Y^{\perp} = I - P_Y = I - Y(Y^*Y)^{-1}Y^*$, with the property (18) and the fact $(I-P_Y)^*Y = 0$, the FOT can be bounded as follows:

$$|\mathrm{FOT}| = \frac{\left|g_Y^3((I-P_Y)\nabla f(YY^*)(I-P_Y)\bar{\xi}_Y(Y^*Y)^{-1},\bar{\xi}_Y)\right|}{g_Y^3(\bar{\xi}_Y,\bar{\xi}_Y)} = \frac{2\left|\left\langle P_Y^{\perp}\nabla f(YY^*)P_Y^{\perp}\bar{\xi}_Y,\bar{\xi}_Y\right\rangle_{\mathbb{C}^{n\times p}}\right|}{g_Y^3(\bar{\xi}_Y,\bar{\xi}_Y)}$$

$$= \frac{2\left|\langle\nabla f(YY^*)Y_\perp K, Y_\perp K\rangle_{\mathbb{C}^{n\times p}}\right|}{g_Y^3(\bar{\xi}_Y,\bar{\xi}_Y)} = \frac{2\left|\langle\nabla f(YY^*)Y_\perp K, Y_\perp K\rangle_{\mathbb{C}^{n\times p}}\right|}{\left\|Y\bar{\xi}_Y^*+\bar{\xi}_Y Y^*\right\|_F^2} = \frac{2\left|\langle\nabla f(YY^*)Y_\perp K, Y_\perp K\rangle_{\mathbb{C}^{n\times p}}\right|}{\left\|2YSY^*+Y_\perp KY^*+YK^*Y_\perp^*\right\|_F^2}$$

$$= \frac{2\left|\langle\nabla f(YY^*)Y_\perp K, Y_\perp K\rangle_{\mathbb{C}^{n\times p}}\right|}{\|2YSY^*\|_F^2+\|Y_\perp KY^*\|_F^2+\left\|YK^*Y_\perp^*\right\|_F^2} = \frac{\left|\langle\nabla f(YY^*)Y_\perp K, Y_\perp K\rangle_{\mathbb{C}^{n\times p}}\right|}{2\|YSY^*\|_F^2+\|Y_\perp KY^*\|_F^2} \leq \frac{\left|\langle\nabla f(YY^*)Y_\perp K, Y_\perp K\rangle_{\mathbb{C}^{n\times p}}\right|}{\|Y_\perp KY^*\|_F^2}$$

$$\leq \frac{\|Y_\perp K\|_F^2}{\|Y_\perp KY^*\|_F^2} \|\nabla f(YY^*)\| \leq \frac{1}{\sigma_p} \|\nabla f(YY^*)\|.$$

□

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