A BLOCK COORDINATE DESCENT METHOD FOR NONSMOOTH COMPOSITE OPTIMIZATION UNDER ORTHOGONALITY CONSTRAINTS

Anonymous authors

Paper under double-blind review

ABSTRACT

Nonsmooth composite optimization with orthogonality constraints has a wide range of applications in statistical learning and data science. However, this problem is challenging due to its nonsmooth objective and computationally expensive, non-convex constraints. In this paper, we propose a new approach called **OBCD**, which leverages Block Coordinate Descent to address these challenges. **OBCD** is a feasible method with a small computational footprint. In each iteration, it updates k rows of the solution matrix, where $k \geq 2$, by globally solving a small nonsmooth optimization problem under orthogonality constraints. We prove that the limiting points of **OBCD**, referred to as (global) block-k stationary points, offer stronger optimality than standard critical points. Furthermore, we show that **OBCD** converges to ϵ -block-k stationary points with an iteration complexity of $\mathcal{O}(1/\epsilon)$. Additionally, under the Kurdyka-Lojasiewicz (KL) inequality, we establish the non-ergodic convergence rate of **OBCD**. We also demonstrate how novel breakpoint search methods can be used to solve the subproblem in **OBCD**. Empirical results show that our approach consistently outperforms existing methods.

1 Introduction

We consider the following nonsmooth composite optimization problem under orthogonality constraints ($\stackrel{\triangle}{}$ means define):

$$\min_{\mathbf{X} \in \mathbb{R}^{n \times r}} F(\mathbf{X}) \triangleq f(\mathbf{X}) + h(\mathbf{X}), \ s.t. \, \mathbf{X}^\mathsf{T} \mathbf{X} = \mathbf{I}_r. \tag{1}$$

Here, $n \geq r$, $n \geq 2$, and \mathbf{I}_r is a $r \times r$ identity matrix. We do not assume convexity of $f(\mathbf{X})$ and $h(\mathbf{X})$. For brevity, the orthogonality constraints $\mathbf{X}^\mathsf{T}\mathbf{X} = \mathbf{I}_r$ in Problem (1) is rewritten as $\mathbf{X} \in \mathrm{St}(n,r) \triangleq \{\mathbf{X} \in \mathbb{R}^{n \times r} \mid \mathbf{X}^\mathsf{T}\mathbf{X} = \mathbf{I}_r\}$, where $\mathcal{M} \triangleq \mathrm{St}(n,r)$ is the Stiefel manifold in the literature (Edelman et al., 1998; Absil et al., 2008; Wen & Yin, 2013; Hu et al., 2020). We impose the following assumptions on Problem (1) throughout this paper. (Asm-i) For any \mathbf{X} and \mathbf{X}^+ , where \mathbf{X} and \mathbf{X}^+ only differ at most by k rows with $k \geq 2$, we assume $f: \mathbb{R}^{n \times r} \mapsto \mathbb{R}$ is \mathbf{H} -smooth with $\mathbf{0} \preceq \mathbf{H} \in \mathbb{R}^{nr \times nr}$ such that:

$$f(\mathbf{X}^+) \le \mathcal{Q}(\mathbf{X}^+; \mathbf{X}) \triangleq f(\mathbf{X}) + \langle \mathbf{X}^+ - \mathbf{X}, \nabla f(\mathbf{X}) \rangle + \frac{1}{2} \|\mathbf{X}^+ - \mathbf{X}\|_{\mathbf{H}}^2,$$
 (2)

where $\|\mathbf{H}\|_{sp} \leq L_f$ for some constant $L_f > 0$ and $\|\mathbf{X}\|_{\mathbf{H}}^2 \triangleq \operatorname{vec}(\mathbf{X})^{\mathsf{T}}\mathbf{H}\operatorname{vec}(\mathbf{X})^{\;1}$. Here, $\|\mathbf{H}\|_{sp}$ is the spectral norm of \mathbf{H} . Notably, when $\mathbf{H} = L_f \cdot \mathbf{I}_{nr}$, this condition simplifies to the standard L_f -smoothness (Nesterov, 2003). (Asm-ii) The function $h(\mathbf{X}) : \mathbb{R}^{n \times r} \mapsto \mathbb{R}$ is closed, proper, and lower semicontinuous, and potentially non-smooth. Additionally, it is coordinate-wise separable, such that $h(\mathbf{X}) = \sum_{i,j} h(\mathbf{X}_{ij})$. Typical examples of $h(\mathbf{X})$ include the ℓ_p norm function $h(\mathbf{X}) = \|\mathbf{X}\|_p$ with $p \in \{0,1\}$, and the indicator function for non-negativity constraints $h(\mathbf{X}) = \iota_{\geq 0}(\mathbf{X})$. (Asm-iii) The following small-sized subproblem can be solved exactly and efficiently:

$$\min_{\mathbf{V} \in St(k,k)} \mathcal{P}(\mathbf{V}) \triangleq \frac{1}{2} \|\mathbf{V}\|_{\tilde{\mathbf{Q}}}^2 + \langle \mathbf{V}, \mathbf{P} \rangle + h(\mathbf{V}\mathbf{Z})$$
(3)

for any given $\mathbf{Z} \in \mathbb{R}^{k \times r}$, $\mathbf{P} \in \mathbb{R}^{k \times k}$, and $\tilde{\mathbf{Q}} \in \mathbb{R}^{k^2 \times k^2}$. Here, we employ a notational simplification by defining $h(\mathbf{VZ}) \triangleq \sum_{i,j} h([\mathbf{VZ}]_{ij})$, given the coordinate-wise separability of the function $h(\cdot)$.

Problem (1) is an optimization framework that plays a crucial role in a variety of statistical learning and data science models, such as sparse Principal Component Analysis (PCA) (Journée et al.,

¹We let $f(\mathbf{X}) = \frac{1}{2} \operatorname{tr}(\mathbf{X}^\mathsf{T} \mathbf{C} \mathbf{X} \mathbf{D}) = \frac{1}{2} ||\mathbf{X}||_{\mathbf{H}}^2$, where $\mathbf{H} = \mathbf{D} \otimes \mathbf{C}$, and $\mathbf{C} \in \mathbb{R}^{n \times n}$ and $\mathbf{D} \in \mathbb{R}^{r \times r}$ are symmetric. Clearly, $f(\mathbf{X})$ satisfies (2) with equality, as $f(\mathbf{X}^+) = \mathcal{Q}(\mathbf{X}^+; \mathbf{X})$ holds for all \mathbf{X} and \mathbf{X}^+ .

2010; Shalit & Chechik, 2014), nonnegative PCA (Zass & Shashua, 2006; Qian et al., 2021), deep neural networks (Cogswell et al., 2016; Cho & Lee, 2017; Xie et al., 2017; Bansal et al., 2018; Massart & Abrol, 2022; Huang & Gao, 2023), electronic structure calculation (Zhang et al., 2014; Liu et al., 2014), Fourier transforms approximation (Frerix & Bruna, 2019), phase synchronization (Liu et al., 2017), orthogonal nonnegative matrix factorization (Jiang et al., 2022), *K*-indicators clustering (Jiang et al., 2016), and dictionary learning (Zhai et al., 2020).

1.1 MOTIVATING APPLICATIONS

Many machine learning and data science models can be formulated as Problem (1). Below, we present two examples.

- ▶ L_0 Norm-based SPCA. L_0 norm-based Sparse PCA (SPCA) is a method that uses ℓ_0 norm to produce modified principal components with sparse loadings, which helps reduce model complexity and increase model interpretability (d'Aspremont et al., 2008; Chen et al., 2016). It can be formulated as: $\min_{\mathbf{X} \in \mathrm{St}(n,r)} -\langle \mathbf{X}, \mathbf{C} \mathbf{X} \rangle + \lambda \|\mathbf{X}\|_0$, where $\mathbf{C} = \mathbf{A}^\mathsf{T} \mathbf{A} \in \mathbb{R}^{n \times n}$ is the covariance of the data matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ and $\lambda > 0$.
- ▶ L_1 Norm-based SPCA. As the L_1 norm provides the tightest convex relaxation for the L_0 -norm over the unit ball in the sense of L_∞ -norm, some researchers replace the non-convex and discontinuous L_0 norm function with a convex but non-smooth function (Chen et al., 2016; Vu et al., 2013; Lu & Zhang, 2012). This leads to the following optimization problem of L_1 norm-based SPCA: $\min_{\mathbf{X} \in \mathrm{St}(n,r)} \langle \mathbf{X}, \mathbf{C} \mathbf{X} \rangle + \lambda \|\mathbf{X}\|_1$, where $\mathbf{C} \in \mathbb{R}^{n \times n}$ is the covariance matrix of the data, and $\lambda > 0$.

1.2 RELATED WORK

We now present some related algorithms in the literature.

- ▶ Minimizing Smooth Functions under Orthogonality Constraints. One of the main challenges in solving Problem (1) stems from the nonconvexity of the orthogonality constraints. Existing approaches for addressing this difficulty can be broadly categorized into three classes: (i) Geodesic-like methods (Abrudan et al., 2008; Edelman et al., 1998; Absil et al., 2008). Computing exact geodesics typically involves solving ordinary differential equations, which can be computationally expensive. To avoid this, geodesic-like methods approximate the geodesic path by computing the geodesic logarithm using simpler linear algebraic operations. (ii) Projection-like methods (Absil et al., 2008; Golub & Van Loan, 2013; Jiang & Dai, 2015). These include techniques such as projection onto the nearest orthogonal matrix, polar decomposition, and QR-based projection. At each iteration, these methods descend along the Euclidean or Riemannian gradient direction and subsequently apply a projection step to enforce orthogonality. (iii) Multiplier correction methods (Gao et al., 2018; 2019; Xiao et al., 2022). These methods exploit the fact that the Lagrange multiplier associated with the orthogonality constraint is symmetric and admits a closed-form expression at first-order stationarity. They update the multiplier after achieving sufficient decrease in the objective, resulting in efficient feasible or infeasible first-order methods.
- ▶ Minimizing Nonmooth Functions under Orthogonality Constraints. Another major challenge in solving Problem (1) arises from the nonsmoothness of the objective function. Existing approaches for handling this issue can be broadly categorized into four classes: (i) Subgradient methods (Hwang et al., 2015; Li et al., 2021; Cheung et al., 2024). These methods generalize gradient descent to nonsmooth settings. Many of the previously mentioned geodesic-like and projection-based strategies can be incorporated into subgradient frameworks on manifolds. (ii) Proximal gradient methods (Chen et al., 2020; Li et al., 2024b). These methods compute a descent direction by solving a strongly convex subproblem over the tangent space, often using a semi-smooth Newton method. The resulting point is then mapped back onto the manifold via a retraction to preserve orthogonality. (iii) Block Majorization Minimization (BMM) on Riemannian manifolds (Li et al., 2024b; 2023; Breloy et al., 2021; Gutman & Ho-Nguyen, 2023). This class of methods iteratively constructs a tangential majorizing surrogate for a block of the objective, takes an approximate descent step in the corresponding tangent space, and retracts the iterate back to the manifold. (iv) Operator splitting methods (Lai & Osher, 2014; Chen et al., 2016; Zhang et al., 2019). These methods reformulate the original problem by introducing auxiliary variables and linear constraints, decomposing it into simpler subproblems that can be solved separately and often exactly. Prominent examples include the Alternating Direction Method of Multipliers (ADMM) (He & Yuan, 2012), Riemannian ADMM (RADMM) (Li et al., 2024a), and Smoothing Penalty Methods (SPM) (Chen, 2012).

109

110

111

112

113

114

115

116

117

118

119

120

121

122

123

124

125

126

127

128

129

130

131

133

134 135

136

137

138

139

140 141

142

143

144

145

146

152

153

154

155

156

157

158

159

160 161

- ▶ Block Coordinate Descent Methods. (Block) coordinate descent is a classical and powerful algorithm that solves optimization problems by iteratively performing minimization along (block) coordinate directions (Tseng & Yun, 2009; Xu & Yin, 2013). The BCD methods have recently gained attention in solving nonconvex optimization problems, including sparse optimization (Yuan, 2024), k-means clustering (Nie et al., 2022), recurrent neural network (Massart & Abrol, 2022), and multi-layer convolutional networks (Bibi et al., 2019; Zeng et al., 2019). BCD methods have also been used in (Shalit & Chechik, 2014; Massart & Abrol, 2022) for solving optimization problems with orthogonal group constraints. However, their column-wise BCD methods are limited only to solve smooth minimization problems with k=2 and r=n (Refer to Section 4.2 in (Shalit & Chechik, 2014)). Our row-wise BCD methods can solve general nonsmooth problems with $k \ge 2$ and $r \leq n$. The work of (Gao et al., 2019) proposes a parallelizable column-wise BCD scheme for solving the subproblems of their proximal linearized augmented Lagrangian algorithm. Impressive parallel scalability in a parallel environment of their algorithm is demonstrated. We stress that our **row-wise** BCD methods differ from the two **column-wise** counterparts.
- ▶ Summary. Existing solutions have one or more of the following limitations: (i) They rely on full gradient information, incurring high computational costs per iteration. (ii) They cannot handle general nonsmooth composite problems. (iii) They lack descent properties, even worse, they are infeasible methods, achieving solution feasibility only at the limit point. (iv) They often lack rigorous convergence guarantees. (v) They only establish weak optimality at critical points. \bigstar To our knowledge, this represents the first application of BCD methods to solve nonsmooth composite optimization problems under orthogonality constraints, demonstrating strong optimality and convergence guarantees.

1.3 Contributions and Notations

This paper makes the following contributions. (i) Algorithmically: We propose a Block Coordinate Descent (BCD) algorithm tailored for nonsmooth composite optimization under orthogonality constraints (Section 2). (ii) Theoretically: We provide comprehensive optimality and convergence analyses of our methods (Sections 3 and 4). (iii) Empirically: Extensive experiments demonstrate that our methods surpass existing solutions in terms of accuracy and/or efficiency (Section 5).

We define $[n] \triangleq \{1, 2, ..., n\}$, and denote the Stiefel manifold as $\mathcal{M} \triangleq \operatorname{St}(n, r)$. Matlab-style colon notation is used to describe submatrices. For a matrix $\mathbf{X} \in \mathbb{R}^{n \times r}$, let $\text{vec}(\mathbf{X}) \in \mathbb{R}^{nr \times 1}$ denote the vector formed by stacking its columns, and let $mat(\mathbf{x}) \in \mathbb{R}^{n \times r}$ denote the inverse operator, such that $mat(vec(\mathbf{X})) = \mathbf{X}$. We use $\mathbb{A} + \mathbb{B}$ and $\mathbb{A} - \mathbb{B}$ to denote standard Minkowski addition and subtraction between sets \mathbb{A} and \mathbb{B} , and $\mathbb{A} \oplus \mathbb{B}$ and $\mathbb{A} \ominus \mathbb{B}$ to denote element-wise addition and subtraction, respectively. Additional notations are summarized in Appendix A.1.

THE PROPOSED **OBCD** ALGORITHM

In this section, we introduce **OBCD**, a Block Coordinate Descent algorithm for solving general nonsmooth composite problems under Orthogonality constraints, as defined in Problem (1).

We start by presenting a new update scheme designed to maintain the orthogonality constraint.

 \triangleright A New Constraint-Preserving Update Scheme. For any partition of the index vector [1, 2, ..., n]into $[B,B^c]$ with $B\in\mathbb{N}^k$, $B^c\in\mathbb{N}^{n-k}$, we define $U_B\in\mathbb{R}^{n\times k}$ and $U_{B^c}\in\mathbb{R}^{n\times (n-k)}$ as: $(U_B)_{ji}=\left\{\begin{array}{l} 1, & B_i=j; \\ 0, & \text{else.} \end{array}\right., (U_{B^c})_{ji}=\left\{\begin{array}{l} 1, & B_i^c=j; \\ 0, & \text{else.} \end{array}\right.$ Therefore, we have the following variable splitting for any $\mathbf{X}\in\mathbb{R}^{n\times r}$: $\mathbf{X}=\mathbf{I}_n\mathbf{X}=(U_BU_B^\mathsf{T}+U_{B^c}U_{B^c}^\mathsf{T})\mathbf{X}=U_B\mathbf{X}(B,:)+U_{B^c}\mathbf{X}(B^c,:),$ where $\mathbf{X}(B,:)=U_B^\mathsf{T}\mathbf{X}\in\mathbb{R}^{k\times r}$ and $\mathbf{X}(B^c,:)=U_{B^c}^\mathsf{T}\mathbf{X}\in\mathbb{R}^{(n-k)\times r}.$

In each iteration t, the indices $\{1, 2, ..., n\}$ of the rows of decision variable $\mathbf{X} \in \mathrm{St}(n, r)$ are separated to two sets B and B^c , where B is the working set with |B| = k and $B^c = \{1, 2, ..., n\} \setminus B$. To simplify notation, we use B instead of B^t , as t can be inferred from the context. We only update k rows of the variable \mathbf{X} via $\mathbf{X}^{t+1}(\mathsf{B},:) \leftarrow \mathbf{V}\mathbf{X}^t(\mathsf{B},:)$ for some appropriate matrix $\mathbf{V} \in \mathbb{R}^{k \times k}$. The following equivalent expressions hold:

$$\mathbf{X}^{t+1}(\mathsf{B},:) = \mathbf{V}\mathbf{X}^{t}(\mathsf{B},:) \quad \Leftrightarrow \quad \mathbf{X}^{t+1} = (\mathbf{U}_{\mathsf{B}}\mathbf{V}\mathbf{U}_{\mathsf{B}}^{\mathsf{T}} + \mathbf{U}_{\mathsf{B}^{c}}\mathbf{U}_{\mathsf{B}^{c}}^{\mathsf{T}})\mathbf{X}^{t}$$

$$\Leftrightarrow \quad \mathbf{X}^{t+1} = \mathbf{X}^{t} + \mathbf{U}_{\mathsf{B}}(\mathbf{V} - \mathbf{I}_{k})\mathbf{U}_{\mathsf{B}}^{\mathsf{T}}\mathbf{X}^{t}.$$
(4)

$$\Leftrightarrow \mathbf{X}^{t+1} = \mathbf{X}^t + \mathbf{U}_{\mathrm{B}}(\mathbf{V} - \mathbf{I}_k)\mathbf{U}_{\mathrm{B}}^{\mathsf{T}}\mathbf{X}^t.$$
 (5)

We consider the following minimization procedure to iteratively solve Problem (1):

$$\min_{\mathbf{V}} F(\mathcal{X}_{\mathrm{B}}^{t}(\mathbf{V})), \ s.t. \ \mathcal{X}_{\mathrm{B}}^{t}(\mathbf{V}) \in \mathrm{St}(n,r), \ \text{where} \ \mathcal{X}_{\mathrm{B}}^{t}(\mathbf{V}) \triangleq \mathbf{X}^{t} + \mathrm{U}_{\mathrm{B}}(\mathbf{V} - \mathbf{I}_{k})\mathrm{U}_{\mathrm{B}}^{\mathsf{T}}\mathbf{X}^{t}. \tag{6}$$

The following lemma shows that the orthogonality constraint for $\mathbf{X}^+ = \mathbf{X} + \mathbf{U}_{\mathbb{B}}(\mathbf{V} - \mathbf{I}_k)\mathbf{U}_{\mathbb{B}}^\mathsf{T}\mathbf{X}$ can be preserved by choosing suitable \mathbf{V} and \mathbf{X} .

Lemma 2.1. (Proof in Appendix D.1) We let $\mathbb{B} \in \{\mathcal{B}_i\}_{i=1}^{\mathbb{C}_n^k}$, where the set $\{\mathcal{B}_1, \mathcal{B}_2, ..., \mathcal{B}_{\mathbb{C}_n^k}\}$ denotes all possible combinations of the index vectors choosing k items from n without repetition. We let $\mathbf{V} \in \operatorname{St}(k,k)$. We define $\mathbf{X}^+ \triangleq \mathcal{X}_{\mathbb{B}}(\mathbf{V}) \triangleq \mathbf{X} + \operatorname{U}_{\mathbb{B}}(\mathbf{V} - \mathbf{I}_k)\operatorname{U}_{\mathbb{B}}^{\mathsf{T}}\mathbf{X}$. (a) For any $\mathbf{X} \in \mathbb{R}^{n \times r}$, we have $[\mathbf{X}^+]^{\mathsf{T}}\mathbf{X}^+ = \mathbf{X}^{\mathsf{T}}\mathbf{X}$. (b) If $\mathbf{X} \in \operatorname{St}(n,r)$, then $\mathbf{X}^+ \in \operatorname{St}(n,r)$.

Thanks to Lemma 2.1, we can now explore the following alternative formulation for Problem (6).

$$\bar{\mathbf{V}}^t \in \arg\min_{\mathbf{V}} F(\mathcal{X}_{\mathrm{B}}^t(\mathbf{V})), \ s.t. \ \mathbf{V} \in \mathrm{St}(k,k). \tag{7}$$

Then the solution matrix is updated via: $\mathbf{X}^{t+1} = \mathcal{X}_{\mathrm{B}}^t(\bar{\mathbf{V}}^t)$.

The following lemma offers important properties for the update rule $\mathbf{X}^+ = \mathbf{X} + \mathbf{U}_{\mathbb{B}}(\mathbf{V} - \mathbf{I}_k)\mathbf{U}_{\mathbb{B}}^\mathsf{T}\mathbf{X}$. Lemma 2.2. (Proof in Appendix D.2) We define $\mathbf{X}^+ = \mathbf{X} + \mathbf{U}_{\mathbb{B}}(\mathbf{V} - \mathbf{I}_k)\mathbf{U}_{\mathbb{B}}^\mathsf{T}\mathbf{X}$. For any $\mathbf{X} \in \mathrm{St}(n,r)$, $\mathbf{V} \in \mathrm{St}(k,k)$, $\mathbf{B} \in \{\mathcal{B}_i\}_{i=1}^{C_k^k}$, and symmetric matrix $\mathbf{H} \in \mathbb{R}^{nr \times nr}$, we have: (a) $\frac{1}{2}\|\mathbf{X}^+ - \mathbf{X}\|_{\mathbf{H}}^2 = \frac{1}{2}\|\mathbf{V} - \mathbf{I}_k\|_{\mathbf{Q}}^2$, where $\mathbf{Q} \triangleq (\mathbf{Z}^\mathsf{T} \otimes \mathbf{U}_{\mathbb{B}})^\mathsf{T}\mathbf{H}(\mathbf{Z}^\mathsf{T} \otimes \mathbf{U}_{\mathbb{B}})$, $\mathbf{Z} \triangleq \mathbf{U}_{\mathbb{B}}^\mathsf{T}\mathbf{X} \in \mathbb{R}^{k \times r}$, and $\mathbf{X} \otimes \mathbf{Y}$ is the Kronecker product of \mathbf{X} and \mathbf{Y} . (b) $\frac{1}{2}\|\mathbf{X}^+ - \mathbf{X}\|_{\mathsf{F}}^2 = \langle \mathbf{I}_k - \mathbf{V}, \mathbf{U}_{\mathbb{B}}^\mathsf{T}\mathbf{X}\mathbf{X}^\mathsf{T}\mathbf{U}_{\mathbb{B}}\rangle$. (c) $\frac{1}{2}\|\mathbf{X}^+ - \mathbf{X}\|_{\mathsf{F}}^2 \leq \frac{1}{2}\|\mathbf{V} - \mathbf{I}_k\|_{\mathsf{F}}^2 = \langle \mathbf{I}_k, \mathbf{I}_k - \mathbf{V}\rangle$.

▶ The Main Algorithm. The proposed algorithm **OBCD** is an iterative procedure that sequentially minimizes the objective function along block coordinate directions within a sub-manifold of \mathcal{M} .

Starting with an initial feasible solution, **OBCD** iteratively determines a working set \mathbb{B}^t using specific strategies. It then solves the small-sized subproblem in Problem (7) through successive Majorization Minimization (MM). This method iteratively constructs a surrogate function that majorizes the objective function, driving it to decrease as expected (Mairal, 2013; Razaviyayn et al., 2013; Sun et al., 2016; Breloy et al., 2021), and it has proven effective for minimizing complex functions.

We now demonstrate how to derive the majorization function for $F(\mathcal{X}_{\mathbb{B}}^t(\mathbf{V}))$ in Problem (7). Initially, for any $\mathbf{X}^t \in \operatorname{St}(n,r)$ and $\mathbf{V} \in \operatorname{St}(k,k)$, we establish following inequalities: $f(\mathcal{X}_{\mathbb{B}}^t(\mathbf{V})) - f(\mathbf{X}^t) \leq \langle \mathcal{X}_{\mathbb{B}}^t(\mathbf{V}) - \mathbf{X}^t, \nabla f(\mathbf{X}^t) \rangle + \frac{1}{2} \|\mathcal{X}_{\mathbb{B}}^t(\mathbf{V}) - \mathbf{X}^t\|_{\mathbf{H}}^2 \stackrel{@}{=} \langle \mathbf{U}_{\mathbb{B}}(\mathbf{V} - \mathbf{I}_k) \mathbf{U}_{\mathbb{B}}^\mathsf{T} \mathbf{X}^t, \nabla f(\mathbf{X}^t) \rangle + \frac{1}{2} \|\mathbf{V} - \mathbf{I}_k\|_{\mathbf{Q}}^2 \leq \langle \mathbf{V} - \mathbf{I}_k, [\nabla f(\mathbf{X}^t)(\mathbf{X}^t)^\mathsf{T}]_{\mathbb{B}\mathbb{B}} \rangle + \frac{1}{2} \|\mathbf{V} - \mathbf{I}_k\|_{\mathbf{Q} + \alpha \mathbf{I}}^2$, where step ① uses Inequality (2); step ② uses Claim (a) of Lemma 2.2; step ③ uses $\alpha > 0$ and $\mathbf{Q} \leq \mathbf{Q}$, which can be ensured by choosing \mathbf{Q} using one of the following methods:

$$\mathbf{Q} = \underline{\mathbf{Q}} \triangleq (\mathbf{Z}^{\mathsf{T}} \otimes \mathbf{U}_{\mathsf{B}})^{\mathsf{T}} \mathbf{H} (\mathbf{Z}^{\mathsf{T}} \otimes \mathbf{U}_{\mathsf{B}}), \tag{8}$$

$$\mathbf{Q} = \varsigma \mathbf{I}, \text{ with } \|\mathbf{Q}\|_{\mathsf{sp}} \le \varsigma \le L_f. \tag{9}$$

where $\mathbf{Z} \triangleq \mathbf{U}_{\mathrm{B}}^{\mathsf{T}} \mathbf{X}^t$. Then, we apply the MM technique to the smooth function $f(\mathbf{X})$, while keeping the nonsmooth component $h(\mathbf{X})$ unchanged, leading to a function $\mathcal{K}(\mathbf{V}; \mathbf{X}^t, \mathbf{B})$ that majorizes $F(\mathcal{X}_{\mathrm{B}}^t(\mathbf{V})) = f(\mathcal{X}_{\mathrm{B}}^t(\mathbf{V})) + h(\mathcal{X}_{\mathrm{B}}^t(\mathbf{V}))$:

$$F(\mathcal{X}_{\mathrm{B}}^{t}(\mathbf{V})) \leq f(\mathbf{X}^{t}) + \langle \mathbf{V} - \mathbf{I}_{k}, [\nabla f(\mathbf{X}^{t})(\mathbf{X}^{t})^{\mathsf{T}}]_{\mathrm{BB}} \rangle + \frac{1}{2} \|\mathbf{V} - \mathbf{I}_{k}\|_{\mathbf{Q} + \alpha \mathbf{I}}^{2} + h(\mathbf{V}\mathbf{U}_{\mathrm{B}}^{\mathsf{T}}\mathbf{X}^{t})$$

$$\leq \mathcal{K}(\mathbf{V}; \mathbf{X}^{t}, \mathbf{B}) \triangleq \frac{1}{2} \|\mathbf{V} - \mathbf{I}_{k}\|_{\mathbf{Q} + \alpha \mathbf{I}}^{2} + \langle \mathbf{V}, [\nabla f(\mathbf{X}^{t})(\mathbf{X}^{t})^{\mathsf{T}}]_{\mathrm{BB}} \rangle + h(\mathbf{V}\mathbf{U}_{\mathrm{B}}^{\mathsf{T}}\mathbf{X}^{t}) + \ddot{c}, \qquad (10)$$

where $\ddot{c} = f(\mathbf{X}^t) + h(\mathbf{U}_{\mathbb{B}^c}^\mathsf{T}\mathbf{X}^t) - \langle \mathbf{I}_k, [\nabla f(\mathbf{X}^t)(\mathbf{X}^t)^\mathsf{T}]_{\mathbb{B}\mathbb{B}} \rangle$ is a constant. Here, we use the coordinate-wise separable property of $h(\cdot)$ as follows: $h(\mathcal{X}_{\mathbb{B}}^t(\mathbf{V})) = h(\mathbf{U}_{\mathbb{B}^c}\mathbf{U}_{\mathbb{B}^c}^\mathsf{T}\mathbf{X}^t + \mathbf{U}_{\mathbb{B}}\mathbf{V}\mathbf{U}_{\mathbb{B}}^\mathsf{T}\mathbf{X}^t) = h(\mathbf{U}_{\mathbb{B}^c}^\mathsf{T}\mathbf{X}^t) + h(\mathbf{V}\mathbf{U}_{\mathbb{B}}^\mathsf{T}\mathbf{X}^t)$. We minimize the upper bound of the right-hand side of Inequality (10), resulting in the minimization problem that $\bar{\mathbf{V}}^t \in \arg\min_{\mathbf{V} \in \mathrm{St}(k,k)} \mathcal{K}(\mathbf{V};\mathbf{X}^t,\mathbb{B})$, which can be efficiently and exactly solved due to our assumption.

Two simple strategies to find the working set B with |B| = k can be considered. (i) Random strategy: B is randomly selected from $\{\mathcal{B}_1, \mathcal{B}_2, ..., \mathcal{B}_{C_n^k}\}$ with equal probability $1/C_n^k$. (ii) Cyclic strategy: B^t takes all possible combinations in cyclic order, such as $\mathcal{B}_1 \to \mathcal{B}_2 \to ... \to \mathcal{B}_{C_n^k} \to \mathcal{B}_1 \to ...$.

The proposed **OBCD** algorithm is summarized in Algorithm 1. Importantly, **OBCD** is a partial gradient method with low iterative computational complexity as it only assesses k rows of the Euclidean

Algorithm 1 OBCD: Block Coordinate Descent for Problem (1)

- 1: **Input:** initial feasible solution \mathbf{X}^0 ; choose $k \geq 2$; set t = 0.
- 2: for t = 0 to T do
- 3: (S1) Select working set $\mathcal{B}^t \in \{1, \dots, n\}^k$. Let $\mathcal{B} = \mathcal{B}^t$ and $\mathcal{B}^c = \{1, \dots, n\} \setminus \mathcal{B}$.
- 4: (S2) Choose $\mathbf{Q} \in \mathbb{R}^{k^2 \times k^2}$ using (8) or (9).
- 5: (S3) Define $\mathcal{K}(\cdot,;\cdot,\cdot)$ as in Equation (10). Compute $\bar{\mathbf{V}}^t$ as the global minimizer

$$\bar{\mathbf{V}}^t \in \arg\min_{\mathbf{V} \in \operatorname{St}(k,k)} \mathcal{K}(\mathbf{V}; \mathbf{X}^t, \mathcal{B}).$$
 (11)

Alternatively, find a local solution $\bar{\mathbf{V}}^t$ such that $\mathcal{K}(\bar{\mathbf{V}}^t; \mathbf{X}^t, \mathbf{B}) \leq \mathcal{K}(\mathbf{I}_k; \mathbf{X}^t, \mathbf{B})$.

- 6: (S4) $\mathbf{X}^{t+1}(\mathcal{B},:) \leftarrow \bar{\mathbf{V}}^t \mathbf{X}^t(\mathcal{B},:)$
- 226 6: (S4) 7: end for

gradient of $\nabla f(\mathbf{X}^t)$ and the solution \mathbf{X}^t to compute the linear term $\langle [\nabla f(\mathbf{X}^t)(\mathbf{X}^t)^\mathsf{T}]_{\mathbb{BB}}, \mathbf{V} \rangle = \langle [\nabla f(\mathbf{X}^t)]_{\mathbb{B},:}^\mathsf{T}[\mathbf{X}^t]_{\mathbb{B},:}, \mathbf{V} \rangle$, as shown in Equation (10). Appendix C.3 details the complexity comparison between **OBCD** and full gradient methods for some quadratic function $f(\mathbf{X})$.

► Solving the General OBCD Subproblems. The following lemma outlines key properties of the OBCD subproblems.

Lemma 2.3. (Proof in Appendix D.3) We define $\mathbf{P} \triangleq [\nabla f(\mathbf{X}^t)(\mathbf{X}^t)^\mathsf{T}]_{BB} - \max(\mathbf{Q}\text{vec}(\mathbf{I}_k)) - \alpha \mathbf{I}_k$, and $\mathbf{Z} = \mathbf{U}_B^\mathsf{T} \mathbf{X}^t$. We have:

- (a) The subproblem $\bar{\mathbf{V}}^t \in \arg\min_{\mathbf{V} \in \operatorname{St}(k,k)} \mathcal{K}(\mathbf{V}; \mathbf{X}^t, \mathbf{B})$ in Algorithm 1 is equivalent to Problem (3) with $\tilde{\mathbf{Q}} = \mathbf{Q} + \alpha \mathbf{I}$, $\mathbf{P} = [\nabla f(\mathbf{X}^t)(\mathbf{X}^t)^{\mathsf{T}}]_{\mathrm{BB}}$, and $\mathbf{Z} = \mathbf{U}_{\mathrm{B}}^{\mathsf{T}} \mathbf{X}^t$.
- (b) Assume that Formula (9) is used to choose \mathbf{Q} . Problem (3) further reduces to the following problem: $\bar{\mathbf{V}}^t \in \arg\min_{\mathbf{V} \in \mathrm{St}(k,k)} \mathcal{P}(\mathbf{V}) \triangleq \langle \mathbf{V}, \mathbf{P} \rangle + h(\mathbf{VZ})$. In particular, when $h(\mathbf{X}) \triangleq 0$, we obtain: $\bar{\mathbf{V}}^t = -\mathbb{P}_{\mathcal{M}}(\mathbf{P})$. Here, $\mathbb{P}_{\mathcal{M}}(\mathbf{P})$ is the nearest orthogonality matrix to \mathbf{P} .
- Remark 2.4. (a) By Claim (b) of Lemma 2.3, when k > 2, $h(\mathbf{X}) = 0$, and \mathbf{Q} is chosen to be a diagonal matrix as in Equation (9), the subproblem $\bar{\mathbf{V}}^t \in \arg\min_{\mathbf{V} \in \mathrm{St}(k,k)} \mathcal{K}(\mathbf{V}; \mathbf{X}^t, \mathbf{B})$ in Algorithm 1 can be solved exactly and efficiently due to our assumption, see Remark 2.6. (b) For general k and $h(\cdot)$, the subproblem may not admit a global solution. However, if a **local** stationary solution $\bar{\mathbf{V}}^t$ satisfying $(\bar{\mathbf{V}}^t; \mathbf{X}^t, \mathbf{B}) \leq \mathcal{K}(\mathbf{I}_k; \mathbf{X}^t, \mathbf{B})$ can be found, then the sufficient descent condition remains valid, and convergence to a weaker optimality condition for the final solution \mathbf{X}^{∞} is still achievable (see Inequalities (42), (44)).
- ▶ Smallest Possible Subproblems When k=2. We now discuss how to solve the subproblems exactly when k=2 and $h(\cdot) \neq 0$. The following lemma reveals an equivalent expression for any $\mathbf{V} \in \mathrm{St}(2,2)$.
- **Lemma 2.5.** (Proof in Appendix D.4) Any orthogonal matrix $\mathbf{V} \in \operatorname{St}(2,2)$ can be expressed as $\mathbf{V} = \mathbf{V}^{\operatorname{rot}}_{\theta}$ or $\mathbf{V} = \mathbf{V}^{\operatorname{rot}}_{\theta}$ for some $\theta \in \mathbb{R}$, where $\mathbf{V}^{\operatorname{rot}}_{\theta} \triangleq \begin{pmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{pmatrix}$, $\mathbf{V}^{\operatorname{ref}}_{\theta} \triangleq \begin{pmatrix} -\cos(\theta) & \sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix}$. We have $\det(\mathbf{V}^{\operatorname{rot}}_{\theta}) = 1$ and $\det(\mathbf{V}^{\operatorname{ref}}_{\theta}) = -1$ for any θ .

Using Lemma 2.5, we can reformulate Problem (3) as the following one-dimensional problem:

$$\bar{\theta} \in \arg\min_{\theta} \mathcal{P}(\mathbf{V}), s.t. \mathbf{V} \in \{\mathbf{V}_{\theta}^{\text{rot}}, \mathbf{V}_{\theta}^{\text{ref}}\}.$$

The optimal solution $\bar{\theta}$ can be identified even if $h(\cdot) \neq 0$ using a novel breakpoint searching method, which is discussed later in Section B in the Appendix.

Remark 2.6. (i) $\mathbf{V}_{\theta}^{\mathrm{rot}}$ and $\mathbf{V}_{\theta}^{\mathrm{ref}}$ are called Givens rotation matrix and Jacobi reflection matrix respectively in the literature (Sun & Bischof, 1995). Previous research only considered $\{\mathbf{V}_{\theta}^{\mathrm{rot}}\}$ for solving symmetric linear eigenvalue problems (Golub & Van Loan, 2013) and sparse PCA problems (Shalit & Chechik, 2014), while we use $\{\mathbf{V}_{\theta}^{\mathrm{ref}}, \mathbf{V}_{\theta}^{\mathrm{rot}}\}$ for solving Problem (1). (ii) We show the necessity of using $\{\mathbf{V}_{\theta}^{\mathrm{ref}}, \mathbf{V}_{\theta}^{\mathrm{rot}}\}$ in the following two examples of 2×2 optimization problems with orthogonality constraints: $\min_{\mathbf{V} \in \mathrm{St}(2,2)} F(\mathbf{V}) \triangleq \|\mathbf{V} - \mathbf{A}\|_{\mathrm{F}}^2$, and $\min_{\mathbf{V} \in \mathrm{St}(2,2)} F(\mathbf{V}) \triangleq \|\mathbf{V} - \mathbf{B}\|_{\mathrm{F}}^2 + 5\|\mathbf{V}\|_1$, where $\mathbf{A} = \begin{pmatrix} 1 & 0 \\ -1 & -1 \end{pmatrix}$ and $\mathbf{B} = \begin{pmatrix} 1 & 0 \\ 1 & 2 \end{pmatrix}$. The use of the reflection matrix $\mathbf{V}_{\theta}^{\mathrm{ref}}$ is essential in these examples because it results in lower objective values. See Section C.1 in the Appendix for more details.

3 OPTIMALITY ANALYSIS

This section provides the optimality analysis for **OBCD**. First, we establish the completeness of the proposed update scheme, showing that **OBCD** can reach any feasible point from an arbitrary initialization. Second, we analyze the optimality conditions of both Problem (1) and the associated subproblems of **OBCD**. Finally, by comparing these two sets of conditions, we derive a hierarchy of optimality, illustrating how the algorithm's stationarity relates to that of Problem (1).

- ▶ Basis Representation of Orthogonal Matrices. The following theorem is used to characterize any orthogonal matrix $\mathbf{D} \in \operatorname{St}(n,n)$ and $\mathbf{X} \in \operatorname{St}(n,r)$.
- **Theorem 3.1.** (*Proof in Appendix E.1*, Basis Representation of Orthogonal Matrices) Assume k = 2. For all $i \in [C_n^k]$, we define $\mathcal{W}_i \triangleq \mathbf{I}_n + \mathbf{U}_{\mathcal{B}_i}(\mathcal{V}_i \mathbf{I}_k)\mathbf{U}_{\mathcal{B}_i}^\mathsf{T} = \mathbf{U}_{\mathcal{B}_i}\mathcal{V}_i\mathbf{U}_{\mathcal{B}_i}^\mathsf{T} + \mathbf{U}_{\mathcal{B}_i^c}\mathbf{U}_{\mathcal{B}_i^c}^\mathsf{T}$, where $\mathcal{V}_i \in \mathrm{St}(2,2)$. We have:
- (a) Any matrix $\mathbf{D} \in \mathrm{St}(n,n)$ can be expressed as $\mathbf{D} = \mathcal{W}_{\mathrm{C}_n^k}...\mathcal{W}_2\mathcal{W}_1$ using suitable \mathcal{W}_i (which depends on \mathcal{V}_i). Furthermore, if $\forall i,\ \mathcal{V}_i = \mathbf{I}_2$, then $\mathbf{D} = \mathbf{I}_n$.
- (b) Any matrix $\mathbf{X} \in \operatorname{St}(n,r)$ can be expressed as $\mathbf{X} = \mathcal{W}_{C_n^k}...\mathcal{W}_2\mathcal{W}_1\mathbf{X}^0$ using suitable \mathcal{W}_i and any fixed constant matrix $\mathbf{X}^0 \in \operatorname{St}(n,r)$.
- **Remark 3.2.** (i) We use both Givens rotation and Jacobi reflection matrices to compute $\mathbf{D} \in \mathrm{St}(n,n)$. This is necessary since a reflection matrix cannot be represented through a sequence of rotations. (ii) The result in Claim (b) of Theorem 3.1 indicates that the proposed update scheme $\mathbf{X}^+ \Leftarrow \mathbf{X} + \mathrm{U_B}(\mathbf{V} \mathbf{I_k})\mathrm{U_B}^\mathsf{T}\mathbf{X}$ as shown in Formula (5) can reach any orthogonal matrix $\mathbf{X} \in \mathrm{St}(n,r)$ for any starting solution $\mathbf{X}^0 \in \mathrm{St}(n,r)$.
- ▶ First-Order Optimality Conditions for Problem (1). We provide the first-order optimality condition of Problem (1) (Wen & Yin, 2013; Chen et al., 2020). We use $\partial F(\mathbf{X})$ to denote the limiting subdifferential of $F(\mathbf{X})$ (Mordukhovich, 2006; Rockafellar & Wets., 2009), which is always nonempty since $F(\mathbf{X})$ is closed, proper, and lower semicontinuous. Given $f(\mathbf{X})$ is differentiable, we have $\partial F(\mathbf{X}) = \partial (f+h)(\mathbf{X}) = \nabla f(\mathbf{X}) + \partial h(\mathbf{X})$ (Rockafellar & Wets., 2009). We extend the definition of limiting subdifferential to introduce $\partial_{\mathcal{M}} F(\mathbf{X})$ as the Riemannian limiting subdifferential of $F(\mathbf{X})$ at \mathbf{X} , defined as $\partial_{\mathcal{M}} F(\mathbf{X}) \triangleq \partial F(\mathbf{X}) \ominus (\mathbf{X}[\partial F(\mathbf{X})]^{\mathsf{T}}\mathbf{X})$, where \ominus is the element-wise subtraction between sets.
- Introducing a Lagrangian multiplier matrix $\Lambda \in \mathbb{R}^{r \times r}$ for the orthogonality constraint, we define the following Lagrangian function of Problem (1): $\mathcal{L}(\mathbf{X}, \Lambda) = F(\mathbf{X}) + \frac{1}{2} \langle \mathbf{I}_r \mathbf{X}^\mathsf{T} \mathbf{X}, \Lambda \rangle$. Notably, the matrix Λ is symmetric, as $\mathbf{X}^\mathsf{T} \mathbf{X}$ is symmetric. We state the following definition of first-order optimality condition.
- **Definition 3.3.** Critical Point (Wen & Yin, 2013; Chen et al., 2020). A solution $\check{\mathbf{X}} \in \operatorname{St}(n,r)$ is a critical point of Problem (1) if: $\mathbf{0} \in \partial_{\mathcal{M}} F(\check{\mathbf{X}}) \triangleq \partial F(\check{\mathbf{X}}) \ominus (\check{\mathbf{X}}[\partial F(\check{\mathbf{X}})]^{\mathsf{T}}\check{\mathbf{X}})$, where $(\partial F(\check{\mathbf{X}}) \ominus \check{\mathbf{X}}[\partial F(\check{\mathbf{X}})]^{\mathsf{T}}\check{\mathbf{X}}) \triangleq \{\mathbf{G} \check{\mathbf{X}}\mathbf{G}^{\mathsf{T}}\check{\mathbf{X}} \mid \mathbf{G} \in \partial F(\check{\mathbf{X}})\}$. Furthermore, $\mathbf{\Lambda} \in [\partial F(\check{\mathbf{X}})]^{\mathsf{T}}\check{\mathbf{X}}$.
- **Remark 3.4.** The critical point condition in Lemma 3.3 can be equivalently expressed as (Absil et al., 2008; Jiang & Dai, 2015; Liu et al., 2016): $\mathbf{0} \in \mathbb{P}_{\mathbf{T}_{\mathbf{X}}\mathcal{M}}(\partial F(\mathbf{X}))$. Here, $\mathbf{T}_{\mathbf{X}}\mathcal{M}$ is the tangent space to \mathcal{M} at $\mathbf{X} \in \mathcal{M}$ with $\mathbf{T}_{\mathbf{X}}\mathcal{M} = \{\mathbf{Y} \in \mathbb{R}^{n \times r} \, | \, \mathbf{X}^\mathsf{T}\mathbf{Y} + \mathbf{Y}^\mathsf{T}\mathbf{X} = \mathbf{0}\}$.
- ▶ Optimality Conditions for the Subproblems. The Euclidean subdifferential of $\mathcal{K}(\mathbf{V}; \mathbf{X}^t, \mathsf{B}^t)$ w.r.t. \mathbf{V} can be computed as follows: $\ddot{\mathbf{G}}(\mathbf{V}) \triangleq \ddot{\mathbf{\Delta}} + \mathbf{U}_{\mathsf{B}}^{\mathsf{T}} [\nabla f(\mathbf{X}^t) + \partial h(\mathbf{X}^{t+1})] (\mathbf{X}^t)^{\mathsf{T}} \mathbf{U}_{\mathsf{B}}$, where $\ddot{\mathbf{\Delta}} = \max((\mathbf{Q} + \alpha \mathbf{I}_k) \mathrm{vec}(\mathbf{V} \mathbf{I}_k))$, and $\mathbf{X}^{t+1} = \mathbf{X}^t + \mathbf{U}_{\mathsf{B}} (\mathbf{V} \mathbf{I}_k) \mathbf{U}_{\mathsf{B}}^{\mathsf{T}} \mathbf{X}^t$. Using Lemma 3.3, we set the Riemannian subdifferential of $\mathcal{K}(\mathbf{V}; \mathbf{X}^t, \mathsf{B}^t)$ w.r.t. \mathbf{V} to zero and obtain the following first-order optimality condition for $\bar{\mathbf{V}}^t$: $\mathbf{0} \in \partial_{\mathcal{M}} \mathcal{K}(\bar{\mathbf{V}}^t; \mathbf{X}^t, \mathsf{B}^t) \triangleq \ddot{\mathbf{G}}(\bar{\mathbf{V}}^t) \ominus \bar{\mathbf{V}}^t \ddot{\mathbf{G}}(\bar{\mathbf{V}}^t)^{\mathsf{T}} \bar{\mathbf{V}}^t$.
- ▶ Optimality Conditions and Their Hierarchy. We introduce the following new optimality condition of block-k stationary points.
- **Definition 3.5.** (Global) Block-k Stationary Point, abbreviated as BS_k -point. Let $\alpha > 0$ and $k \geq 2$. A solution $\ddot{\mathbf{X}} \in St(n,r)$ is called a block-k stationary point if: $\forall \mathbf{B} \in \{\mathcal{B}_i\}_{i=1}^{C_n^k}$, $\mathbf{I}_k \in \arg\min_{\mathbf{V} \in St(k,k)} \mathcal{K}(\mathbf{V}; \ddot{\mathbf{X}}, \mathbf{B})$, where $\mathcal{K}(\cdot; \cdot, \cdot)$ is defined in Equation (10).

Remarks. BS_k-point states that if we *globally* minimize the majorization function $\mathcal{K}(\mathbf{V}; \ddot{\mathbf{X}}, \mathbb{B})$, there is no possibility of improving the objective function value for $\mathcal{K}(\mathbf{V}; \ddot{\mathbf{X}}, \mathbb{B})$ across all $\mathbb{B} \in \{\mathcal{B}_i\}_{i=1}^{C_n^k}$.

The following theorem establishes the relation between BS_k -points, standard critical points, and global optimal points.

Theorem 3.6. (*Proof in Appendix E.2*) We establish the following relationships:

(a) {critical points $\check{\mathbf{X}}$ } \supseteq {BS₂-points $\ddot{\mathbf{X}}$ }.

- (b) $\{BS_2\text{-points }\ddot{\mathbf{X}}\} \supseteq \{\text{global optimal points }\bar{\mathbf{X}}\}.$
- (c) $\{BS_k\text{-points }\ddot{\mathbf{X}}\}\supseteq \{BS_{k+1}\text{-points }\ddot{\mathbf{X}}\}$, where $k\in \{2,3,\ldots,n-1\}$.
- (d) The reverse of the above three inclusions may not always hold true.

Remark 3.7. (i) The optimality of BS_2 -points is stronger than that of standard critical points (Wen & Yin, 2013; Chen et al., 2020; Absil et al., 2008). (ii) Testing whether a solution $\mathbf X$ is a BS_k -points deterministically requires solving all C_n^k subproblems. However, by randomly selecting the working set B from the C_n^k possible combinations $\{\mathcal{B}_i\}_{i=1}^{C_n^k}$, one can test whether $\mathbf X$ is a BS_k -point in expectation.

4 Convergence Analysis

This section establishes the iteration complexity and last-iterate (non-ergodic) convergence rates of the proposed **OBCD** algorithm. We first prove a sufficient descent property, followed by an ergodic convergence rate typical in nonconvex optimization. We then analyze iteration complexity under the Riemannian subgradient condition, commonly used in nonsmooth manifold settings. Finally, we derive a last-iterate convergence rate based on the KL inequality.

Throughout this section, we assume that the working set is determined by a random strategy and that the global minimizer $\bar{\mathbf{V}}^t \in \arg\min_{\mathbf{V} \in \mathrm{St}(k,k)} \mathcal{K}(\mathbf{V}; \mathbf{X}^t, \mathcal{B})$ can be computed. The algorithm **OBCD** then generates a random output $(\bar{\mathbf{V}}^t, \mathbf{X}^{t+1})$ for $t = 0, 1, \ldots, \infty$, depending on the realization of the random variable $\xi^t \triangleq (\mathbb{B}^1, \mathbb{B}^2, \ldots, \mathbb{B}^t)$. We denote \mathbf{X}^∞ as an arbitrary limit point of **OBCD**.

4.1 ITERATION COMPLEXITY Initially, we introduce the notation of ϵ -B

Initially, we introduce the notation of ϵ -BS $_k$ -point as follows.

Definition 4.1. $(\epsilon \text{-BS}_k \text{-point})$ Given any constant $\epsilon > 0$, a point $\ddot{\mathbf{X}}$ is called an $\epsilon \text{-BS}_k \text{-point}$ if: $\frac{1}{C_n^k} \sum_{i=1}^{C_n^k} \operatorname{dist}(\mathbf{I}_k, \arg\min_{\mathbf{V}} \mathcal{K}(\mathbf{V}; \ddot{\mathbf{X}}, \mathcal{B}_i))^2 \leq \epsilon$, where $\mathcal{K}(\cdot; \cdot, \cdot)$ is defined in Equation (10). Here, the set $\{\mathcal{B}_1, \mathcal{B}_2, ..., \mathcal{B}_{C_n^k}\}$ denotes all possible combinations of the index vectors choosing k items from n without repetition, and $\operatorname{dist}(\Xi, \Xi')$ denotes the distance between two sets Ξ and Ξ' .

Using the optimality measure from Definition 4.1, we establish the iteration complexity of **OBCD**.

Theorem 4.2. (Proof in Appendix F.1) We define $\tilde{c} \triangleq \frac{2}{\alpha} \cdot (F(\mathbf{X}^0) - F(\mathbf{X}^\infty)) \geq 0$. We have:

(a) The following sufficient decrease condition holds for all $t \geq 0$:

$$\frac{\alpha}{2} \|\mathbf{X}^{t+1} - \mathbf{X}^t\|_{\mathsf{F}}^2 \leq \frac{\alpha}{2} \|\bar{\mathbf{V}}^t - \mathbf{I}_k\|_{\mathsf{F}}^2 \leq F(\mathbf{X}^t) - F(\mathbf{X}^{t+1}).$$

(b) If the B^t is selected from $\{\mathcal{B}_i\}_{i=1}^{C_n^k}$ randomly and uniformly, **OBCD** finds an ϵ -BS_k-point of Problem (1) in at most T iterations in the sense of expectation, where $T \geq \lceil \frac{\tilde{c}}{\epsilon} \rceil$.

Remark 4.3. Theorem 4.2 shows that **OBCD** converges to ϵ -block-k stationary points with an iteration complexity of $\mathcal{O}(1/\epsilon)$, which is typical for general nonconvex optimization.

Apart from Definition 4.1, another common optimality measure relies on the Riemannian subgradient. To this end, we present the following lemma.

Lemma 4.4. (Proof in Appendix F.2, Riemannian Subgradient Lower Bound for the Iterates Gap) Assume $\|\nabla f(\mathbf{X})\|_{sp} \leq l_f$, $\|\partial h(\mathbf{X})\|_{sp} \leq l_h$ for all $\mathbf{X} \in \operatorname{St}(n,r)$ with $l_f, l_h > 0$. The Riemannian subdifferential of $\mathcal{K}(\mathbf{V}; \mathbf{X}^t, \mathbb{B}^t)$ at the point $\mathbf{V} = \mathbf{I}_k$ can be computed as: $\partial_{\mathcal{M}} \mathcal{K}(\mathbf{I}_k; \mathbf{X}^t, \mathbb{B}^t) = \mathbf{U}_{\mathbb{B}^t}^{\mathsf{T}}(\mathbb{D} \ominus \mathbb{D}^{\mathsf{T}})\mathbf{U}_{\mathbb{B}^t}$, where $\mathbb{D} = [\nabla f(\mathbf{X}^t) + \partial h(\mathbf{X}^t)][\mathbf{X}^t]^{\mathsf{T}}$. We have:

 $\textbf{(a)} \ \ \mathbb{E}_{\xi^{t+1}}[\mathrm{dist}(\mathbf{0},\partial_{\mathcal{M}}\mathcal{K}(\mathbf{I}_k;\mathbf{X}^{t+1},\mathbf{B}^{t+1}))] \leq \phi \cdot \mathbb{E}_{\xi^t}[\|\bar{\mathbf{V}}^t - \mathbf{I}_k\|_{\mathsf{F}}], \text{ where } \phi \triangleq 4(l_f + l_h + L_f) + 2\alpha.$

```
(b) \mathbb{E}_{\xi^t}[\operatorname{dist}(\mathbf{0}, \partial_{\mathcal{M}} F(\mathbf{X}^t))] \leq \gamma \cdot \mathbb{E}_{\xi^t}[\operatorname{dist}(\mathbf{0}, \partial_{\mathcal{M}} \mathcal{K}(\mathbf{I}_k; \mathbf{X}^t, \mathbf{B}^t))], \text{ where } \gamma \triangleq (\mathbf{C}_n^k / \mathbf{C}_{n-2}^{k-2})^{1/2}.
```

Remark 4.5. The important class of nonsmooth ℓ_1 norm function $h(\mathbf{X}) = \|\mathbf{X}\|_1$ (Chen et al., 2020; 2024) satisfies the assumption made in Lemma 4.4.

We establish the iteration complexity of **OBCD** using the optimality measure of Riemannian subgradient (Chen et al., 2020; Cheung et al., 2024; Li et al., 2024b).

Theorem 4.6. (Proof in Appendix F.3) We define $\tilde{c} \triangleq \frac{2}{\alpha} \cdot (F(\mathbf{X}^0) - F(\mathbf{X}^\infty))$, and $\{\phi, \gamma\}$ as in Lemma 4.4. **OBCD** finds an ϵ -critical point of Problem (1) satisfying $\mathbb{E}_{\xi^{\bar{t}}}[\operatorname{dist}^2(\mathbf{0}, \partial_{\mathcal{M}} F(\mathbf{X}^{\bar{t}+1}))] \leq \epsilon$ in at most T+1 iterations in the sense of expectation, where $T \geq \lceil \frac{\gamma^2 \phi^2 \tilde{c}}{\epsilon} \rceil$.

4.2 Convergence Rate under KL Inequality

We establish the non-ergodic convergence rate of **OBCD** using the Kurdyka-Łojasiewicz inequality, a key tool in non-convex analysis (Attouch et al., 2010; Bolte et al., 2014; Liu et al., 2016).

Initially, we make the following additional assumption.

Assumption 4.7. The function $F_{\iota}(\mathbf{X}) = F(\mathbf{X}) + \iota_{\mathcal{M}}(\mathbf{X})$ is a KL function.

We present the following useful proposition, due to (Attouch et al., 2010; Bolte et al., 2014).

Proposition 4.8. (Kurdyka-Łojasiewicz Property). For a KL function $F_{\iota}(\mathbf{X})$ with $\mathbf{X} \in \text{dom } F_{\iota}$, there exists $\sigma \in [0,1), \ \eta \in (0,+\infty]$, a neighborhood Υ of \mathbf{X}^{∞} , and a concave continuous function $\varphi(t) = ct^{1-\sigma}, \ c > 0, \ t \in [0,\eta)$ such that for all $\mathbf{X}' \in \Upsilon$ that satisfies $F_{\iota}(\mathbf{X}') \in (F_{\iota}(\mathbf{X}^{\infty}), F_{\iota}(\mathbf{X}^{\infty}) + \eta)$, it holds that $\operatorname{dist}(\mathbf{0}, \partial F_{\iota}(\mathbf{X}')) \varphi'(F_{\iota}(\mathbf{X}') - F_{\iota}(\mathbf{X}^{\infty})) \geq 1$.

Utilizing the Kurdyka-Łojasiewicz property, one can establish a finite-length property of **OBCD**, a result considerably stronger than that of Theorem 4.2.

Theorem 4.9. (Proof in Appendix F.4, A Finite Length Property). We define $E_{t+1} \triangleq \mathbb{E}_{\xi^t}[\|\bar{\mathbf{V}}^t - \mathbf{I}_k\|_{\mathsf{F}}]$, and $D_i = \sum_{j=i}^{\infty} E_{j+1}$. Based on the continuity assumption made in Lemma 4.4, We have:

- (a) It holds that $(E_{t+1})^2 \leq \kappa E_t(\varphi^t \varphi^{t+1})$, where $\varphi^t \triangleq \varphi(F(\mathbf{X}^t) F(\mathbf{X}^\infty))$, $\kappa \triangleq \frac{2\gamma\phi}{\alpha}$ is a positive constant, $\gamma \triangleq (C_n^k/C_{n-2}^{k-2})^{1/2}$, ϕ is defined in Lemma 4.4, and $\varphi(\cdot)$ is the desingularization function defined in Proposition 4.8.
- (b) It holds that $\forall t \geq 1$, $D_t \leq E_t + 2\kappa \varphi^t$. The sequence $\{E_t\}_{t=1}^{\infty}$ has the finite length property that $D_t \triangleq \sum_{i=t}^{\infty} E_{i+1}$ is always upper-bounded by a certain constant for all t > 1.

Finally, we establish the last-iterate convergence rate for **OBCD**.

Theorem 4.10. (Proof in Appendix F.5). Based on the continuity assumption made in Lemma 4.4, there exists t' such that for all t > t', we have:

- (a) If $\sigma = 0$, then the sequence \mathbf{X}^t converges in a finite number of steps in expectation.
- (b) If $\sigma \in (0, \frac{1}{2}]$, then there exist $\dot{c} > 0$ and $\dot{\tau} \in [0, 1)$ such that $\mathbb{E}_{\varepsilon^{t-1}}[\|\mathbf{X}^t \mathbf{X}^{\infty}\|_{\mathsf{F}}] \leq \dot{c}\dot{\tau}^t$.
- (c) If $\sigma \in (\frac{1}{2}, 1)$, then there exist $\dot{c} > 0$ such that $\mathbb{E}_{\varepsilon^{t-1}}[\|\mathbf{X}^t \mathbf{X}^{\infty}\|_{\mathsf{F}}] \leq \mathcal{O}(t^{-(1-\sigma)/(2\sigma-1)})$.

Remark 4.11. When $F(\mathbf{X})$ is a semi-algebraic function and the desingularising function is $\varphi(t) = ct^{1-\sigma}$ for some c>0 and $\sigma\in[0,1)$, Theorem 4.10 shows that **OBCD** converges in finite iterations when $\sigma=0$, with linear convergence when $\sigma\in(0,\frac{1}{2}]$, and sublinear convergence when $\sigma\in(\frac{1}{2},1)$ for the gap $\|\mathbf{X}^t-\mathbf{X}^\infty\|_{\mathsf{F}}$ in expectation. These results are consistent with those in (Attouch et al., 2010).

5 EXPERIMENTS

This section presents numerical comparisons between **OBCD** and state-of-the-art methods on both real-world and synthetic data for L_0 norm-based Sparse PCA (SPCA). Appendix Section G.1 describes how to generate the data sets in the experiments.

▶ Compared Methods. We compare against three operator splitting methods: Linearized ADMM (LADMM) (Lai & Osher, 2014; He & Yuan, 2012), Riemannian ADMM (RADMM) (Li et al., 2024a), and the Smoothing Penalty Method (SPM) (Lai & Osher, 2014; Chen, 2012). Each method is initialized with either a random or identity matrix, yielding six variants: LADMM(id), RADMM(id), SPM(id), LADMM(rnd), RADMM (rnd), and SPM(rnd). For OBCD, we adopt a random working set strategy with identity initialization, denoted as OBCD-R(id).

data-m-n	LADMM	RADMM	SPM	LADMM	RADMM	SPM	OBCD-R	data-m-n	LADMM	RADMM	SPM	LADMM	RADMM	SPM	OBCD-R
	(id)	(id)	(id)	(rnd)	(rnd)	(rnd)	(id)	cuttu III II	(id)	(id)	(id)	(rnd)	(rnd)	(rnd)	(id)
$r = 20$, $\lambda = 10$, time limit=30							$r = 20$, $\lambda = 50$, time limit=30								
w1a-2477-300	199.897	219.698	199.897	259.825	239.717	259.672	199.667	w1a-2477-300	999.891	1099.730	1099.889	1249.723	1049.707	1649.675	999.667
TDT2-500-1000	199.997	359.382	199.997	389.376	269.292	389.260	199.258	TDT2-500-1000	1049.997	1099.288	999.460	1049.282	1249.280	2149.271	999.257
20News-8000-1000	199.995	219.673	199.995	239.301	219.243	349.228	199.222	20News-8000-1000	1149.995	1149.501	999.549	3649.247	1049.326	1799.228	999.222
sector-6412-1000	199.980	349.793	199.980	749.996	249.813	369.651	199.649	sector-6412-1000	2449.886	1799.904	999.816	1549.998	1749.952	1399.651	999.649
E2006-2000-1000	199.999	239.115	199.999	269.128	219.084	709.095	199.077	E2006-2000-1000	1099.283	1249.109	999.284	1849.115	1349.085	2549.136	999.077
MNIST-60000-784	199.985	379.893	199.985	289.917	339.910	1339.774	199.896	MNIST-60000-784	999.985	1699.913	2849.852	1399.921	1649.905	4349.781	999.896
Gisette-3000-1000	199.980	339.979	199.980	539.979	369.981	1639.952	199.979	Gisette-3000-1000	999.980	1649.980	999.980	10399.983	2249.976	6899.967	999.979
CnnCal-3000-1000	199.981	429.979	199.981	689.970	379.979	909.931	199.946	CnnCal-3000-1000	999.981	2499.981	1049.969	4599.973	2649.981	3499.938	999.946
Cifar-1000-1000	199.979	479.979	199.979	1449.982	429.975	2169.934	199.974	Cifar-1000-1000	1099.979	1449.978	999.979	2149.979	3149.974	4349.972	999.974
randn-500-1000	199.980	469.980	199.980	409.980	389.980	1349.975	199.977	randn-500-1000	1349.980	2449.980	3949.977	1299.981	1749.980	4249.976	999.977
	LADMM	RADMM	SPM	LADMM	RADMM	SPM	OBCD-R		LADMM	RADMM	SPM	LADMM	RADMM	SPM	OBCD-R
· · · · · · ·	(id)	(id)	(id)	(rnd)	(rnd)	(rnd)	(id)	data-m-n	(id)	(id)	(id)	(rnd)	(rnd)	(rnd)	(id)
	(id)			(rnd)				data-m-n		(id)		(rnd)			
w1a-2477-300	(id) 2499.912		(id)	(rnd)				data-m-n w1a-2477-300		(id)	(id)	(rnd)			
	<u> </u>	r = 20	(id) $\lambda = 100$, tir	(rnd) ne limit=30	(rnd)	(rnd)	(id)		(id)	(id) $r = 20$,	(id) $\lambda = 500$, tin	(rnd) ne limit=30	(rnd)	(rnd)	(id)
w1a-2477-300	2499.912	r = 20, 2799.713	(id) $\lambda = 100$, tin 2199.819	(rnd) ne limit=30 2399.723	(rnd) 2499.708	(rnd) 3299.662	(id) 1999.667	w1a-2477-300	(id) 11999.706	(id) r = 20, 10999.702	(id) , λ = 500, tin 16499.714	(rnd) ne limit=30 10499.702	(rnd) 9999.711	(rnd) 14499.667	(id) 9999.667
w1a-2477-300 TDT2-500-1000	2499.912 2199.515	r = 20, 2799.713 2199.302	(id) $\lambda = 100$, tir 2199.819 1999.432	(rnd) ne limit=30 2399.723 8799.310	(rnd) 2499.708 2699.278	(rnd) 3299.662 2499.257	(id) 1999.667 1999.258	w1a-2477-300 TDT2-500-1000	(id) 11999.706 10499.273	(id) r = 20, 10999.702 15999.294	(id) , λ = 500, tir 16499.714 10999.395	(rnd) ne limit=30 10499.702 10499.368	(rnd) 9999.711 15499.281	(rnd) 14499.667 12499.256	(id) 9999.667 9999.258
w1a-2477-300 TDT2-500-1000 20News-8000-1000	2499.912 2199.515 2699.480	r = 20, 2799.713 2199.302 2199.262	(id) $\lambda = 100$, tir 2199.819 1999.432 1999.440	(rnd) ne limit=30 2399.723 8799.310 2099.242	(rnd) 2499.708 2699.278 1999.230	3299.662 2499.257 3999.224	1999.667 1999.258 1999.222	w1a-2477-300 TDT2-500-1000 20News-8000-1000	(id) 11999.706 10499.273 9999.347	r = 20, 10999.702 15999.294 11499.281	(id) , λ = 500, tin 16499.714 10999.395 11499.328	rnd) ne limit=30 10499.702 10499.368 10999.454	9999.711 15499.281 10499.258	(rnd) 14499.667 12499.256 14499.232	(id) 9999.667 9999.258 9999.222
w1a-2477-300 TDT2-500-1000 20News-8000-1000 sector-6412-1000	2499.912 2199.515 2699.480 7799.995	r = 20, 2799.713 2199.302 2199.262 4599.977	(id) $\lambda = 100$, tir 2199.819 1999.432 1999.440 2099.716	(rnd) ne limit=30 2399.723 8799.310 2099.242 3099.999	(rnd) 2499.708 2699.278 1999.230 4399.973	3299.662 2499.257 3999.224 2199.651	1999.667 1999.258 1999.222 1999.649	w1a-2477-300 TDT2-500-1000 20News-8000-1000 sector-6412-1000	(id) 11999.706 10499.273 9999.347 13999.997	r = 20, 10999.702 15999.294 11499.281 16999.992	(id) λ = 500, tin 16499.714 10999.395 11499.328 12999.660	rnd) ne limit=30 10499.702 10499.368 10999.454 22999.999	9999.711 15499.281 10499.258 18999.986	(rnd) 14499.667 12499.256 14499.232 13499.649	9999.667 9999.258 9999.222 9999.649
w1a-2477-300 TDT2-500-1000 20News-8000-1000 sector-6412-1000 E2006-2000-1000	2499.912 2199.515 2699.480 7799.995 2099.207	r = 20, 2799.713 2199.302 2199.262 4599.977 3199.083	(id) $\lambda = 100$, tir 2199.819 1999.432 1999.440 2099.716 1999.284	(rnd) ne limit=30 2399.723 8799.310 2099.242 3099.999 2599.106	2499.708 2699.278 1999.230 4399.973 2299.085	3299.662 2499.257 3999.224 2199.651 4399.081	1999.667 1999.258 1999.222 1999.649 1999.077	w1a-2477-300 TDT2-500-1000 20News-8000-1000 sector-6412-1000 E2006-2000-1000	(id) 11999.706 10499.273 9999.347 13999.997 9999.918	$\begin{array}{c} (\text{id}) \\ \hline r = 20, \\ \hline 10999.702 \\ 15999.294 \\ 11499.281 \\ 16999.992 \\ 14499.080 \\ \end{array}$	(id) $\lambda = 500$, tir 16499.714 10999.395 11499.328 12999.660 9999.284	(rnd) ne limit=30 10499.702 10499.368 10999.454 22999.999 26499.095	9999.711 15499.281 10499.258 18999.986 10499.082	14499.667 12499.256 14499.232 13499.649 21499.081	9999.667 9999.258 9999.222 9999.649 9999.077
w1a-2477-300 TDT2-500-1000 20News-8000-1000 sector-6412-1000 E2006-2000-1000 MNIST-60000-784	2499.912 2199.515 2699.480 7799.995 2099.207 1999.984	r = 20, 2799.713 2199.302 2199.262 4599.977 3199.083 3199.904	(id) $\lambda = 100$, tir 2199.819 1999.432 1999.440 2099.716 1999.284 11799.715	(rnd) ne limit=30 2399.723 8799.310 2099.242 3099.999 2599.106 3199.922	2499.708 2699.278 1999.230 4399.973 2299.085 3599.907	3299.662 2499.257 3999.224 2199.651 4399.081 8299.829	1999.667 1999.258 1999.222 1999.649 1999.077 1999.896	w1a-2477-300 TDT2-500-1000 20News-8000-1000 sector-6412-1000 E2006-2000-1000 MNIST-60000-784	(id) 11999.706 10499.273 9999.347 13999.997 9999.918 19499.965	$\begin{array}{c} (\mathrm{id}) \\ \hline r = 20, \\ 10999.702 \\ 15999.294 \\ 11499.281 \\ 16999.992 \\ 14499.080 \\ 20499.886 \\ \end{array}$	(id) , $\lambda = 500$, tii 16499.714 10999.395 11499.328 12999.660 9999.284 39499.844	(rnd) ne limit=30 10499.702 10499.368 10999.454 22999.999 26499.095 11999.911	9999.711 15499.281 10499.258 18999.986 10499.082 16999.905	14499.667 12499.256 14499.232 13499.649 21499.081 47999.705	9999.667 9999.258 9999.222 9999.649 9999.077 9999.896
w1a-2477-300 TDT2-500-1000 20News-8000-1000 sector-6412-1000 E2006-2000-1000 MNIST-60000-784 Gisette-3000-1000	2499.912 2199.515 2699.480 7799.995 2099.207 1999.984 2199.980	r = 20, 2799.713 2199.302 2199.262 4599.977 3199.083 3199.904 4299.979	(id) $\lambda = 100$, tin 2199.819 1999.432 1999.440 2099.716 1999.284 11799.715 1999.980	(rnd) me limit=30 2399.723 8799.310 2099.242 3099.999 2599.106 3199.922 2499.982	(rnd) 2499.708 2699.278 1999.230 4399.973 2299.085 3599.907 2799.981	(md) 3299.662 2499.257 3999.224 2199.651 4399.081 8299.829 11499.971	1999.667 1999.258 1999.222 1999.649 1999.077 1999.896 1999.979	w1a-2477-300 TDT2-500-1000 20News-8000-1000 sector-6412-1000 E2006-2000-1000 MNIST-60000-784 Gisette-3000-1000	(id) 11999.706 10499.273 9999.347 13999.997 9999.918 19499.965 14999.980	r = 20, 10999.702 15999.294 11499.281 16999.992 14499.080 20499.886 16499.979	(id) \$\lambda = 500, \text{ tir} 16499.714 10999.395 11499.328 12999.660 9999.284 39499.844 9999.980	(md) me limit=30 10499.702 10499.368 10999.454 22999.999 26499.095 11999.911 15499.980	9999.711 15499.281 10499.258 18999.986 10499.082 16999.905 16999.978	(rnd) 14499.667 12499.256 14499.232 13499.649 21499.081 47999.705 36499.977	9999.667 9999.258 9999.222 9999.649 9999.077 9999.896 9999.979

Table 1: Comparisons of objective values for L_0 norm-based SPCA. The 1^{st} , 2^{nd} , and 3^{rd} best results are colored with red. green and blue, respectively.

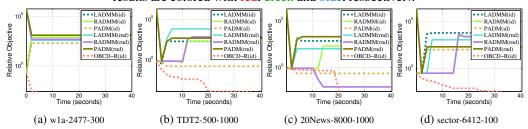


Figure 1: The convergence curve for solving L_0 norm-based SPCA with $\lambda = 100$. No matter how long the algorithms run, the other methods remain trapped in poor local minima.

- ▶ Implementations. All methods are implemented in MATLAB on an Intel 2.6 GHz CPU with 32 GB RAM. However, our breakpoint searching procedure is developed in C++ and integrated into the MATLAB environment ², as it requires inefficient element-wise loops in native MATLAB. Code to reproduce the experiments can be found in the **supplemental material**.
- ▶ Experiment Settings. We compare objective values $F(\mathbf{X})$ for different methods after running for 30 seconds. For numerical stability in reporting the objectives, we use the count of elements with absolute values greater than a threshold of 10^{-6} instead of the original ℓ_0 norm function $\|\mathbf{X}\|_0$. We set $\alpha = 10^{-5}$ for **OBCD**. Full-gradient methods have higher per-iteration complexity but require fewer iterations, while **OBCD**, as a partial-gradient method, has lower per-iteration costs but needs more iterations. Thus, we compare based on CPU time rather than iteration count.
- ▶ Experiment Results. Table 1 and Figure 1 display accuracy and computational efficiency results for L_0 norm-based SPCA, yielding the following observations: (i) OBCD-R delivers the best performance. (ii) Unlike other methods where objectives fluctuate during iterations, OBCD-R monotonically decreases the objective function while maintaining the orthogonality constraint. This is because OBCD is a greedy descent method for this problem class. (iii) While other methods often get stuck in poor local minima, OBCD-R escapes from such minima and generally finds lower objectives, aligning with our theory that our methods locate stronger stationary points.

6 CONCLUSIONS

In this paper, we introduced **OBCD**, a new block coordinate descent method for nonsmooth composite optimization under orthogonality constraints. **OBCD** operates on k rows of the solution matrix, offering lower computational complexity per iteration for $k \geq 2$. We also provide a novel optimality analysis, showing how **OBCD** exploits problem structure to escape bad local minima and find better stationary points than methods focused on critical points. Under the Kurdyka-Lojasiewicz (KL) inequality, we establish strong limit-point convergence. Additionally, we show how novel breakpoint search methods can be used to solve the subproblem when k=2. Extensive experiments demonstrate that **OBCD** outperforms existing methods.

7 LLM USAGE

A large language model (LLM) was used to assist in refining the writing of this paper.

²Although we prioritize accuracy over speed, the comparisons remain fair, as the other methods based on matrix multiplication and SVD rely on highly optimized BLAS and LAPACK libraries.

REFERENCES

- Traian E Abrudan, Jan Eriksson, and Visa Koivunen. Steepest descent algorithms for optimization under unitary matrix constraint. *IEEE Transactions on Signal Processing*, 56(3):1134–1147, 2008.
- Pierre-Antoine Absil, Robert E. Mahony, and Rodolphe Sepulchre. *Optimization Algorithms on Matrix Manifolds*. Princeton University Press, 2008.
 - Hedy Attouch, Jérôme Bolte, Patrick Redont, and Antoine Soubeyran. Proximal alternating minimization and projection methods for nonconvex problems: An approach based on the kurdykalojasiewicz inequality. *Mathematics of Operations Research*, 35(2):438–457, 2010.
 - Nitin Bansal, Xiaohan Chen, and Zhangyang Wang. Can we gain more from orthogonality regularizations in training deep networks? *Advances in Neural Information Processing Systems*, 31, 2018.
 - Adel Bibi, Bernard Ghanem, Vladlen Koltun, and René Ranftl. Deep layers as stochastic solvers. In *International Conference on Learning Representations (ICLR)*, 2019.
 - Jérôme Bolte, Shoham Sabach, and Marc Teboulle. Proximal alternating linearized minimization for nonconvex and nonsmooth problems. *Mathematical Programming*, 146(1-2):459–494, 2014.
 - Arnaud Breloy, Sandeep Kumar, Ying Sun, and Daniel P Palomar. Majorization-minimization on the stiefel manifold with application to robust sparse pca. *IEEE Transactions on Signal Processing*, 69:1507–1520, 2021.
 - Shixiang Chen, Shiqian Ma, Anthony Man-Cho So, and Tong Zhang. Proximal gradient method for nonsmooth optimization over the stiefel manifold. *SIAM Journal on Optimization*, 30(1): 210–239, 2020.
 - Shixiang Chen, Shiqian Ma, Anthony Man-Cho So, and Tong Zhang. Nonsmooth optimization over the stiefel manifold and beyond: Proximal gradient method and recent variants. *SIAM Review*, 66 (2):319–352, 2024.
 - Weiqiang Chen, Hui Ji, and Yanfei You. An augmented lagrangian method for ℓ_1 -regularized optimization problems with orthogonality constraints. *SIAM Journal on Scientific Computing*, 38(4): B570–B592, 2016.
 - Xiaojun Chen. Smoothing methods for nonsmooth, nonconvex minimization. *Mathematical programming*, 134:71–99, 2012.
 - Andy Yat-Ming Cheung, Jinxin Wang, Man-Chung Yue, and Anthony Man-Cho So. Randomized submanifold subgradient method for optimization over stiefel manifolds. *arXiv preprint arXiv:2409.01770*, 2024.
 - Minhyung Cho and Jaehyung Lee. Riemannian approach to batch normalization. *Advances in Neural Information Processing Systems*, 30, 2017.
 - Michael Cogswell, Faruk Ahmed, Ross B. Girshick, Larry Zitnick, and Dhruv Batra. Reducing overfitting in deep networks by decorrelating representations. In Yoshua Bengio and Yann LeCun (eds.), *International Conference on Learning Representations (ICLR)*, 2016.
 - Alexandre d'Aspremont, Francis Bach, and Laurent El Ghaoui. Optimal solutions for sparse principal component analysis. *Journal of Machine Learning Research*, 9(7), 2008.
 - Alan Edelman, Tomás A. Arias, and Steven Thomas Smith. The geometry of algorithms with orthogonality constraints. *SIAM Journal on Matrix Analysis and Applications*, 20(2):303–353, 1998.
 - Thomas Frerix and Joan Bruna. Approximating orthogonal matrices with effective givens factorization. In *International Conference on Machine Learning (ICML)*, pp. 1993–2001, 2019.
 - Bin Gao, Xin Liu, Xiaojun Chen, and Ya-xiang Yuan. A new first-order algorithmic framework for optimization problems with orthogonality constraints. *SIAM Journal on Optimization*, 28(1): 302–332, 2018.

- Bin Gao, Xin Liu, and Ya-xiang Yuan. Parallelizable algorithms for optimization problems with orthogonality constraints. *SIAM Journal on Scientific Computing*, 41(3):A1949–A1983, 2019.
- Gene H Golub and Charles F Van Loan. Matrix computations. 2013.
 - David H Gutman and Nam Ho-Nguyen. Coordinate descent without coordinates: Tangent subspace descent on riemannian manifolds. *Mathematics of Operations Research*, 48(1):127–159, 2023.
 - Bingsheng He and Xiaoming Yuan. On the $\mathcal{O}(1/n)$ convergence rate of the douglas-rachford alternating direction method. SIAM Journal on Numerical Analysis, 50(2):700–709, 2012.
 - Jiang Hu, Xin Liu, Zai-Wen Wen, and Ya-Xiang Yuan. A brief introduction to manifold optimization. *Journal of the Operations Research Society of China*, 8(2):199–248, 2020.
 - Feihu Huang and Shangqian Gao. Gradient descent ascent for minimax problems on riemannian manifolds. *IEEE Trans. Pattern Anal. Mach. Intell.*, 45(7):8466–8476, 2023.
 - Seong Jae Hwang, Maxwell D. Collins, Sathya N. Ravi, Vamsi K. Ithapu, Nagesh Adluru, Sterling C. Johnson, and Vikas Singh. A projection free method for generalized eigenvalue problem with a nonsmooth regularizer. In *IEEE International Conference on Computer Vision (ICCV)*, pp. 1841–1849, 2015.
 - Bo Jiang and Yu-Hong Dai. A framework of constraint preserving update schemes for optimization on stiefel manifold. *Mathematical Programming*, 153(2):535–575, 2015.
 - Bo Jiang, Ya-Feng Liu, and Zaiwen Wen. ℓ_p -norm regularization algorithms for optimization over permutation matrices. *SIAM Journal on Optimization*, 26(4):2284–2313, 2016.
 - Bo Jiang, Xiang Meng, Zaiwen Wen, and Xiaojun Chen. An exact penalty approach for optimization with nonnegative orthogonality constraints. *Mathematical Programming*, pp. 1–43, 2022.
 - Michel Journée, Yurii Nesterov, Peter Richtárik, and Rodolphe Sepulchre. Generalized power method for sparse principal component analysis. *Journal of Machine Learning Research*, 11 (2), 2010.
 - Rongjie Lai and Stanley Osher. A splitting method for orthogonality constrained problems. *Journal of Scientific Computing*, 58(2):431–449, 2014.
 - Jiaxiang Li, Shiqian Ma, and Tejes Srivastava. A riemannian alternating direction method of multipliers. *Mathematics of Operations Research*, 2024a.
 - Xiao Li, Shixiang Chen, Zengde Deng, Qing Qu, Zhihui Zhu, and Anthony Man-Cho So. Weakly convex optimization over stiefel manifold using riemannian subgradient-type methods. *SIAM Journal on Optimization*, 31(3):1605–1634, 2021.
 - Yuchen Li, Laura Balzano, Deanna Needell, and Hanbaek Lyu. Convergence and complexity of block majorization-minimization for constrained block-riemannian optimization. *arXiv* preprint arXiv:2312.10330, 2023.
 - Yuchen Li, Laura Balzano, Deanna Needell, and Hanbaek Lyu. Convergence and complexity guarantee for inexact first-order riemannian optimization algorithms. In *International Conference on Machine Learning (ICML)*, 2024b.
 - Huikang Liu, Weijie Wu, and Anthony Man-Cho So. Quadratic optimization with orthogonality constraints: Explicit lojasiewicz exponent and linear convergence of line-search methods. In *International Conference on Machine Learning (ICML)*, pp. 1158–1167, 2016.
 - Huikang Liu, Man-Chung Yue, and Anthony Man-Cho So. On the estimation performance and convergence rate of the generalized power method for phase synchronization. *SIAM Journal on Optimization*, 27(4):2426–2446, 2017.
 - Xin Liu, Xiao Wang, Zaiwen Wen, and Yaxiang Yuan. On the convergence of the self-consistent field iteration in kohn–sham density functional theory. *SIAM Journal on Matrix Analysis and Applications*, 35(2):546–558, 2014.

- Zhihua Lu and Yi Zhang. An augmented lagrangian approach for sparse principal component analysis. *Mathematical Programming*, 135(1-2):149–193, 2012.
 - Julien Mairal. Optimization with first-order surrogate functions. In *International Conference on Machine Learning (ICML)*, volume 28, pp. 783–791, 2013.
 - Estelle Massart and Vinayak Abrol. Coordinate descent on the orthogonal group for recurrent neural network training. In *Proceedings of the AAAI Conference on Artificial Intelligence (AAAI)*, volume 36, pp. 7744–7751, 2022.
 - Boris S. Mordukhovich. Variational analysis and generalized differentiation i: Basic theory. *Berlin Springer*, 330, 2006.
 - Yurii Nesterov. *Introductory lectures on convex optimization: A basic course*, volume 87. Springer Science & Business Media, 2003.
 - Feiping Nie, Jingjing Xue, Danyang Wu, Rong Wang, Hui Li, and Xuelong Li. Coordinate descent method for k-means. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 44(5): 2371–2385, 2022.
 - Yitian Qian, Shaohua Pan, and Lianghai Xiao. Exact penalty methods for minimizing a smooth function over the nonnegative orthogonal set. *arXiv*, 11 2021.
 - Meisam Razaviyayn, Mingyi Hong, and Zhi-Quan Luo. A unified convergence analysis of block successive minimization methods for nonsmooth optimization. *SIAM Journal on Optimization*, 23(2):1126–1153, 2013.
 - R. Tyrrell Rockafellar and Roger J-B. Wets. Variational analysis. *Springer Science & Business Media*, 317, 2009.
 - Uri Shalit and Gal Chechik. Coordinate-descent for learning orthogonal matrices through givens rotations. In *International Conference on Machine Learning (ICML)*, pp. 548–556. PMLR, 2014.
 - Xiaobai Sun and Christian Bischof. A basis-kernel representation of orthogonal matrices. *SIAM Journal on Matrix Analysis and Applications*, 16(4):1184–1196, 1995.
 - Ying Sun, Prabhu Babu, and Daniel P Palomar. Majorization-minimization algorithms in signal processing, communications, and machine learning. *IEEE Transactions on Signal Processing*, 65 (3):794–816, 2016.
 - Paul Tseng and Sangwoon Yun. A coordinate gradient descent method for nonsmooth separable minimization. *Mathematical Programming*, 117(1-2):387–423, 2009.
 - Vincent Q Vu, Juhee Cho, Jing Lei, and Karl Rohe. Fantope projection and selection: A near-optimal convex relaxation of sparse pca. *Advances in Neural Information Processing Systems (NeurIPS)*, 26, 2013.
 - Zaiwen Wen and Wotao Yin. A feasible method for optimization with orthogonality constraints. *Mathematical Programming*, 142(1-2):397, 2013.
 - WikiContributors. Quartic equation: https://en.wikipedia.org/wiki/Quartic_equation. pp. Last edited in March, 2023.
 - Nachuan Xiao, Xin Liu, and Ya-xiang Yuan. A class of smooth exact penalty function methods for optimization problems with orthogonality constraints. *Optimization Methods and Software*, 37 (4):1205–1241, 2022.
 - Di Xie, Jiang Xiong, and Shiliang Pu. All you need is beyond a good init: Exploring better solution for training extremely deep convolutional neural networks with orthonormality and modulation. In *IEEE Conference on Computer Vision and Pattern Recognition*, pp. 6176–6185, 2017.
 - Yangyang Xu and Wotao Yin. A block coordinate descent method for regularized multiconvex optimization with applications to nonnegative tensor factorization and completion. *SIAM Journal on Imaging Sciences*, 6(3):1758–1789, 2013.

Under review as a conference paper at ICLR 2026 Ganzhao Yuan. Smoothing proximal gradient methods for nonsmooth sparsity constrained optimiza-tion: Optimality conditions and global convergence. In International Conference on Machine Learning, 2024. Ron Zass and Amnon Shashua. Nonnegative sparse PCA. Advances in Neural Information Process-ing Systems (NeurIPS), pp. 1561-1568, 2006. Jinshan Zeng, Tim Tsz-Kit Lau, Shaobo Lin, and Yuan Yao. Global convergence of block coordinate descent in deep learning. In International Conference on Machine Learning (ICML), pp. 7313-7323. PMLR, 2019. Yuexiang Zhai, Zitong Yang, Zhenyu Liao, John Wright, and Yi Ma. Complete dictionary learning via 14-norm maximization over the orthogonal group. Journal of Machine Learning Research, 21 (165):1–68, 2020. Junyu Zhang, Shiqian Ma, and Shuzhong Zhang. Primal-dual optimization algorithms over rieman-nian manifolds: an iteration complexity analysis. *Mathematical Programming*, pp. 1–46, 2019. Xin Zhang, Jinwei Zhu, Zaiwen Wen, and Aihui Zhou. Gradient type optimization methods for electronic structure calculations. SIAM Journal on Scientific Computing, 36(3):265–289, 2014.

Appendix

702

703 704

705

706 707

708

709 710

711

712

713 714

715 716

717 718

719 720

721

722

723

724

725

726

727

728

729 730

731

732

733

735 736

739

740

741 742

743

744

745

746 747

748

749

750

751

752

754

755

The appendix section is organized as follows.

Section A covers notations, technical preliminaries, and relevant lemmas.

Section B shows how to solve the subproblem when k = 2.

Section C offers further discussions on the proposed algorithm.

Section D contains proofs from Section 2.

Section E contains proofs from Section 3.

Section F contains proofs from Section 4.

Section G presents additional experiment details and results.

A NOTATIONS, TECHNICAL PRELIMINARIES, AND RELEVANT LEMMAS

A.1 NOTATIONS

Throughout this paper, $\mathcal{M} \triangleq \operatorname{St}(n,r)$ denotes the Stiefel manifold, which is an embedded submanifold of the Euclidean space $\mathbb{R}^{n \times r}$. Boldfaced lowercase letters denote vectors and uppercase letters denote real-valued matrices. We adopt the Matlab colon notation to denote indices that describe submatrices. For given natural numbers n and k, we use $\{\mathcal{B}_1,\mathcal{B}_2,...,\mathcal{B}_{C_n^k}\}$ to denote all the possible combinations of the index vectors choosing k items from n without repetition, where C_n^k is the total number of such combinations and $\mathcal{B}_i \in \mathbb{N}^k$, $\forall i \in [C_n^k]$. For any one-dimensional function $p(t) : \mathbb{R} \mapsto \mathbb{R}$, we define: $p(\pm x \mp y) \triangleq \min\{p(x-y), p(-x+y)\}$. We use the following notations in this paper.

- [n]: $\{1, 2, ..., n\}$
- $\|\mathbf{x}\|$: Euclidean norm: $\|\mathbf{x}\| = \|\mathbf{x}\|_2 = \sqrt{\langle \mathbf{x}, \mathbf{x} \rangle}$
- x_i : the *i*-th element of vector x
- $\mathbf{X}_{i,j}$ or \mathbf{X}_{ij} : the (i^{th}, j^{th}) element of matrix \mathbf{X}
- $\text{vec}(\mathbf{X}): \text{vec}(\mathbf{X}) \in \mathbb{R}^{nr \times 1}$, the vector formed by stacking the column vectors of \mathbf{X}
- $mat(\mathbf{x}) : mat(\mathbf{x}) \in \mathbb{R}^{n \times r}$, Convert $\mathbf{x} \in \mathbb{R}^{nr \times 1}$ into a matrix with $mat(vec(\mathbf{X})) = \mathbf{X}$
- \mathbf{X}^{T} : the transpose of the matrix \mathbf{X}
- $\operatorname{sign}(t)$: the signum function, $\operatorname{sign}(t) = 1$ if $t \ge 0$ and $\operatorname{sign}(t) = -1$ otherwise
- $\det(\mathbf{D})$: Determinant of a square matrix $\mathbf{D} \in \mathbb{R}^{n \times n}$
 - C_n^k : the number of possible combinations choosing k items from n without repetition
 - $\mathbf{0}_{n,r}$: A zero matrix of size $n \times r$; the subscript is omitted sometimes
 - $\mathbf{I}_r : \mathbf{I}_r \in \mathbb{R}^{r \times r}$, Identity matrix
 - $X \succeq 0$ (or $\succ 0$): the Matrix X is symmetric positive semidefinite (or definite)
 - $tr(\mathbf{A})$: Sum of the elements on the main diagonal \mathbf{X} : $tr(\mathbf{A}) = \sum_i \mathbf{A}_{i,i}$
 - $\langle \mathbf{X}, \mathbf{Y} \rangle$: Euclidean inner product, i.e., $\langle \mathbf{X}, \mathbf{Y} \rangle = \sum_{ij} \mathbf{X}_{ij} \mathbf{Y}_{ij}$
 - $\mathbf{X} \otimes \mathbf{Y}$: Kronecker product of \mathbf{X} and \mathbf{Y}
 - $\|\mathbf{X}\|_{\mathsf{F}}$: Frobenius norm: $(\sum_{i,j} \mathbf{X}_{i,j}^2)^{1/2}$
 - $\|\mathbf{X}\|_{\mathsf{sp}}$: Operator/Spectral norm: the largest singular value of \mathbf{X}
 - $\|\mathbf{X}\|_0$: the number of non-zero elements in the matrix \mathbf{X}
 - $\|\mathbf{X}\|_1$: the absolute sum of the elements in the matrix \mathbf{X} with $\|\mathbf{X}\|_1 = \sum_{i,j} |\mathbf{X}_{i,j}|$
- $\nabla f(\mathbf{X})$: Euclidean gradient of $f(\mathbf{X})$ at \mathbf{X}
 - $\nabla_{\mathcal{M}} f(\mathbf{X})$: Riemannian gradient of $f(\mathbf{X})$ at \mathbf{X}
 - $\partial F(\mathbf{X})$: limiting Euclidean subdifferential of $F(\mathbf{X})$ at \mathbf{X}

- $\partial_{\mathcal{M}} F(\mathbf{X})$: limiting Riemannian subdifferential of $F(\mathbf{X})$ at \mathbf{X}
- $\iota_{\Xi}(\mathbf{X})$: the indicator function of a set Ξ with $\iota_{\Xi}(\mathbf{X}) = 0$ if $\mathbf{X} \in \Xi$ and otherwise $+\infty$
- $\iota_{\geq 0}(\mathbf{X})$: indicator function of non-negativity constraint with $\iota_{\geq 0}(\mathbf{X}) = \{ \begin{array}{cc} 0, & \mathbf{X} \geq \mathbf{0}; \\ \infty, & \text{else.} \end{array} \}$
- $\mathbb{P}_{\Xi}(\mathbf{Z})$: Orthogonal projection of \mathbf{Z} with $\mathbb{P}_{\Xi}(\mathbf{Z}) = \arg\min_{\mathbf{X} \in \Xi} \|\mathbf{Z} \mathbf{X}\|_{\mathsf{F}}^2$
- $\mathbb{P}_{\mathcal{M}}(\mathbf{Y})$: Nearest orthogonal matrix of \mathbf{Y} with $\mathbb{P}_{\mathcal{M}}(\mathbf{Y}) = \arg\min_{\mathbf{X}^{\mathsf{T}}\mathbf{X} = \mathbf{I}_r} \|\mathbf{X} \mathbf{Y}\|_{\mathsf{F}}^2$
- $\operatorname{dist}(\Xi,\Xi')$: the distance between two sets with $\operatorname{dist}(\Xi,\Xi') \triangleq \inf_{\mathbf{X} \in \Xi, \mathbf{X}' \in \Xi'} \|\mathbf{X} \mathbf{X}'\|_{\mathsf{F}}$
- $\mathbb{A} + \mathbb{B}$, $\mathbb{A} \mathbb{B}$: standard Minkowski addition and subtraction between sets \mathbb{A} and \mathbb{B}
- $\mathbb{A} \oplus \mathbb{B}$, $\mathbb{A} \ominus \mathbb{B}$: element-wise addition and subtraction between sets \mathbb{A} and \mathbb{B}
- $\|\partial F(\mathbf{X})\|_{\mathsf{F}}$: the distance from the origin to the set $\partial F(\mathbf{X})$ with $\|\partial F(\mathbf{X})\|_{\mathsf{F}} = \inf_{\mathbf{Y} \in \partial F(\mathbf{X})} \|\mathbf{Y}\|_{\mathsf{F}} = \operatorname{dist}(\mathbf{0}, \partial F(\mathbf{X}))$

A.2 TECHNICAL PRELIMINARIES

As the function $F(\cdot)$ can be non-convex and non-smooth, we introduce some tools in non-smooth analysis (Mordukhovich, 2006; Rockafellar & Wets., 2009). The domain of any extended real-valued function $F: \mathbb{R}^{n \times r} \to (-\infty, +\infty]$ is defined as $\mathrm{dom}(F) \triangleq \{\mathbf{X} \in \mathbb{R}^{n \times r} : |F(\mathbf{X})| < +\infty\}$. The Fréchet subdifferential of F at $\mathbf{X} \in \mathrm{dom}(F)$ is defined as

$$\hat{\partial} F(\mathbf{X}) \triangleq \{ \boldsymbol{\xi} \in \mathbb{R}^{n \times r} : \lim_{\mathbf{Z} \to \mathbf{X}} \inf_{\mathbf{Z} \neq \mathbf{X}} \frac{F(\mathbf{Z}) - F(\mathbf{X}) - \langle \boldsymbol{\xi}, \mathbf{Z} - \mathbf{X} \rangle}{\|\mathbf{Z} - \mathbf{X}\|_{\mathsf{F}}} \ge 0 \},$$

while the limiting subdifferential of $F(\mathbf{X})$ at $\mathbf{X} \in \text{dom}(F)$ is denoted as

$$\partial F(\mathbf{X}) \triangleq \{ \boldsymbol{\xi} \in \mathbb{R}^n : \exists \mathbf{X}^t \to \mathbf{X}, F(\mathbf{X}^t) \to F(\mathbf{X}), \boldsymbol{\xi}^t \in \hat{\partial} F(\mathbf{X}^t) \to \boldsymbol{\xi}, \forall t \}.$$

We denote $\nabla F(\mathbf{X})$ as the gradient of $F(\cdot)$ at \mathbf{X} in the Euclidean space. We have the following relation between $\hat{\partial}F(\mathbf{X})$, $\partial F(\mathbf{X})$, and $\nabla F(\mathbf{X})$. (i) It holds that $\hat{\partial}F(\mathbf{X})\subseteq \partial F(\mathbf{X})$. (ii) If the function $F(\cdot)$ is convex, $\partial F(\mathbf{X})$ and $\hat{\partial}F(\mathbf{X})$ essentially the classical subdifferential for convex functions, i.e.,

$$\partial F(\mathbf{X}) = \hat{\partial} F(\mathbf{X}) = \{ \boldsymbol{\xi} \in \mathbb{R}^{n \times r} : F(\mathbf{Z}) \ge F(\mathbf{X}) + \langle \boldsymbol{\xi}, \mathbf{Z} - \mathbf{X} \rangle, \forall \mathbf{Z} \in \mathbb{R}^{n \times r} \}.$$

(iii) If the function $F(\cdot)$ is differentiable, then $\hat{\partial}F(\mathbf{X}) = \partial F(\mathbf{X}) = \{\nabla F(\mathbf{X})\}.$

We need some prerequisite knowledge in optimization with orthogonality constraints (Absil et al., 2008). The nearest orthogonality matrix to an arbitrary matrix $\mathbf{Y} \in \mathbb{R}^{n \times r}$ is given by $\mathbb{P}_{\mathcal{M}}(\mathbf{Y}) = \hat{\mathbf{U}}\hat{\mathbf{V}}^\mathsf{T}$, where $\mathbf{Y} = \hat{\mathbf{U}}\mathrm{Diag}(\mathbf{s})\hat{\mathbf{V}}^\mathsf{T}$ is the singular value decomposition of \mathbf{Y} . We use $\mathcal{N}_{\mathcal{M}}(\mathbf{X})$ to denote the limiting normal cone to \mathcal{M} at \mathbf{X} , leading to

$$\mathcal{N}_{\mathcal{M}}(\mathbf{X}) = \partial \iota_{\mathcal{M}}(\mathbf{X}) = \{ \mathbf{Z} \in \mathbb{R}^{n \times r} : \langle \mathbf{Z}, \mathbf{X} \rangle \ge \langle \mathbf{Z}, \mathbf{Y} \rangle, \, \forall \mathbf{Y} \in \mathcal{M} \}.$$

The tangent and norm space to \mathcal{M} at $\mathbf{X} \in \mathcal{M}$ are denoted as $T_{\mathbf{X}}\mathcal{M}$ and $N_{\mathbf{X}}\mathcal{M}$, respectively. For a given $\mathbf{X} \in \mathcal{M}$, we let $\mathcal{A}_{\mathbf{X}}(\mathbf{Y}) \triangleq \mathbf{X}^{\mathsf{T}}\mathbf{Y} + \mathbf{Y}^{\mathsf{T}}\mathbf{X}$ for $\mathbf{Y} \in \mathbb{R}^{n \times r}$, and we have $T_{\mathbf{X}}\mathcal{M} = \{\mathbf{Y} \in \mathbb{R}^{n \times r} | \mathcal{A}_{X}(\mathbf{Y}) = \mathbf{0}\}$ and $N_{\mathbf{X}}\mathcal{M} = \{2\mathbf{X}\mathbf{\Lambda} | \mathbf{\Lambda} = \mathbf{\Lambda}^{\mathsf{T}}, \mathbf{\Lambda} \in \mathbb{R}^{r \times r}\}$. For any non-convex and non-smooth function $F(\mathbf{X})$, we use $\partial_{\mathcal{M}}F(\mathbf{X})$ to denote the limiting Riemannian gradient of $F(\mathbf{X})$ at \mathbf{X} , and obtain $\partial_{\mathcal{M}}F(\mathbf{X}) = \mathbb{P}_{\mathbf{T}_{\mathbf{X}}\mathcal{M}}(\partial F(\mathbf{X}))$. We denote $\partial F(\mathbf{X}) \ominus \mathbf{X}[\partial F(\mathbf{X})]^{\mathsf{T}}\mathbf{X} \triangleq \{\mathbb{E} | \mathbb{E} = \mathbf{G} - \mathbf{X}\mathbf{G}^{\mathsf{T}}\mathbf{X}, \mathbf{G} \in \partial F(\mathbf{X})\}$.

A.3 RELEVANT LEMMAS

We offer a set of useful lemmas, each of which stands independently of context and specific methodology.

Lemma A.1. Let $k \geq 2$ and $\mathbf{W} \in \mathbb{R}^{n \times n}$. If $\mathbf{0}_{k,k} = \mathbf{U}_{\mathrm{B}}^{\mathsf{T}} \mathbf{W} \mathbf{U}_{\mathrm{B}}$ for all $\mathrm{B} \in \{\mathcal{B}_i\}_{i=1}^{\mathrm{C}_n^k}$, then $\mathbf{W} = \mathbf{0}$. Here, the set $\{\mathcal{B}_1, \mathcal{B}_2, ..., \mathcal{B}_{\mathrm{C}_n^k}\}$ represents all possible combinations of the index vectors choosing k items from n without repetition.

Proof. The proof is straightforward and relies on elementary reasoning.

Notably, the conclusion of this lemma does not necessarily hold if |B| = k = 1. This is because any matrix $\mathbf{W} \in \mathbb{R}^{n \times n}$ with $\mathbf{W}_{ii} = 0$ for all $i \in [n]$ satisfies the condition of this lemma but is not necessary a zero matrix.

Lemma A.2. For any matrices $\mathbf{A} \in \mathbb{R}^{k \times k}$ and $\mathbf{C} \in \mathbb{R}^{k \times k}$, we have: $\|\mathbf{A} - \mathbf{A}^{\mathsf{T}}\|_{\mathsf{F}} \leq 2\|\mathbf{A} - \mathbf{C}\|_{\mathsf{F}} + \|\mathbf{C} - \mathbf{C}^{\mathsf{T}}\|_{\mathsf{F}}$.

Proof. We derive:
$$\|\mathbf{A} - \mathbf{A}^{\mathsf{T}}\|_{\mathsf{F}} = \|(\mathbf{A} - \mathbf{C}) + (\mathbf{C} - \mathbf{C}^{\mathsf{T}}) + (\mathbf{C}^{\mathsf{T}} - \mathbf{A}^{\mathsf{T}})\|_{\mathsf{F}} \stackrel{\textcircled{\tiny{0}}}{\leq} \|\mathbf{A} - \mathbf{C}\|_{\mathsf{F}} + \|\mathbf{C} - \mathbf{C}^{\mathsf{T}}\|_{\mathsf{F}} + \|\mathbf{C}^{\mathsf{T}} - \mathbf{A}^{\mathsf{T}}\|_{\mathsf{F}} = 2\|\mathbf{A} - \mathbf{C}\|_{\mathsf{F}} + \|\mathbf{C} - \mathbf{C}^{\mathsf{T}}\|_{\mathsf{F}}, \text{ where step } \textcircled{\tiny{0}} \text{ uses the triangle inequality.}$$

Lemma A.3. Let $\tau \in \mathbb{R}$, and $\mathbf{A} \in \mathbb{R}^{2 \times 2}$ be any skey-symmetric matrix with $\mathbf{A}^{\mathsf{T}} = -\mathbf{A}$. The matrix $\mathbf{Q} = [(\mathbf{I}_2 + \frac{\tau}{2}\mathbf{A})^{-1}(\mathbf{I}_k - \frac{\tau}{2}\mathbf{A})]$ is always a rotation matrix with $\det(\mathbf{Q}) = 1$.

Proof. Since **A** is a two-dimensional matrix, it can be expressed in the form: $\mathbf{A} = \begin{pmatrix} 0 & a \\ -a & 0 \end{pmatrix}$ for some $a \in \mathbb{R}$. Letting $b = \frac{\tau}{2}a$, we derive:

$$\mathbf{Q} = (\mathbf{I}_2 + \tfrac{\tau}{2}\mathbf{A})^{-1}(\mathbf{I}_k - \tfrac{\tau}{2}\mathbf{A}) \stackrel{\textcircled{\tiny 3}}{=} \left(\begin{smallmatrix} 1 & b \\ -b & 1 \end{smallmatrix} \right)^{-1} \left(\begin{smallmatrix} 1 & -b \\ b & 1 \end{smallmatrix} \right) \stackrel{\textcircled{\tiny 2}}{=} \tfrac{1}{1+b^2} \left(\begin{smallmatrix} 1 & -b \\ b & 1 \end{smallmatrix} \right) \left(\begin{smallmatrix} 1 & -b \\ b & 1 \end{smallmatrix} \right) = \tfrac{1}{1+b^2} \left(\begin{smallmatrix} 1-b^2 & -2b \\ 2b & 1-b^2 \end{smallmatrix} \right),$$

where step ① uses $\frac{\tau}{2}\mathbf{A} = \left(\begin{smallmatrix} 0 & b \\ -b & 0 \end{smallmatrix} \right)$; step ② uses the fact that $\left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix} \right)^{-1} = \frac{1}{ad-bc} \left(\begin{smallmatrix} d & -b \\ -c & a \end{smallmatrix} \right)^{-1}$ for all $a,b,c,d \in \mathbb{R}$. We further obtain: $\det(\mathbf{Q}) \stackrel{@}{=} \frac{1-b^2}{1+b^2} \cdot \frac{1-b^2}{1+b^2} - \frac{2b}{1+b^2} \cdot \frac{-2b}{1+b^2} = \frac{(1-b^2)^2+4b^2}{(1+b^2)^2} = \frac{(1+b^2)^2}{(1+b^2)^2} = 1$, where step ① uses the fact that $\det(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}) = ad - bc$ for all $a,b,c,d \in \mathbb{R}$.

Lemma A.4. For any $\mathbf{W} \in \mathbb{R}^{n \times n}$, we have $\sum_{i=1}^{C_n^k} \|\mathbf{W}(\mathcal{B}_i, \mathcal{B}_i)\|_{\mathsf{F}}^2 = C_{n-2}^{k-2} \sum_i \sum_{j,j \neq i} \mathbf{W}_{ij}^2 + \frac{k}{n} C_n^k \sum_i \mathbf{W}_{ii}^2$. Here, the set $\{\mathcal{B}_1, \mathcal{B}_2, ..., \mathcal{B}_{C_n^k}\}$ represents all possible combinations of the index vectors choosing k items from n without repetition.

Proof. For any matrix $\mathbf{W} \in \mathbb{R}^{n \times n}$, we define: $\mathbf{w} \triangleq \operatorname{diag}(\mathbf{W}) \in \mathbb{R}^n$, and $\mathbf{W}' \triangleq \mathbf{W} - \operatorname{Diag}(\mathbf{w})$.

We have: $\mathbf{W} = \mathrm{Diag}(\mathbf{w}) + \mathbf{W}'$, this leads to the following decomposition:

$$\sum_{i=1}^{C_n^k} \|\mathbf{U}_{\mathcal{B}_i}^\mathsf{T} \mathbf{W} \mathbf{U}_{\mathcal{B}_i}\|_{\mathsf{F}}^2 = \sum_{i=1}^{C_n^k} \|\mathbf{U}_{\mathcal{B}_i}^\mathsf{T} (\mathrm{Diag}(\mathbf{w}) + \mathbf{W}') \mathbf{U}_{\mathcal{B}_i}\|_{\mathsf{F}}^2$$

$$= \underbrace{\sum_{i=1}^{C_n^k} \|\mathbf{U}_{\mathcal{B}_i}^\mathsf{T} \mathrm{Diag}(\mathbf{w}) \mathbf{U}_{\mathcal{B}_i}\|_{\mathsf{F}}^2}_{\Gamma_1} + \underbrace{\sum_{i=1}^{C_n^k} \|\mathbf{U}_{\mathcal{B}_i}^\mathsf{T} \mathbf{W}' \mathbf{U}_{\mathcal{B}_i}\|_{\mathsf{F}}^2}_{\Gamma_2}. \quad (12)$$

We first focus on the term Γ_1 . We have:

$$\Gamma_1 = \sum_{i=1}^{C_n^k} \|\mathbf{U}_{\mathcal{B}_i}^\mathsf{T} \mathrm{Diag}(\mathbf{w}) \mathbf{U}_{\mathcal{B}_i}\|_\mathsf{F}^2 \stackrel{\textcircled{\tiny{1}}}{=} \sum_{i=1}^{C_n^k} \|\mathbf{w}_{\mathcal{B}_i}\|_2^2 \stackrel{\textcircled{\tiny{2}}}{=} C_n^k \cdot \frac{k}{n} \cdot \|\mathbf{w}\|_2^2 = C_n^k \cdot \frac{k}{n} \cdot \sum_i \mathbf{W}_{ii}^2, \quad (13)$$

where step ① uses the fact that $\|\mathbf{B}^\mathsf{T}\mathrm{Diag}(\mathbf{w})\mathbf{B}\|_\mathsf{F}^2 = \|[\mathrm{Diag}(\mathbf{w})]_{\mathsf{BB}}\|_\mathsf{F}^2 = \|\mathbf{w}_{\mathsf{B}}\|_2^2$ for any $\mathbf{B} \in \{\mathcal{B}_i\}_{i=1}^{\mathsf{C}_n^k}$; step ② uses the observation that \mathbf{w}_i appears in the term $\sum_{i=1}^{\mathsf{C}_n^k} \|\mathbf{w}_{\mathcal{B}_i}\|_2^2$ a total of $(\mathsf{C}_n^k \cdot \frac{k}{n})$ times, which can be deduced using basic induction.

We now focus on the term Γ_2 . Noticing that $\mathbf{W}'_{ii} = 0$ for all $i \in [n]$, we have:

$$\Gamma_{2} = \sum_{i=1}^{C_{n}^{k}} \|\mathbf{U}_{\mathcal{B}_{i}}^{\mathsf{T}} \mathbf{W}' \mathbf{U}_{\mathcal{B}_{i}}\|_{\mathsf{F}}^{2} \stackrel{@}{=} \sum_{i} \sum_{j \neq i} \left[C_{n-2}^{k-2} (\mathbf{W}_{ij}')^{2} \right] \stackrel{@}{=} C_{n-2}^{k-2} \sum_{i} \sum_{j,j \neq i} (\mathbf{W}_{ij})^{2}, \tag{14}$$

where step ① uses the fact that the term $\sum_{i=1}^{C_n^k} \|\mathbf{U}_{\mathcal{B}_i}^\mathsf{T} \mathbf{W}' \mathbf{U}_{\mathcal{B}_i}\|_\mathsf{F}^2$ comprises C_{n-2}^{k-2} distinct patterns, each including $\{i,j\}$ with $i \neq j$; step ② uses $\sum_{i,j \neq i} (\mathbf{W}_{ij})^2 = \sum_{i,j \neq i} (\mathbf{W}_{ij}')^2$.

In view of Equalities (12), (13), and (14), we complete the proof of this lemma. \Box

Lemma A.5. Assume $\mathbf{Q}\mathbf{R} = \mathbf{X} \in \mathbb{R}^{n \times n}$, where $\mathbf{Q} \in \mathrm{St}(n,n)$ and \mathbf{R} is a lower triangular matrix with $\mathbf{R}_{i,j} = 0$ for all i < j. If $\mathbf{X} \in \mathrm{St}(n,n)$, then \mathbf{R} is a diagonal matrix with $\mathbf{R}_{i,i} \in \{-1,+1\}$ for all $i \in [n]$.

Proof. We derive: $\mathbf{R}\mathbf{R}^{\mathsf{T}} \stackrel{\textcircled{\tiny{0}}}{=} (\mathbf{Q}\mathbf{X})(\mathbf{Q}\mathbf{X})^{\mathsf{T}} = \mathbf{Q}\mathbf{X}\mathbf{X}^{\mathsf{T}}\mathbf{Q}^{\mathsf{T}} \stackrel{\textcircled{\tiny{0}}}{=} \mathbf{I}$, where step $\textcircled{\tiny{0}}$ uses $\mathbf{R} = \mathbf{Q}^{\mathsf{T}}\mathbf{X}$; step $\textcircled{\tiny{0}}$ uses $\mathbf{X} \in \mathrm{St}(n,n)$ and $\mathbf{Q} \in \mathrm{St}(n,n)$. First, given $\|\mathbf{R}(1,:)\| = 1$ and $\mathbf{R}(1,2:n) = 0$, we have $\mathbf{R}_{1,1} \in \{-1,+1\}$. Second, we have $\|\mathbf{R}(2,:)\| = 1$ and $\mathbf{R}(1,:)^{\mathsf{T}}\mathbf{R}(:,2) = 0$, leading to $\mathbf{R}_{1,2} = 0$ and $\mathbf{R}_{2,2} \in \{-1,+1\}$. Finally, using similar recursive strategy, we conclude that \mathbf{R} is a diagonal matrix with $\mathbf{R}_{i,i} \in \{-1,+1\}$ for all $i \in [n]$.

 Lemma A.6. We define $T_{\mathbf{X}}\mathcal{M} \triangleq \{\mathbf{Y} \in \mathbb{R}^{n \times r} \mid \mathcal{A}_X(\mathbf{Y}) = \mathbf{0}\}$ and $\mathcal{A}_{\mathbf{X}}(\mathbf{Y}) \triangleq \mathbf{X}^\mathsf{T}\mathbf{Y} + \mathbf{Y}^\mathsf{T}\mathbf{X}$. For any $\mathbf{G} \in \mathbb{R}^{n \times r}$ and $\mathbf{X} \in \mathrm{St}(n,k)$, we have: $(\mathbf{G} - \frac{1}{2}\mathbf{X}\mathcal{A}_{\mathbf{X}}(\mathbf{G})) = \arg\min_{\mathbf{Y} \in T_{\mathbf{X}}\mathcal{M}} \|\mathbf{Y} - \mathbf{G}\|_{\mathsf{F}}^2$.

Proof. The conclusion of this lemma can be found in (Absil et al., 2008). For completeness, we present a short proof.

Consider the convex problem: $\bar{\mathbf{Y}} = \arg\min_{\mathbf{Y}} \|\mathbf{Y} - \mathbf{G}\|_{\mathsf{F}}^2, s.t. \mathbf{X}^\mathsf{T}\mathbf{Y} + \mathbf{Y}^\mathsf{T}\mathbf{X} = \mathbf{0}.$ Introducing a multiplier $\mathbf{\Lambda} \in \mathbb{R}^{r \times r}$ for the linear constraints leads to the following Lagrangian function: $\tilde{\mathcal{L}}(\mathbf{Y}; \mathbf{\Lambda}) = \|\mathbf{Y} - \mathbf{G}\|_{\mathsf{F}}^2 + \langle \mathbf{X}^\mathsf{T}\mathbf{Y} + \mathbf{Y}^\mathsf{T}\mathbf{X}, \mathbf{\Lambda} \rangle.$ We derive the subsequent first-order optimality condition: $2(\mathbf{Y} - \mathbf{G}) + \mathbf{X}(\mathbf{\Lambda} + \mathbf{\Lambda}^\mathsf{T}) = \mathbf{0}$, and $\mathbf{X}^\mathsf{T}\mathbf{Y} + \mathbf{Y}^\mathsf{T}\mathbf{X} = \mathbf{0}$. Given $\mathbf{\Lambda}$ is symmetric, we have $\mathbf{Y} = \mathbf{G} - \mathbf{X}\mathbf{\Lambda}$. Incorporating this result into $\mathbf{X}^\mathsf{T}\mathbf{Y} + \mathbf{Y}^\mathsf{T}\mathbf{X} = \mathbf{0}$, we obtain: $\mathbf{X}^\mathsf{T}(\mathbf{G} - \mathbf{X}\mathbf{\Lambda}) + (\mathbf{G} - \mathbf{X}\mathbf{\Lambda})^\mathsf{T}\mathbf{X} = \mathbf{0}$. Given $\mathbf{X} \in \mathrm{St}(n,r)$, we have $\mathbf{X}^\mathsf{T}\mathbf{G} - \mathbf{\Lambda} + \mathbf{G}^\mathsf{T}\mathbf{X} - \mathbf{\Lambda}^\mathsf{T} = \mathbf{0}$, leading to: $\mathbf{\Lambda} = \frac{1}{2}(\mathbf{X}^\mathsf{T}\mathbf{G} + \mathbf{G}^\mathsf{T}\mathbf{X})$. Therefore, the optimal solution $\bar{\mathbf{Y}}$ can be computed as $\bar{\mathbf{Y}} = \mathbf{G} - \mathbf{X}\mathbf{\Lambda} = \mathbf{G} - \frac{1}{2}\mathbf{X}(\mathbf{X}^\mathsf{T}\mathbf{G} + \mathbf{G}^\mathsf{T}\mathbf{X})$.

Lemma A.7. Consider the following problem: $\min_{\mathbf{X}} F_{\iota}(\mathbf{X}) \triangleq F(\mathbf{X}) + \iota_{\mathcal{M}}(\mathbf{X})$, where $F(\mathbf{X})$ is defined in Equation (1). For any $\mathbf{X} \in \operatorname{St}(n,r)$, it holds that $\operatorname{dist}(\mathbf{0}, \partial F_{\iota}(\mathbf{X})) \leq \operatorname{dist}(\mathbf{0}, \partial_{\mathcal{M}} F(\mathbf{X}))$.

Proof. We let $G \in \partial F(X)$ and define $A_X(G) \triangleq X^TG + G^TX$.

Recall that the following first-order optimality conditions are equivalent for all $\mathbf{X} \in \operatorname{St}(n,r)$: $(\mathbf{0} \in \partial F_{\iota}(\mathbf{X})) \Leftrightarrow (\mathbf{0} \in \mathbb{P}_{\mathbf{T}_{\mathbf{X}}\mathcal{M}}(\partial F(\mathbf{X})))$. Therefore, we derive:

$$\begin{aligned}
\operatorname{dist}(\mathbf{0}, \partial F_{\iota}(\mathbf{X})) &= \inf_{\mathbf{Y} \in \partial F_{\iota}(\mathbf{X})} \|\mathbf{Y}\|_{\mathsf{F}} = \inf_{\mathbf{Y} \in \mathbb{P}_{(\mathbf{T}_{\mathbf{X}}\mathcal{M})}(\partial F(\mathbf{X}))} \|\mathbf{Y}\|_{\mathsf{F}} \\
&\stackrel{\textcircled{\tiny{1}}}{=} \|\mathbb{P}_{(\mathbf{T}_{\mathbf{X}}\mathcal{M})}(\mathbf{G})\|_{\mathsf{F}} \\
&\stackrel{\textcircled{\tiny{2}}}{=} \|\mathbf{G} - \frac{1}{2}\mathbf{X}\mathcal{A}_{\mathbf{X}}(\mathbf{G})\|_{\mathsf{F}} \\
&\stackrel{\textcircled{\tiny{3}}}{=} \|\mathbf{G} - \frac{1}{2}\mathbf{X}(\mathbf{X}^{\mathsf{T}}\mathbf{G} + \mathbf{G}^{\mathsf{T}}\mathbf{X})\|_{\mathsf{F}} \\
&\stackrel{\textcircled{\tiny{4}}}{=} \|(\mathbf{I} - \frac{1}{2}\mathbf{X}\mathbf{X}^{\mathsf{T}})(\mathbf{G} - \mathbf{X}\mathbf{G}^{\mathsf{T}}\mathbf{X})\|_{\mathsf{F}} \\
&\stackrel{\textcircled{\tiny{5}}}{=} \|\mathbf{G} - \mathbf{X}\mathbf{G}^{\mathsf{T}}\mathbf{X}\|_{\mathsf{F}}.
\end{aligned}$$

where step ① uses $\mathbf{G} \in \partial F(\mathbf{X})$; step ② uses Lemma A.6; step ③ uses the definition of $\mathcal{A}_{\mathbf{X}}(\mathbf{G})$; step ④ uses the identity that $\mathbf{G} - \frac{1}{2}\mathbf{X}(\mathbf{X}^\mathsf{T}\mathbf{G} + \mathbf{G}^\mathsf{T}\mathbf{X}) = (\mathbf{I} - \frac{1}{2}\mathbf{X}\mathbf{X}^\mathsf{T})(\mathbf{G} - \mathbf{X}\mathbf{G}^\mathsf{T}\mathbf{X})$; step ⑤ uses the norm inequality and fact that the matrix $\mathbf{I} - \frac{1}{2}\mathbf{X}\mathbf{X}^\mathsf{T}$ only contains eigenvalues that are $\frac{1}{2}$ or 1.

Lemma A.8. Assume $\cos(\theta) \neq 0$. Any pair of trigonometric functions $(\cos(\theta), \sin(\theta))$ can be represented as follows:

$$\begin{array}{l} \textbf{\textit{a})} \; \cos(\theta) = \frac{1}{\sqrt{1 + \tan^2(\theta)}}, \, \textit{and} \, \sin(\theta) = \frac{\tan(\theta)}{\sqrt{1 + \tan^2(\theta)}}. \\ \textbf{\textit{b})} \; \cos(\theta) = \frac{-1}{\sqrt{1 + \tan^2(\theta)}}, \, \textit{and} \, \sin(\theta) = \frac{-\tan(\theta)}{\sqrt{1 + \tan^2(\theta)}}. \end{array}$$

Proof. For all values of θ where $\cos(\theta) \neq 0$, the trigonometric functions $\{\sin(\theta), \cos(\theta), \tan(\theta)\}$ are well-defined. Utilizing the identity $\sin^2(\theta) + \cos^2(\theta) = 1$ and $\tan(\theta)\cos(\theta) = \sin(\theta)$, we derive: $(\tan(\theta) \cdot \cos(\theta))^2 + \cos^2(\theta) = 1$. Consequently, we find: $\cos(\theta) = \frac{\pm 1}{\sqrt{\tan^2(\theta) + 1}}$. Finally, we

can express
$$\sin(\theta)$$
 as $\sin(\theta) = \tan(\theta) \cdot \cos(\theta) = \frac{\tan(\theta)}{\sqrt{\tan^2(\theta)+1}}$.

Lemma A.9. Let $A \in \mathbb{R}$ and $B \in \mathbb{R}$. The minimizer of the following one-dimensional problem:

$$\bar{\theta} \in \arg\min_{\theta} h(\theta) = A\cos(\theta) + B\sin(\theta)$$
 (15)

will be achieved at $\bar{\theta}$, where $\cos(\bar{\theta}) = -\frac{A}{\sqrt{A^2 + B^2}}$, $\sin(\bar{\theta}) = -\frac{B}{\sqrt{A^2 + B^2}}$, and $h(\bar{\theta}) = -\sqrt{A^2 + B^2}$.

Proof. Initially, we consider the special case when $cos(\theta) = 0$ or A = 0. Problem (15) reduces to:

$$\bar{\theta} \in \arg\min_{\theta} h(\theta) = B\sin(\theta).$$

Clearly, we have: $\sin(\bar{\theta}) = -\frac{B}{|B|}$, $\cos(\bar{\theta}) = 0$, and $h(\bar{\theta}) = -|B|$. The conclusion of this lemma holds.

We now assume that $A \neq 0$ and $\cos(\theta) \neq 0$ for all θ . Using the fact that $\tan(\theta) = \frac{\sin(\theta)}{\cos(\theta)}$ and $\cos(\theta)^2 + \sin(\theta)^2 = 1$, we have the following two cases for $\cos(\theta)$ and $\sin(\theta)$:

a)
$$\cos(\theta) = \frac{1}{\sqrt{1 + \tan^2(\theta)}}$$
, and $\sin(\theta) = \frac{\tan(\theta)}{\sqrt{1 + \tan^2(\theta)}}$

b)
$$\cos(\theta) = \frac{-1}{\sqrt{1 + \tan^2(\theta)}}$$
, and $\sin(\theta) = \frac{-\tan(\theta)}{\sqrt{1 + \tan^2(\theta)}}$.

Therefore, Problem (15) reduces to the following equivalent minimization problem:

$$\bar{\theta} \in \arg\min_{\theta} \frac{\pm A \pm \tan(\theta)B}{\sqrt{1 + \tan^2(\theta)}}$$

Using the variable substitution that $tan(\theta) = t$, we have the following equivalent problem:

$$\bar{t} \in \arg\min_{t} h(t) \triangleq \frac{\pm (A+Bt)}{\sqrt{1+t^2}}.$$

For any optimal solution \bar{t} , we have the following necessary first-order optimality condition:

$$\begin{split} 0 &\in \partial h(\bar{t}) = \frac{\pm B\sqrt{1+\bar{t}^2} \mp (A+B\bar{t}) \cdot (1+\bar{t}^2)^{-1/2}\bar{t}}{1+\bar{t}^2} \\ \Rightarrow \quad 0 &\in \pm B\sqrt{1+\bar{t}^2} \mp \frac{(A+B\bar{t})\bar{t}}{\sqrt{1+\bar{t}^2}} \\ \Rightarrow \quad B\sqrt{1+\bar{t}^2} &= \frac{(A+B\bar{t})\bar{t}}{\sqrt{1+t^2}} \\ \Rightarrow \quad \bar{t} &= \frac{B}{4} \end{split}$$

Therefore, we have: $\bar{t} = \frac{B}{A} = \tan(\bar{\theta})$. The optimal solution pair $[\cos(\bar{\theta}), \sin(\bar{\theta})]$ for Problem (15) can be computed as one of the following two cases:

a)
$$\cos(\bar{\theta}) = \frac{A}{\sqrt{A^2 + B^2}}$$
, and $\sin(\bar{\theta}) = \frac{B}{\sqrt{A^2 + B^2}}$.

b)
$$\cos(\bar{\theta}) = \frac{-A}{\sqrt{A^2 + B^2}}$$
, and $\sin(\bar{\theta}) = \frac{-B}{\sqrt{A^2 + B^2}}$.

In view of the original problem $\bar{\theta} = \arg\min_{\theta} h(\theta) = A\cos(\theta) + B\sin(\theta)$, we conclude that $\cos(\bar{\theta}) = \frac{-A}{\sqrt{A^2 + B^2}}$, and $\sin(\bar{\theta}) = \frac{-B}{\sqrt{A^2 + B^2}}$.

Lemma A.10. Assume $(E_{t+1})^2 \leq E_t(p^t - p^{t+1})$ and $p^t \geq p^{t+1}$, where $\{E_t, p^t\}_{t=0}^{\infty}$ are two nonnegative sequences. For all $i \geq 1$, we have: $\sum_{t=i}^{\infty} E_{t+1} \leq E_i + 2p^i$.

Proof. We define $w_t \triangleq p^t - p^{t+1}$. We let $1 \leq i < T$.

First, for any $i \ge 1$, we have:

$$\sum_{t=i}^{T} w_t = \sum_{t=i}^{T} (p^t - p^{t+1}) = p^i - p^{T+1} \stackrel{\textcircled{i}}{\leq} p^i, \tag{16}$$

where step ① uses $p^i \ge 0$ for all i.

Second, we obtain:

$$E_{t+1} \stackrel{\circ}{\leq} \sqrt{E_t w_t}$$

$$\stackrel{\circ}{\leq} \sqrt{\frac{\alpha}{2} (E_t)^2 + (w_t)^2 / (2\alpha)}, \, \forall \alpha > 0$$

$$\stackrel{\circ}{\leq} \sqrt{\frac{\alpha}{2}} \cdot E_t + w_t \sqrt{1 / (2\alpha)}, \, \forall \alpha > 0.$$

$$(17)$$

Here, step ① uses $(E_{t+1})^2 \leq E_t(p^t-p^{t+1})$ and $w_t \triangleq p^t-p^{t+1}$; step ② uses the fact that $ab \leq \frac{\alpha}{2}a^2 + \frac{1}{2\alpha}b^2$ for all $\alpha > 0$; step ③ uses the fact that $\sqrt{a+b} \leq \sqrt{a} + \sqrt{b}$ for all $a,b \geq 0$.

 Assume $1 - \sqrt{\frac{\alpha}{2}} > 0$. Telescoping Inequality (17) over t from i to T, we have:

$$\begin{split} &\sum_{t=i}^{T} w_t \sqrt{1/(2\alpha)} \\ &\geq \{\sum_{t=i}^{T} E_{t+1}\} - \sqrt{\frac{\alpha}{2}} \{\sum_{t=i}^{T} E_t\} \\ &= \{E_{T+1} + \sum_{t=i}^{T-1} E_{t+1}\} - \sqrt{\frac{\alpha}{2}} \{E_i + \sum_{t=i}^{T-1} E_{t+1}\} \\ &= E_{T+1} - \sqrt{\frac{\alpha}{2}} E_i + (1 - \sqrt{\frac{\alpha}{2}}) \sum_{t=i}^{T-1} E_{t+1} \\ &\stackrel{\textcircled{0}}{\geq} - \sqrt{\frac{\alpha}{2}} E_i + (1 - \sqrt{\frac{\alpha}{2}}) \sum_{t=i}^{T-1} E_{t+1}, \end{split}$$

where step ① uses $E_{T+1} \ge 0$ and $1 - \sqrt{\frac{\alpha}{2}} > 0$. This leads to:

$$\sum_{t=i}^{T-1} E_{t+1} \leq (1 - \sqrt{\frac{\alpha}{2}})^{-1} \cdot \{\sqrt{\frac{\alpha}{2}} E_i + \sqrt{\frac{1}{2\alpha}} \sum_{t=i}^{T} w_t \}$$

$$\stackrel{@}{=} E_i + 2 \sum_{t=i}^{T} w_t$$

$$\stackrel{@}{\leq} E_i + 2p^i,$$

step ① uses the fact that $(1-\sqrt{\frac{\alpha}{2}})^{-1}\cdot\sqrt{\frac{\alpha}{2}}=1$ and $(1-\sqrt{\frac{\alpha}{2}})^{-1}\cdot\sqrt{\frac{1}{2\alpha}}=2$ when $\alpha=\frac{1}{2}$; step ② uses Inequalities (16). Letting $T\to\infty$, we conclude this lemma.

Lemma A.11. Assume that $[D_t]^{\tau+1} \leq a(D_{t-1} - D_t)$, where $\tau, a > 0$, and $\{D_t\}_{t=0}^{\infty}$ is a nonnegative sequence. We have: $D_T \leq \mathcal{O}(T^{-1/\tau})$.

Proof. We let $\kappa > 1$ be any constant. We define $h(s) = s^{-\tau - 1}$, where $\tau > 0$.

We consider two cases for $r^t \triangleq h(D_t)/h(D_{t-1})$.

Case (1). $r^t \leq \kappa$. We define $\check{h}(s) \triangleq -\frac{1}{\tau} \cdot s^{-\tau}$. We derive:

$$1 \stackrel{\textcircled{\tiny 0}}{\leq} a(D_{t-1} - D_t) \cdot h(D_t)$$

$$\stackrel{\textcircled{\tiny 2}}{\leq} a(D_{t-1} - D_t) \cdot \kappa h(D_{t-1})$$

$$\stackrel{\textcircled{\tiny 3}}{\leq} a\kappa \int_{D_t}^{D_{t-1}} h(s) ds$$

$$\stackrel{\textcircled{\tiny 0}}{=} a\kappa \cdot (\check{h}(D_{t-1}) - \check{h}(D_t))$$

$$\stackrel{\textcircled{\tiny 5}}{=} a\kappa \cdot \frac{1}{\tau} \cdot ([D_t]^{-\tau} - [D_{t-1}]^{-\tau}),$$

where step ① uses $[D_t]^{\tau+1} \leq a(D_{t-1}-D_t)$; step ② uses $h(D_t) \leq \kappa h(D_{t-1})$; step ③ uses the fact that h(s) is a nonnegative and increasing function that $(a-b)h(a) \leq \int_b^a h(s)ds$ for all $a,b \in [0,\infty)$; step ④ uses the fact that $\nabla \check{h}(s) = h(s)$; step ⑤ uses the definition of $\check{h}(\cdot)$. This leads to:

$$[D_t]^{-\tau} - [D_{t-1}]^{-\tau} \ge \frac{\tau}{\kappa \alpha}.$$
 (18)

Case (2). $r^t > \kappa$. We have:

$$h(D_{t}) > \kappa h(D_{t-1}) \stackrel{\textcircled{0}}{\Rightarrow} [D_{t}]^{-(\tau+1)} > \kappa \cdot [D_{t-1}]^{-(\tau+1)}$$

$$\stackrel{\textcircled{2}}{\Rightarrow} ([D_{t}]^{-(\tau+1)})^{\frac{\tau}{\tau+1}} > \kappa^{\frac{\tau}{\tau+1}} \cdot ([D_{t-1}]^{-(\tau+1)})^{\frac{\tau}{\tau+1}}$$

$$\Rightarrow [D_{t}]^{-\tau} > \kappa^{\frac{\tau}{\tau+1}} \cdot [D_{t-1}]^{-\tau}, \tag{19}$$

where step ① uses the definition of $h(\cdot)$; step ② uses the fact that if a > b > 0, then $a^{\dot{\tau}} > b^{\dot{\tau}}$ for any exponent $\dot{\tau} \triangleq \frac{\tau}{\tau+1} \in (0,1)$. For any $t \geq 1$, we derive:

$$[D_{t}]^{-\tau} - [D_{t-1}]^{-\tau} \stackrel{\text{@}}{\geq} (\kappa^{\frac{\tau}{\tau+1}} - 1) \cdot [D_{t-1}]^{-\tau}$$

$$\stackrel{\text{@}}{\geq} (\kappa^{\frac{\tau}{\tau+1}} - 1) \cdot [D_{0}]^{-\tau}, \tag{20}$$

where step ① uses Inequality (19); step ② uses $\tau > 0$ and $D_{t-1} \le D_0$ for all $t \ge 1$.

In view of Inequalities (18) and (20), we have:

$$[D_t]^{-\tau} - [D_{t-1}]^{-\tau} \ge \underbrace{\min(\frac{\tau}{\kappa\alpha}, (\kappa^{\frac{\tau}{\tau+1}} - 1) \cdot [D_0]^{-\tau})}_{\triangleq \varepsilon}.$$
 (21)

Telescoping Inequality (21) over t from 1 to T, we have:

$$[D_T]^{-\tau} - [D_0]^{-\tau} \ge T\ddot{c}.$$

This leads to:

$$D_T = ([D_T]^{-\tau})^{-1/\tau} \le \mathcal{O}(T^{-1/\tau}).$$

B SOLVING THE SUBPROBLEM WHEN k=2

This section presents a novel Breakpoint Searching Method (**BSM**) to find the *global optimal solution* of Problem (3) when k=2.

Initially, Problem (3) boils down to the following one-dimensional subproblem: $\min_{\theta} \frac{1}{2} \|\mathbf{V}\|_{\mathbf{Q}}^2 + \langle \mathbf{V}, \mathbf{P} \rangle + h(\mathbf{V}\mathbf{Z}), s.t. \mathbf{V} \in \{\mathbf{V}_{\theta}^{\mathrm{rot}}, \mathbf{V}_{\theta}^{\mathrm{ref}}\}$, which can be further rewritten as: $\bar{\theta} \in \arg\min_{\theta} \frac{1}{2} \mathrm{vec}(\mathbf{V})^{\mathsf{T}} \mathbf{Q} \mathrm{vec}(\mathbf{V}) + \langle \mathbf{V}, \mathbf{P} \rangle + h(\mathbf{V}\mathbf{Z}), s.t. \mathbf{V} \triangleq (\frac{\pm \cos(\theta) \sin(\theta)}{\mp \sin(\theta) \cos(\theta)})$, where $\mathbf{Q} \in \mathbb{R}^{4 \times 4}$, $\mathbf{P} \in \mathbb{R}^{2 \times 2}$, and $\mathbf{Z} \in \mathbb{R}^{2 \times r}$. Given $h(\cdot)$ is coordinate-wise separable, we have the following equivalent optimization problem:

$$\min_{\theta} h\left(\cos(\theta)\mathbf{x} + \sin(\theta)\mathbf{y}\right) + a\cos(\theta) + b\sin(\theta) + c\cos^{2}(\theta) + d\cos(\theta)\sin(\theta) + e\sin^{2}(\theta), \quad (22)$$

where
$$a = \mathbf{P}_{22} \pm \mathbf{P}_{11}$$
, $b = \mathbf{P}_{12} \mp \mathbf{P}_{21}$, $c = 0.5(\mathbf{Q}_{11} + \mathbf{Q}_{44}) \pm \mathbf{Q}_{14}$, $d = -\mathbf{Q}_{12} \pm \mathbf{Q}_{13} \mp \mathbf{Q}_{24} + \mathbf{Q}_{34}$, $e = 0.5(\mathbf{Q}_{22} + \mathbf{Q}_{33}) \mp \mathbf{Q}_{23}$, $\mathbf{r} = \pm \mathbf{Z}(1,:)$, $\mathbf{s} = \mathbf{Z}(2,:)$, $\mathbf{p} = \mathbf{Z}(2,:)$, $\mathbf{u} = \mp \mathbf{Z}(1,:)$, $\mathbf{x} \triangleq [\mathbf{r}; \mathbf{p}] \in \mathbb{R}^{2r \times 1}$, and $\mathbf{y} \triangleq [\mathbf{s}; \mathbf{u}] \in \mathbb{R}^{2r \times 1}$.

Our key strategy is to perform a variable substitution to convert Problem (22) into an equivalent problem that depends on the variable $\tan(\theta) \triangleq t$. The substitution is based on the trigonometric identities that $\cos(\theta) = \pm 1/\sqrt{1+\tan^2(\theta)}$ and $\sin(\theta) = \pm \tan(\theta)/\sqrt{1+\tan^2(\theta)}$.

The following lemma provides a characterization of the global optimal solution for Problem (22).

Lemma B.1. We define $\check{F}(\tilde{c},\tilde{s}) \triangleq a\tilde{c} + b\tilde{s} + c\tilde{c}^2 + d\tilde{c}\tilde{s} + e\tilde{s}^2 + h\left(\tilde{c}\mathbf{x} + \tilde{s}\mathbf{y}\right)$, and $w \triangleq c - e$. The optimal solution $\bar{\theta}$ to (22) can be computed as: $[\cos(\bar{\theta}),\sin(\bar{\theta})] \in \arg\min_{[c,s]} \check{F}(c,s)$, s.t. $[c,s] \in \{[c_1,s_1],[c_2,s_2],[0,1],[0,-1]\}$, where $c_1 \triangleq \frac{1}{\sqrt{1+(\bar{t}_+)^2}}$, $s_1 = \frac{\bar{t}_+}{\sqrt{1+(\bar{t}_+)^2}}$, $c_2 \triangleq \frac{-1}{\sqrt{1+(\bar{t}_-)^2}}$, and $s_2 \triangleq \frac{-\bar{t}_-}{\sqrt{1+(\bar{t}_-)^2}}$. Furthermore, \bar{t}_+ and \bar{t}_- are respectively defined as:

$$\bar{t}_{+} \in \operatorname{arg\,min}_{t} \ p(t) \triangleq \frac{a+bt}{\sqrt{1+t^{2}}} + \frac{w+dt}{1+t^{2}} + h(\frac{\mathbf{x}+t\mathbf{y}}{\sqrt{1+t^{2}}}), \tag{23}$$

$$\bar{t}_{-} \in \operatorname{arg\,min}_{t} \, \tilde{p}(t) \triangleq \frac{-a - bt}{\sqrt{1 + t^{2}}} + \frac{w + dt}{1 + t^{2}} + h(\frac{-\mathbf{x} - t\mathbf{y}}{\sqrt{1 + t^{2}}}). \tag{24}$$

Proof. We define $w \triangleq c - e$. We define $F(\tilde{c}, \tilde{s}) \triangleq a\tilde{c} + b\tilde{s} + c\tilde{c}^2 + d\tilde{c}\tilde{s} + e\tilde{s}^2 + h(\tilde{c}\mathbf{x} + \tilde{s}\mathbf{y})$.

Initially, using $\sin^2(\theta) = 1 - \cos^2(\theta)$, we obtain the following problem, which is equivalent to Problem (22):

$$\bar{\theta} \in \arg\min_{\alpha} a \cos(\theta) + b \sin(\theta) + w \cos^{2}(\theta) + d \cos(\theta) \sin(\theta) + e + h(\cos(\theta)\mathbf{x} + \sin(\theta)\mathbf{y}). \tag{25}$$

We assume $\cos(\theta) \neq 0$. Using Lemma A.8, we consider the two cases for $(\cos(\theta), \sin(\theta))$ in Problem (25).

1080 Case a). $\cos(\theta) = \frac{1}{\sqrt{1+\tan^2(\theta)}}$, and $\sin(\theta) = \frac{\tan(\theta)}{\sqrt{1+\tan^2(\theta)}}$. Problem (22) reduces to:

$$\bar{\theta}_+ \in \arg\min_{\theta} \tfrac{a + \tan(\theta)b}{\sqrt{1 + \tan^2(\theta)}} + \tfrac{w + \tan(\theta)d}{1 + \tan^2(\theta)} + h(\tfrac{\mathbf{x} + \tan(\theta)\mathbf{y}}{\sqrt{1 + \tan^2(\theta)}}).$$

Defining $t = \tan(\theta)$, we have the following equivalent problem:

$$\bar{t}_+ \in \arg\min_t \frac{a+bt}{\sqrt{1+t^2}} + \frac{w+dt}{1+t^2} + h(\frac{\mathbf{x}+\mathbf{y}t}{\sqrt{1+t^2}}).$$

Therefore, the optimal solution $\bar{\theta}_+$ can be computed as:

$$\cos(\bar{\theta}_{+}) = \frac{1}{\sqrt{1 + (\bar{t}_{+})^{2}}}, \ \sin(\bar{\theta}_{+}) = \frac{\bar{t}_{+}}{\sqrt{1 + (\bar{t}_{+})^{2}}}.$$
 (26)

Case b). $\cos(\theta) = \frac{-1}{\sqrt{1+\tan(\theta)^2}}$, and $\sin(\theta) = \frac{-\tan(\theta)}{\sqrt{1+\tan(\theta)^2}}$. Problem (22) boils down to:

$$\bar{\theta}_- \in \arg\min_{\theta} \frac{-a - \tan(\theta)b}{\sqrt{1 + \tan(\theta)^2}} + \frac{w + \tan(\theta)d}{1 + \tan(\theta)^2} + h(\frac{-\mathbf{x} - \tan(\theta)\mathbf{y}}{\sqrt{1 + \tan(\theta)^2}}).$$

Defining $t = \tan(\theta)$, we have the following equivalent problem:

$$\bar{t}_{-} \in \arg\min_{t} \frac{-a - bt}{\sqrt{1 + t^2}} + \frac{w + dt}{1 + t^2} + h(\frac{-\mathbf{x} - \mathbf{y}t}{\sqrt{1 + t^2}}).$$

Therefore, the optimal solution $\bar{\theta}_{-}$ can be computed as:

$$\cos(\bar{\theta}_{-}) = \frac{-1}{\sqrt{1 + (\bar{t}_{-})^2}}, \ \sin(\bar{\theta}_{-}) = \frac{-\bar{t}_{-}}{\sqrt{1 + (\bar{t}_{-})^2}}$$
(27)

In view of (26) and (27), when $\cos(\theta) \neq 0$, the optimal solution $\bar{\theta}$ for Problem (25) is computed as: $[\cos(\bar{\theta}),\sin(\bar{\theta})] \in \arg\min_{c,s} \check{F}(c,s), \ s.t. \ [c,s] \in \{[\cos(\bar{\theta}_+),\sin(\bar{\theta}_+)],[\cos(\bar{\theta}_-),\sin(\bar{\theta}_-)]\}$. Taking into account the case when $\cos(\theta) = 0$, the optimal solution $\bar{\theta}$ for Problem (25) is computed as:

$$\begin{split} &[\cos(\bar{\theta}),\sin(\bar{\theta})] \in \arg\min_{c,s} \, \breve{F}(c,s), \\ &s.t. \, [c,s] \in \{ [\cos(\bar{\theta}_+),\sin(\bar{\theta}_+)], [\cos(\bar{\theta}_-),\sin(\bar{\theta}_-)], [0,1], [0,-1] \}. \end{split}$$

Notably, $\{\cos(\bar{\theta}), \sin(\bar{\theta})\}$ uniquely determines $\bar{\theta}$. Moreover, since the objective function in Problem (22) solely depends on $\{\cos(\theta), \sin(\theta)\}$, computing the exact values of $\bar{\theta}_+$ for (26) and $\bar{\theta}_-$ for (27) is unnecessary.

We describe our **BSM** to solve Problem (23); our approach can be naturally extended to tackle Problem (24). **BSM** first identifies all the possible breakpoints / critical points Θ , and then picks the solution that leads to the lowest value as the optimal solution \bar{t} , i.e., $\bar{t} \in \arg\min_t \ p(t), \ s.t. \ t \in \Theta$.

We assume $y_i \neq 0$. If this is not true and there exists $y_i = 0$ for some i, then $\{x_i, y_i\}$ can be removed since it does not affect the minimizer of the problem.

► Finding the Breakpoint Set for $h(\mathbf{x}) \triangleq \lambda \|\mathbf{x}\|_0$

Since the function $h(\mathbf{x}) \triangleq \lambda \|\mathbf{x}\|_0$ is scale-invariant and symmetric with $\|\pm t\mathbf{x}\|_0 = \|\mathbf{x}\|_0$ for all t > 0, Problem (23) reduces to the following problem:

$$\min_{t} p(t) \triangleq \frac{a+bt}{\sqrt{1+t^2}} + \frac{w+dt}{1+t^2} + \lambda \|\mathbf{x} + t\mathbf{y}\|_{0}.$$
(28)

Given the limiting subdifferential of the ℓ_0 norm function can be computed as $\partial \|t\|_0 \in \{ \frac{\mathbb{R}}{\{0\}}, \frac{t=0}{\text{else.}} \}$ (see Appendix C.5), we consider the following two cases. (i) We assume $(\mathbf{x}+t\mathbf{y})_i=0$ for some i. Then the solution \bar{t} can be determined using $\bar{t}=\frac{\mathbf{x}_i}{\mathbf{y}_i}$. There are 2r breakpoints $\{\frac{\mathbf{x}_1}{\mathbf{y}_1}, \frac{\mathbf{x}_2}{\mathbf{y}_2}, ..., \frac{\mathbf{x}_{2r}}{\mathbf{y}_{2r}}\}$ for this case. (ii) We now assume $(\mathbf{x}+t\mathbf{y})_i\neq 0$ for all i. Then $\lambda \|\mathbf{x}+t\mathbf{y}\|_0=2r\lambda$ becomes a constant. Setting the subgradient of p(t) to zero yields:

 $0 = \nabla p(t) = [b(1+t^2) - (a+bt)t] \cdot \sqrt{1+t^2} \cdot t^\circ + [d(1+t^2) - (w+dt)(2t)] \cdot t^\circ, \text{ where } t^\circ = (1+t^2)^{-2}. \text{ Since } t^\circ > 0, \text{ we obtain: } d(1+t^2) - (w+dt)2t = -(b-at) \cdot \sqrt{1+t^2}.$ Squaring both sides, we obtain the following quartic equation: $c_4t^4 + c_3t^3 + c_2t^2 + c_1t + c_0 = 0$ for some suitable c_4 , c_3 , c_2 , c_1 and c_0 . Solving this equation squartically using Lodovico Ferrari's method (WikiContributors), we obtain all its real roots $\{\bar{t}_1, \bar{t}_2, ..., \bar{t}_j\}$ with $1 \leq j \leq 4$. There are at most 4 breakpoints for this case. Therefore, Problem (28) contains at most 2r + 4 breakpoints $\Theta = \{\frac{\mathbf{x}_1}{\mathbf{y}_1}, \frac{\mathbf{x}_2}{\mathbf{y}_2}, ..., \frac{\mathbf{x}_{2r}}{\mathbf{y}_{2r}}, \bar{t}_1, \bar{t}_2, ..., \bar{t}_j\}.$

▶ Finding the Breakpoint Set for $h(\mathbf{x}) \triangleq \lambda ||\mathbf{x}||_1$

Since the function $h(\mathbf{x}) \triangleq \lambda \|\mathbf{x}\|_1$ is symmetric, Problem (23) reduces to the following problem:

$$\bar{t} \in \arg\min_{t} p(t) \triangleq \frac{a+bt}{\sqrt{1+t^2}} + \frac{w+dt}{1+t^2} + \frac{\lambda \|\mathbf{x} + t\mathbf{y}\|_1}{\sqrt{1+t^2}}.$$
 (29)

Setting the subgradient of $p(\cdot)$ to zero yields: $0 \in \partial p(t) = t^{\circ}[d(1+t^2) - (w+dt)2t + (b-at) \cdot \sqrt{1+t^2}] + t^{\circ}\lambda \cdot \sqrt{1+t^2} \cdot [\langle \operatorname{sign}(\mathbf{x}+t\mathbf{y}),\mathbf{y} \rangle (1+t^2) - \|\mathbf{x}+t\mathbf{y}\|_1 t]$, where $t^{\circ} = (1+t^2)^{-2}$. We consider the following two cases. (i) We assume $(\mathbf{x}+t\mathbf{y})_i = 0$ for some i. Then the solution \bar{t} can be determined using $\bar{t} = \frac{\mathbf{x}_i}{\mathbf{y}_i}$. There are 2r breakpoints $\{\frac{\mathbf{x}_1}{\mathbf{y}_1}, \frac{\mathbf{x}_2}{\mathbf{y}_2}, ..., \frac{\mathbf{x}_{2r}}{\mathbf{y}_{2r}}\}$ for this case. (ii) We now assume $(\mathbf{x}+t\mathbf{y})_i \neq 0$ for all i. We define $\mathbf{z} \triangleq \{+\frac{\mathbf{x}_1}{\mathbf{y}_1}, -\frac{\mathbf{x}_1}{\mathbf{y}_1}, +\frac{\mathbf{x}_2}{\mathbf{y}_2}, -\frac{\mathbf{x}_2}{\mathbf{y}_2}, ..., +\frac{\mathbf{x}_{2r}}{\mathbf{y}_{2r}}, -\frac{\mathbf{x}_{2r}}{\mathbf{y}_{2r}}\} \in \mathbb{R}^{4r \times 1}$, and sort \mathbf{z} in non-descending order. Given $\bar{t} \neq \mathbf{z}_i$ for all i in this case, the domain p(t) can be divided into (4r+1) non-overlapping intervals: $(-\infty,\mathbf{z}_1), (\mathbf{z}_1,\mathbf{z}_2), ..., (\mathbf{z}_{4r},+\infty)$. In each interval, $\operatorname{sign}(\mathbf{x}+t\mathbf{y}) \triangleq \mathbf{o}$ can be determined. Combining with the fact that $t^{\circ} > 0$ and $\|\mathbf{x}+t\mathbf{y}\|_1 = \langle \mathbf{o},\mathbf{x}+t\mathbf{y}\rangle$, the first-order optimality condition reduces to: $0 = [d(1+t^2) - (w+dt)2t + (b-at) \cdot \sqrt{1+t^2}] + \lambda \cdot \sqrt{1+t^2} \cdot [\langle \mathbf{o},\mathbf{y}\rangle(1+t^2) - \langle \mathbf{o},\mathbf{x}+t\mathbf{y}\rangle t]$, which can be simplified as: $(at-b) \cdot \sqrt{1+t^2} - \lambda \cdot \sqrt{1+t^2} \cdot [\langle \mathbf{o},\mathbf{y}-t\mathbf{x}\rangle] = [d(1+t^2) - (w+dt)2t]$. We square both sides and then solve the quartic equation. We obtain obtain all its real roots $\{\bar{t}_1,\bar{t}_2,...,\bar{t}_j\}$ with $1 \leq j \leq 4$. Therefore, Problem (29) contains at most $2r + (4r+1) \times 4$ breakpoints.

► Finding the Breakpoint Set for $h(\mathbf{x}) \triangleq I_{>0}(\mathbf{x})$

Since the function $h(\mathbf{x}) \triangleq \iota_{\geq 0}(\mathbf{x})$ is scale-invariant with $h(t\mathbf{x}) = h(\mathbf{x})$ for all $t \geq 0$, Problem (23) reduces to the following problem:

$$\bar{t} \in \arg\min_{t} p(t) \triangleq \frac{a+bt}{\sqrt{1+t^2}} + \frac{w+dt}{1+t^2}, \, s.t. \, \mathbf{x} + t\mathbf{y} \ge \mathbf{0}. \tag{30}$$

We define $I \triangleq \{i|\mathbf{y}_i>0\}$ and $J \triangleq \{i|\mathbf{y}_i<0\}$. It is not difficult to verity that $\{x+t\mathbf{y}\geq0\}$ \Leftrightarrow $\{-\frac{\mathbf{x}_I}{\mathbf{y}_I}\leq t,t\leq-\frac{\mathbf{x}_J}{\mathbf{y}_J}\}\Leftrightarrow\{lb\triangleq\max(-\frac{\mathbf{x}_I}{\mathbf{y}_I})\leq t\leq\min(-\frac{\mathbf{x}_J}{\mathbf{y}_J})\triangleq ub\}$. When lb>ub, we can directly conclude that the problem has no solution for this case. Now we assume $ub\geq lb$ and define $P(t)\triangleq\min(ub,\max(t,lb))$. We omit the bound constraint and set the gradient of p(t) to zero, which yields: $0=\nabla p(t)=[b(1+t^2)-(a+bt)t]\cdot\sqrt{1+t^2}\cdot t^\circ+[d(1+t^2)-(w+dt)(2t)]\cdot t^\circ$, where $t^\circ=(1+t^2)^{-2}$. We obtain all its real roots $\{\bar{t}_1,\bar{t}_2,...,\bar{t}_j\}$ with $1\leq j\leq 4$ after squaring both sides and solving the quartic equation. Combining with the bound constraints, we conclude that Problem (30) contains at most (4+2) breakpoints $\{P(\bar{t}_1),P(\bar{t}_2),...,P(\bar{t}_j),lb,ub\}$ with $1\leq j\leq 4$.

C ADDITIONAL DISCUSSIONS

This section encompasses various discussions, covering topics such as: (i) simple examples for the optimality hierarchy, (ii) computation of the matrix Q, (iii) complexity comparison between **OBCD** and full gradient methods, (iv) generalization to multiple row updates, and (v) the subdifferential of the cardinality function.

C.1 SIMPLE EXAMPLES FOR THE OPTIMALITY HIERARCHY

To demonstrate the strong optimality of BS_2 -points and the advantages of the proposed method, we examine the following simple examples of 2×2 optimization problems mentioned in the paper:

$$\min_{\mathbf{V} \in \text{St}(2,2)} F(\mathbf{V}) \triangleq \|\mathbf{V} - \mathbf{A}\|_{\mathsf{F}}^2, \text{ with } \mathbf{A} = \begin{pmatrix} 1 & 0 \\ -1 & -1 \end{pmatrix}. \tag{31}$$

$$\min_{\mathbf{V} \in St(2.2)} F(\mathbf{V}) \triangleq \|\mathbf{V} - \mathbf{B}\|_{\mathsf{F}}^2 + 5\|\mathbf{V}\|_1, \text{ with } \mathbf{B} = \begin{pmatrix} 1 & 0 \\ 1 & 2 \end{pmatrix}. \tag{32}$$

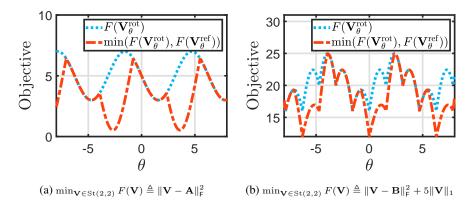


Figure 2: Geometric Visualizations of Two Examples of 2×2 Optimization Problems with Orthogonality Constraints with $\mathbf{A} = \begin{pmatrix} 1 & 0 \\ -1 & -1 \end{pmatrix}$ and $\mathbf{B} = \begin{pmatrix} 1 & 0 \\ 1 & 2 \end{pmatrix}$.

Figure 2 shows the geometric visualizations of Problems (31) and (32) using the relation $\min_{\theta} \min(F(\mathbf{V}_{\theta}^{\text{rot}}), F(\mathbf{V}_{\theta}^{\text{ref}})) = \min_{\mathbf{V} \in \text{St}(2,2)} F(\mathbf{V})$. The two objective functions exhibit periodicity with a period of 2π . Within the interval $[0, 2\pi)$, each of them contains one unique BS₂-point, while the two respective examples contain 4 and 8 critical points. Therefore, the optimality condition of BS₂-points might be much stronger than that of critical points.

BS₂-points vs. Critical Point: Algorithm Instance Study. We briefly analyze methods that find critical points of Problem (31), and demonstrate how they may lead to suboptimal results for Problem (31). We illustrate this with the notable feasible method based on the Cayley transformation (Wen & Yin, 2013). According to Equation (7) from (Wen & Yin, 2013), the update rule is defined as: $\mathbf{X}^{t+1} \Leftarrow \mathbf{Q}\mathbf{X}^t$, where $\mathbf{Q} \triangleq [(\mathbf{I}_2 + \frac{\tau}{2}\mathbf{A})^{-1}(\mathbf{I}_2 - \frac{\tau}{2}\mathbf{A})]$. Here, $\tau \in \mathbb{R}$, and $\mathbf{Q} \in \mathbb{R}^{2 \times 2}$ is a suitable skew-symmetric matrix. Lemma A.3 shows that the matrix \mathbf{Q} consistently functions as a rotation matrix. Consequently, if \mathbf{X}^0 is initialized as a rotation matrix, the resulting solution \mathbf{X}^{t+1} will remain confined to this rotation matrix for all t.

C.2 COMPUTING THE MATRIX Q

Computing the matrix $\mathbf{Q} \in \mathbb{R}^{k^2 \times k^2}$ as in (8) can be a challenging task because it involves the matrix $\mathbf{H} \in \mathbb{R}^{nr \times nr}$. However, in practice, \mathbf{H} often has some special structure that enables fast matrix computation. For example, \mathbf{H} might take a diagonal matrix that is equal to $L\mathbf{I}_{nr}$ for some $L \geq 0$ or has a Kronecker structure where $\mathbf{H} = \mathbf{H}_1 \otimes \mathbf{H}_2$ for some $\mathbf{H}_1 \in \mathbb{R}^{r \times r}$ and $\mathbf{H}_2 \in \mathbb{R}^{n \times n}$. The lemmas provided below demonstrate how to compute the matrix \mathbf{Q} .

Lemma C.1. Assume (8) is used to find \mathbf{Q} . (a) If $\mathbf{H} = \mathbf{H}_1 \otimes \mathbf{H}_2$, we have: $\mathbf{Q} = \mathbf{Q}_1 \otimes \mathbf{Q}_2$, where $\mathbf{Q}_1 = \mathbf{Z}\mathbf{H}_1\mathbf{Z}^{\mathsf{T}} \in \mathbb{R}^{k \times k}$ and $\mathbf{Q}_2 = \mathbf{U}_{\mathsf{B}}^{\mathsf{T}}\mathbf{H}_2\mathbf{U}_{\mathsf{B}} \in \mathbb{R}^{k \times k}$. (b) If $\mathbf{H} = L\mathbf{I}_{nr}$, we have $\mathbf{Q} = (L\mathbf{Z}\mathbf{Z}^{\mathsf{T}}) \otimes \mathbf{I}_k$.

Proof. Recall that for any matrices $\bar{\mathbf{A}}, \bar{\mathbf{B}}, \bar{\mathbf{C}}, \bar{\mathbf{D}}$ of suitable dimensions, we have the following equality: $(\bar{\mathbf{A}} \otimes \bar{\mathbf{B}})(\bar{\mathbf{C}} \otimes \bar{\mathbf{D}}) = (\bar{\mathbf{A}}\bar{\mathbf{C}}) \otimes (\bar{\mathbf{B}}\bar{\mathbf{D}})$.

(a) If
$$\mathbf{H} = \mathbf{H}_1 \otimes \mathbf{H}_2$$
, we derive: $\mathbf{Q} \triangleq (\mathbf{Z}^\mathsf{T} \otimes U_\mathsf{B})^\mathsf{T} \mathbf{H} (\mathbf{Z}^\mathsf{T} \otimes U_\mathsf{B}) = (\mathbf{Z}^\mathsf{T} \otimes U_\mathsf{B})^\mathsf{T} (\mathbf{H}_1 \otimes \mathbf{H}_2) (\mathbf{Z}^\mathsf{T} \otimes U_\mathsf{B}) = (\mathbf{Z}^\mathsf{T} \otimes U_\mathsf{B})^\mathsf{T} [(\mathbf{H}_1 \mathbf{Z}^\mathsf{T}) \otimes (\mathbf{H}_2 U_\mathsf{B})] = (\mathbf{Z} \mathbf{H}_1 \mathbf{Z}^\mathsf{T}) \otimes (U_\mathsf{B}^\mathsf{T} \mathbf{H}_2 U_\mathsf{B}) = \mathbf{Q}_1 \otimes \mathbf{Q}_2.$

(b) If
$$\mathbf{H} = L\mathbf{I}_{nr}$$
, we have: $\mathbf{Q} \triangleq (\mathbf{Z}^{\mathsf{T}} \otimes \mathbf{U}_{\mathsf{B}})^{\mathsf{T}} \mathbf{H} (\mathbf{Z}^{\mathsf{T}} \otimes \mathbf{U}_{\mathsf{B}}) = L(\mathbf{Z}^{\mathsf{T}} \otimes \mathbf{U}_{\mathsf{B}})^{\mathsf{T}} (\mathbf{Z}^{\mathsf{T}} \otimes \mathbf{U}_{\mathsf{B}}) = L(\mathbf{Z}^{\mathsf{T}} \otimes \mathbf{I}_{k})$

Lemma C.2. Assume (9) is used to find \mathbf{Q} . (a) If $\mathbf{H} = \mathbf{H}_1 \otimes \mathbf{H}_2$, we have $\mathbf{Q} = \|\mathbf{Q}_1\|_{\mathsf{sp}} \cdot \|\mathbf{Q}_2\|_{\mathsf{sp}} \cdot \mathbf{I}$, where \mathbf{Q}_1 and \mathbf{Q}_2 are defined in Lemma C.1. (b) If $\mathbf{H} = L\mathbf{I}_{nr}$, we have $\mathbf{Q} = L\|\mathbf{Z}\|_{\mathsf{sp}}^2 \cdot \mathbf{I}$.

1242 Proof. (a) Using the results in Claim (a) of Lemma C.1, we have: $(\mathbf{Z}^{\mathsf{T}} \otimes \mathbf{U}_{\mathsf{B}})^{\mathsf{T}} \mathbf{H} (\mathbf{Z}^{\mathsf{T}} \otimes \mathbf{U}_{\mathsf{B}}) = \mathbf{Q}_1 \otimes \mathbf{Q}_2 \preceq \|\mathbf{Q}_1\|_{\mathsf{sp}} \cdot \|\mathbf{Q}_2\|_{\mathsf{sp}} \cdot \mathbf{I}.$

(b) Using the results in Claim (b) of Lemma C.1, we have: $(\mathbf{Z}^{\mathsf{T}} \otimes \mathbf{U}_{\mathsf{B}})^{\mathsf{T}} \mathbf{H} (\mathbf{Z}^{\mathsf{T}} \otimes \mathbf{U}_{\mathsf{B}}) = L \mathbf{Z} \mathbf{Z}^{\mathsf{T}} \otimes \mathbf{I}_{k} \leq L \|\mathbf{Z}\|_{\mathsf{sp}}^{2} \cdot \mathbf{I}.$

 \Box

C.3 COMPLEXITY COMPARISON BETWEEN **OBCD** AND FULL GRADIENT METHODS

We present a computational complexity comparison with full gradient methods using the linear eigenvalue problem: $\min_{\mathbf{X}} F(\mathbf{X}) \triangleq \frac{1}{2} \langle \mathbf{X}, \mathbf{C} \mathbf{X} \rangle$, s.t. $\mathbf{X}^{\mathsf{T}} \mathbf{X} = \mathbf{I}_r$, where $\mathbf{C} \in \mathbb{R}^{n \times n}$ is given.

We first examine full gradient methods such as the Riemannian gradient method (Jiang & Dai, 2015; Liu et al., 2016). The computation of the Riemannian gradient $\nabla_{\mathcal{M}} F(\mathbf{X}) = \mathbf{C}\mathbf{X} - \mathbf{X}[\mathbf{C}\mathbf{X}]^\mathsf{T}\mathbf{X}$ requires $\mathcal{O}(n^2r)$ time, while the retraction step using SVD, QR, or polar decomposition demands $\mathcal{O}(nr^2)$. Consequently, the overall complexity for Riemannian gradient method is $N_1 \times \mathcal{O}(n^2r)$, where N_1 is the number of iterations required for convergence.

We now consider the proposed **OBCD** method where the matrix \mathbf{Q} is chosen to be a diagonal matrix as in Equality (9). (i) We adopt an incremental update strategy for computing the Euclidean gradient $\nabla F(\mathbf{X}) = \mathbf{C}\mathbf{X}$, maintaining the relationship $\mathbf{Y}^t = \mathbf{C}\mathbf{X}^t$ for all t. The initialization $\mathbf{Y}^0 = \mathbf{C}\mathbf{X}^0$ occurs only once. When \mathbf{X}^t is updated via a k-row change, resulting in $\mathbf{X}^{t+1} = \mathbf{X}^t + \mathbf{U}_{\mathbb{B}}(\mathbf{V} - \mathbf{I})\mathbf{U}_{\mathbb{B}}^{\mathsf{T}}\mathbf{X}^t$, we efficiently reconstruct $\mathbf{C}\mathbf{X}^{t+1}$ by updating $\mathbf{Y}^{t+1} = \mathbf{Y}^t + \mathbf{C}\mathbf{U}_{\mathbb{B}}(\mathbf{V} - \mathbf{I})\mathbf{U}_{\mathbb{B}}^{\mathsf{T}}\mathbf{X}^t$ in $\mathcal{O}(nr)$ time. (ii) Computing the matrix \mathbf{P} as shown in (3) involves matrix multiplication between matrices $[\nabla f(\mathbf{X}^t)]_{\mathbb{B}} \in \mathbb{R}^{k \times r}$ and $[[\mathbf{X}^t]_{\mathbb{B}}]^{\mathsf{T}} \in \mathbb{R}^{r \times k}$, which can be done in $\mathcal{O}(rk^2)$. (iii) Solving the subproblem using small-size SVD takes $\mathcal{O}(k^3)$ time. Thus, the total complexity for **OBCD** is $N_2 \times \mathcal{O}(nr + rk^2 + k^3)$, with N_2 denoting the number of **OBCD** iterations.

C.4 GENERALIZATION TO MULTIPLE ROW UPDATES

The proposed **OBCD** algorithm can be generalized to multiple row updates scheme.

Assume that n is an even number, and k=2. As mentioned in Lemma 2.3, when (9) is used to find \mathbf{Q} , the subproblem $\bar{\mathbf{V}}^t \in \arg\min_{\mathbf{V} \in \operatorname{St}(k,k)} \mathcal{K}(\mathbf{V};\mathbf{X}^t,\mathbf{B})$ in Algorithm 1 reduces to:

$$\min_{\mathbf{V} \in \text{St}(2,2)} \langle \mathbf{V}, (\nabla f(\mathbf{X}^t)[\mathbf{X}^t]^\mathsf{T})_{\text{BB}} \rangle + h(\mathbf{V}\mathbf{U}_{\text{B}}\mathbf{X}^t). \tag{33}$$

One can independently solve (n/2) subproblems, each formulated as follows:

 $\min_{\mathbf{V} \in \text{St}(2,2)} \langle \mathbf{V}, (\nabla f(\mathbf{X}^t)[\mathbf{X}^t]^\mathsf{T})_{\text{BB}} \rangle + h(\mathbf{V}\mathbf{U}_{\text{B}}\mathbf{X}^t) \text{ with } \mathbf{B} = [1,2].$

 $\min_{\mathbf{V} \in \text{St}(2.2)} \langle \mathbf{V}, (\nabla f(\mathbf{X}^t)[\mathbf{X}^t]^\mathsf{T})_{\text{BB}} \rangle + h(\mathbf{V} \mathbf{U}_{\text{B}} \mathbf{X}^t) \text{ with } \mathbf{B} = [3, 4].$

1281 ...

$$\min_{\mathbf{V} \in \text{St}(2,2)} \langle \mathbf{V}, (\nabla f(\mathbf{X}^t)[\mathbf{X}^t]^\mathsf{T})_{\text{BB}} \rangle + h(\mathbf{V} \mathbf{U}_{\text{B}} \mathbf{X}^t) \text{ with } \mathbf{B} = [n-1,n].$$

This approach, known as the Jacobi update in the literature, allows for the parallel update of n rows of the matrix \mathbf{X} .

Notably, one can consider $k \triangleq |B| > 2$ when $h(\cdot) = 0$, and the associated subproblems can be solved using SVD.

C.5 LIMITING SUBDIFFERENTIAL OF THE CARDINALITY FUNCTION

We demonstrate how to calculate the limiting subdifferential of the cardinality function $h(\mathbf{X}) = \|\mathbf{X}\|_0$. Given that $h(\mathbf{X}) = \|\mathbf{X}\|_0$ is coordinate-wise separable, we focus only on the scalar function $h(x) = |x|_0$, where $|x|_0 = \{0, x=0; \\ 1, else.\}$.

The Fréchet subdifferential of the function $h(x) = |x|_0$ at $x \in \text{dom}(h)$ is defined as $\hat{\partial}h(x) \triangleq \{\xi \in \mathbb{R} : \lim_{z \to x} \inf_{z \neq x} \frac{h(z) - h(x) - \langle \xi, z - x \rangle}{|z - x|} \geq 0\}$, while the limiting subdifferential of h(x) at $x \in \mathbb{R}$

dom(h) is denoted as $\partial h(x) \triangleq \{\xi \in \mathbb{R} : \exists x^t \to x, h(x^t) \to h(x), \xi^t \in \hat{\partial} h(x^t) \to \xi, \forall t\}$. We consider the following two cases. (i) $x \neq 0$. We have: $\hat{\partial} h(x) = \{\xi \in \mathbb{R} : \lim_{z \to x} \inf_{z \neq x} \frac{-\langle \xi, z - x \rangle}{|z - x|} \ge 0\} = \{0\}$. (ii) x = 0. We have: $\hat{\partial} h(x) = \{\xi \in \mathbb{R} : \lim_{z \to x} \inf_{z \neq x} \frac{|z|_0 - \langle \xi, z - x \rangle}{|z - x|} \ge 0\} = \{\xi \in \mathbb{R} : \lim_{z \to x} \inf_{z \neq x} \frac{1 - \langle \xi, z \rangle}{|z|} \ge 0\} = \mathbb{R}$.

We therefore conclude that $[\partial \|\mathbf{X}\|_0]_{i,j} \in \{ {\mathbb{R}, \mathbf{X}_{i,j} = 0; \atop \{0\}, \text{else.}} \}$ for all $i \in [n]$ and $j \in [r]$.

D PROOF FOR SECTION 2

D.1 Proof for Lemma 2.1

 Proof. Part (a). For any $\mathbf{V} \in \mathbb{R}^{k \times k}$ and $\mathbf{B} \in \{\mathcal{B}_i\}_{i=1}^{\mathbb{C}_n^k}$, we have:

$$[\mathbf{X}^{+}]^{\mathsf{T}}\mathbf{X}^{+} - \mathbf{X}^{\mathsf{T}}\mathbf{X}$$

$$\stackrel{\textcircled{\tiny }}{=} [\mathbf{X} + \mathbf{U}_{\mathbb{B}}(\mathbf{V} - \mathbf{I}_{k})\mathbf{U}_{\mathbb{B}}^{\mathsf{T}}\mathbf{X}]^{\mathsf{T}}[\mathbf{X} + \mathbf{U}_{\mathbb{B}}(\mathbf{V} - \mathbf{I}_{k})\mathbf{U}_{\mathbb{B}}^{\mathsf{T}}\mathbf{X}] - \mathbf{X}^{\mathsf{T}}\mathbf{X}$$

$$= \mathbf{X}^{\mathsf{T}}\mathbf{U}_{\mathbb{B}}(\mathbf{V} - \mathbf{I}_{k})\mathbf{U}_{\mathbb{B}}^{\mathsf{T}}\mathbf{X} + [\mathbf{U}_{\mathbb{B}}(\mathbf{V} - \mathbf{I}_{k})\mathbf{U}_{\mathbb{B}}^{\mathsf{T}}\mathbf{X}]^{\mathsf{T}}\mathbf{X} + [\mathbf{U}_{\mathbb{B}}(\mathbf{V} - \mathbf{I}_{k})\mathbf{U}_{\mathbb{B}}^{\mathsf{T}}\mathbf{X}]^{\mathsf{T}}[\mathbf{U}_{\mathbb{B}}(\mathbf{V} - \mathbf{I}_{k})\mathbf{U}_{\mathbb{B}}^{\mathsf{T}}\mathbf{X}]$$

$$= \mathbf{X}^{\mathsf{T}}\mathbf{U}_{\mathbb{B}}\left[(\mathbf{V} - \mathbf{I}_{k} + \mathbf{V}^{\mathsf{T}} - \mathbf{I}_{k}) + (\mathbf{V} - \mathbf{I}_{k})^{\mathsf{T}}(\mathbf{V} - \mathbf{I}_{k})\right]\mathbf{U}_{\mathbb{B}}^{\mathsf{T}}\mathbf{X}$$

$$= \mathbf{X}^{\mathsf{T}}\mathbf{U}_{\mathbb{B}}(\mathbf{V} - \mathbf{I}_{k} + \mathbf{V}^{\mathsf{T}} - \mathbf{I}_{k}) + (\mathbf{V} - \mathbf{V}^{\mathsf{T}} - \mathbf{V} + \mathbf{I}_{k})\mathbf{U}_{\mathbb{B}}^{\mathsf{T}}\mathbf{X}$$

$$= \mathbf{X}^{\mathsf{T}}\mathbf{U}_{\mathbb{B}}(\mathbf{V} - \mathbf{I}_{k} + \mathbf{V}^{\mathsf{T}}\mathbf{V})\mathbf{U}_{\mathbb{B}}^{\mathsf{T}}\mathbf{X}$$

$$= \mathbf{X}^{\mathsf{T}}\mathbf{U}_{\mathbb{B}}(-\mathbf{I}_{k} + \mathbf{V}^{\mathsf{T}}\mathbf{V})\mathbf{U}_{\mathbb{B}}^{\mathsf{T}}\mathbf{X}$$

$$\stackrel{\textcircled{\tiny{3}}}{=} \mathbf{X}^{\mathsf{T}}\mathbf{U}_{\mathbb{B}} \cdot \mathbf{0} \cdot \mathbf{U}_{\mathbb{B}}^{\mathsf{T}}\mathbf{X}$$

where step ① uses $\mathbf{X}^+ = \mathbf{X} + \mathbf{U}_{\mathsf{B}}(\mathbf{V} - \mathbf{I}_k)\mathbf{U}_{\mathsf{B}}^\mathsf{T}\mathbf{X}$; step ② uses $\mathbf{U}_{\mathsf{B}}^\mathsf{T}\mathbf{U}_{\mathsf{B}} = \mathbf{I}_k$; step ③ uses $\mathbf{V}^\mathsf{T}\mathbf{V} = \mathbf{I}_k$.

Part (b). Obvious.

D.2 PROOF OF LEMMA 2.2

Proof. We define $\mathbf{X}^+ \triangleq \mathbf{X} + \mathrm{U}_{\mathrm{B}}(\mathbf{V} - \mathbf{I}_k)\mathrm{U}_{\mathrm{B}}^\mathsf{T}\mathbf{X}, \underline{\mathbf{Q}} \triangleq (\mathbf{Z}^\mathsf{T} \otimes \mathrm{U}_{\mathrm{B}})^\mathsf{T}\mathbf{H}(\mathbf{Z}^\mathsf{T} \otimes \mathrm{U}_{\mathrm{B}}), \text{ and } \mathbf{Z} \triangleq \mathrm{U}_{\mathrm{B}}^\mathsf{T}\mathbf{X}.$

Part (a). We derive the following results:

$$\begin{split} \|\mathbf{X}^{+} - \mathbf{X}\|_{\mathbf{H}}^{2} & \stackrel{\textcircled{@}}{=} \|\mathbf{U}_{\mathbb{B}}(\mathbf{V} - \mathbf{I}_{k})\mathbf{Z}\|_{\mathbf{H}}^{2} \\ & \stackrel{\textcircled{@}}{=} \operatorname{vec}(\mathbf{U}_{\mathbb{B}}(\mathbf{V} - \mathbf{I}_{k})\mathbf{Z})^{\mathsf{T}}\mathbf{H}\operatorname{vec}(\mathbf{U}_{\mathbb{B}}(\mathbf{V} - \mathbf{I}_{k})\mathbf{Z}) \\ & \stackrel{\textcircled{@}}{=} \operatorname{vec}(\mathbf{V} - \mathbf{I}_{k})^{\mathsf{T}}(\mathbf{Z}^{\mathsf{T}} \otimes \mathbf{U}_{\mathbb{B}})^{\mathsf{T}}\mathbf{H}(\mathbf{Z}^{\mathsf{T}} \otimes \mathbf{U}_{\mathbb{B}})\operatorname{vec}(\mathbf{V} - \mathbf{I}_{k}) \\ & \stackrel{\textcircled{@}}{=} \|\mathbf{V} - \mathbf{I}_{k}\|_{(\mathbf{Z}^{\mathsf{T}} \otimes \mathbf{U}_{\mathbb{B}})^{\mathsf{T}}\mathbf{H}(\mathbf{Z}^{\mathsf{T}} \otimes \mathbf{U}_{\mathbb{B}})} \\ & \stackrel{\textcircled{@}}{=} \|\mathbf{V} - \mathbf{I}_{k}\|_{\mathbf{Q}}^{2}, \end{split}$$

where step ① uses $\mathbf{X}^+ \triangleq \mathbf{X} + \mathbf{U}_{\mathrm{B}}(\mathbf{V} - \mathbf{I}_k)\mathbf{Z}$; step ② uses $\|\mathbf{X}\|_{\mathbf{H}}^2 = \mathrm{vec}(\mathbf{X})^{\mathsf{T}}\mathbf{H}\mathrm{vec}(\mathbf{X})$; step ③ uses $(\mathbf{Z}^{\mathsf{T}} \otimes \mathbf{R})\mathrm{vec}(\mathbf{U}) = \mathrm{vec}(\mathbf{R}\mathbf{U}\mathbf{Z})$ for all \mathbf{R} , \mathbf{Z} , and \mathbf{U} of suitable dimensions; step ④ uses $\|\mathbf{X}\|_{\mathbf{H}}^2 = \mathrm{vec}(\mathbf{X})^{\mathsf{T}}\mathbf{H}\mathrm{vec}(\mathbf{X})$ again; step ⑤ uses the definition of \mathbf{Q} .

Part (b). We derive the following equalities:

$$\|\mathbf{X}^{+} - \mathbf{X}\|_{\mathsf{F}}^{2} \stackrel{\widehat{\oplus}}{=} \|\mathbf{U}_{\mathsf{B}}(\mathbf{V} - \mathbf{I}_{k})\mathbf{Z}\|_{\mathsf{F}}^{2}$$

$$\stackrel{\widehat{\otimes}}{=} \|(\mathbf{V} - \mathbf{I}_{k})\mathbf{Z}\|_{\mathsf{F}}^{2}$$

$$= \langle(\mathbf{V} - \mathbf{I}_{k})^{\mathsf{T}}(\mathbf{V} - \mathbf{I}_{k}), \mathbf{Z}\mathbf{Z}^{\mathsf{T}}\rangle$$

$$\stackrel{\widehat{\otimes}}{=} 2\langle\mathbf{I}_{k} - \mathbf{V}, \mathbf{Z}\mathbf{Z}^{\mathsf{T}}\rangle + \langle\mathbf{V} - \mathbf{V}^{\mathsf{T}}, \mathbf{Z}\mathbf{Z}^{\mathsf{T}}\rangle.$$

$$\stackrel{\widehat{\oplus}}{=} 2\langle\mathbf{I}_{k} - \mathbf{V}, \mathbf{Z}\mathbf{Z}^{\mathsf{T}}\rangle + 0.$$

where step ① uses $\mathbf{X}^+ \triangleq \mathbf{X} + U_{\mathbb{B}}(\mathbf{V} - \mathbf{I}_k)\mathbf{Z}$; step ② uses the fact that $\|\mathbf{U}_{\mathbb{B}}\mathbf{V}\|_{\mathsf{F}}^2 = \|\mathbf{V}\|_{\mathsf{F}}^2$ for any $\mathbf{V} \in \mathbb{R}^{k \times k}$; step ③ uses

$$(\mathbf{V} - \mathbf{I}_k)^\mathsf{T} (\mathbf{V} - \mathbf{I}_k) = \mathbf{I}_k - \mathbf{V}^\mathsf{T} - \mathbf{V} + \mathbf{I}_k = 2(\mathbf{I}_k - \mathbf{V}) + (\mathbf{V} - \mathbf{V}^\mathsf{T});$$

step 4 uses the fact that $\langle \mathbf{V}, \mathbf{Z}\mathbf{Z}^\mathsf{T} \rangle = \langle \mathbf{V}^\mathsf{T}, (\mathbf{Z}\mathbf{Z}^\mathsf{T})^\mathsf{T} \rangle = \langle \mathbf{V}^\mathsf{T}, \mathbf{Z}\mathbf{Z}^\mathsf{T} \rangle$ which holds true as the matrix $\mathbf{Z}\mathbf{Z}^\mathsf{T}$ is symmetric.

Part (c). We have:

$$\|\mathbf{X}^{+} - \mathbf{X}\|_{\mathsf{F}}^{2} = \|\mathbf{U}_{\mathsf{B}}(\mathbf{V} - \mathbf{I}_{k})\mathbf{U}_{\mathsf{B}}^{\mathsf{T}}\mathbf{X}\|_{\mathsf{F}}^{2}$$

$$\stackrel{\text{\tiny 0}}{\leq} \|\mathbf{U}_{\mathsf{B}}\|_{\mathsf{sp}}^{2} \cdot \|(\mathbf{V} - \mathbf{I}_{k})\mathbf{U}_{\mathsf{B}}^{\mathsf{T}}\mathbf{X}\|_{\mathsf{F}}^{2}$$

$$\stackrel{\text{\tiny 0}}{\leq} \|\mathbf{U}_{\mathsf{B}}\|_{\mathsf{sp}}^{2} \cdot \|\mathbf{V} - \mathbf{I}_{k}\|_{\mathsf{F}}^{2} \cdot \|\mathbf{U}_{\mathsf{B}}^{\mathsf{T}}\|_{\mathsf{sp}}^{2} \cdot \|\mathbf{X}\|_{\mathsf{sp}}^{2}$$

$$\stackrel{\text{\tiny 0}}{=} \|\mathbf{V} - \mathbf{I}_{k}\|_{\mathsf{F}}^{2}$$

$$\stackrel{\text{\tiny 0}}{=} 2\langle \mathbf{I}_{k} - \mathbf{V}, \mathbf{I}_{k} \rangle,$$

where step ① and step ② uses the norm inequality that $\|\mathbf{A}\mathbf{X}\|_{\mathsf{F}} \leq \|\mathbf{A}\|_{\mathsf{F}} \cdot \|\mathbf{X}\|_{\mathsf{sp}}$ for any \mathbf{A} and \mathbf{X} ; step ③ uses $\|\mathbf{U}_{\mathsf{B}}\|_{\mathsf{sp}} = \|\mathbf{U}_{\mathsf{B}}^{\mathsf{T}}\|_{\mathsf{sp}} = \|\mathbf{X}\|_{\mathsf{sp}} = 1$ for any $\mathbf{X} \in \mathrm{St}(n,r)$; step ④ uses the following equalities for any $\mathbf{V} \in \mathrm{St}(k,k)$:

$$\|\mathbf{V} - \mathbf{I}_k\|_{\mathsf{F}}^2 = \|\mathbf{V}\|_{\mathsf{F}}^2 + \|\mathbf{I}_k\|_{\mathsf{F}}^2 - 2\langle \mathbf{I}_k, \mathbf{V} \rangle = \|\mathbf{I}_k\|_{\mathsf{F}}^2 + \|\mathbf{I}_k\|_{\mathsf{F}}^2 - 2\langle \mathbf{I}_k, \mathbf{V} \rangle = 2\langle \mathbf{I}_k, \mathbf{I}_k - \mathbf{V} \rangle.$$

D.3 PROOF OF LEMMA 2.3

Proof. We define $\mathcal{K}(\mathbf{V}; \mathbf{X}^t, \mathbb{B}) \triangleq \frac{1}{2} \|\mathbf{V} - \mathbf{I}_k\|_{\mathbf{Q} + \alpha \mathbf{I}}^2 + h(\mathbf{V}\mathbf{Z}) + \langle \mathbf{V}, [\nabla f(\mathbf{X}^t)(\mathbf{X}^t)^\mathsf{T}]_{\mathbb{B}\mathbb{B}} \rangle + \ddot{c}$, where $\mathbf{Z} \triangleq \mathbf{U}_{\mathbb{B}}^\mathsf{T} \mathbf{X}^t$, and $\ddot{c} = h(\mathbf{U}_{\mathbb{B}^c}^\mathsf{T} \mathbf{X}^t) + f(\mathbf{X}^t) - \langle \mathbf{I}_k, [\nabla f(\mathbf{X}^t)(\mathbf{X}^t)^\mathsf{T}]_{\mathbb{B}\mathbb{B}} \rangle$ is a constant.

Part (a). Using the definition of $\mathcal{K}(\mathbf{V}; \mathbf{X}^t, \mathbf{B})$, we have the following equalities for all $\mathbf{V} \in \mathrm{St}(k, k)$: $\mathcal{K}(\mathbf{V}; \mathbf{X}^t, \mathbf{B})$

$$\stackrel{\triangle}{=} \ddot{c} + \frac{1}{2} \|\mathbf{V} - \mathbf{I}_{k}\|_{\mathbf{Q} + \alpha \mathbf{I}_{k}}^{2} + \langle \mathbf{V}, [\nabla f(\mathbf{X}^{t})(\mathbf{X}^{t})^{\mathsf{T}}]_{\mathsf{BB}} \rangle + h(\mathbf{V}\mathbf{Z})$$

$$= \ddot{c} + \frac{1}{2} \|\mathbf{V} - \mathbf{I}_{k}\|_{\mathbf{Q}}^{2} + \frac{\alpha}{2} \|\mathbf{V} - \mathbf{I}_{k}\|_{\mathsf{F}}^{2} + \langle \mathbf{V}, [\nabla f(\mathbf{X}^{t})(\mathbf{X}^{t})^{\mathsf{T}}]_{\mathsf{BB}} \rangle + h(\mathbf{V}\mathbf{Z})$$

$$\stackrel{\textcircled{\tiny{0}}}{=} \ddot{c} + \frac{1}{2} \|\mathbf{V}\|_{\mathbf{Q}}^{2} - \langle \mathbf{V}, \max(\mathbf{Q}\operatorname{vec}(\mathbf{I}_{k})) \rangle + \frac{1}{2} \|\mathbf{I}_{k}\|_{\mathbf{Q}}^{2} + \alpha \langle \mathbf{I}_{k}, \mathbf{I}_{k} - \mathbf{V} \rangle + \langle \mathbf{V}, [\nabla f(\mathbf{X}^{t})(\mathbf{X}^{t})^{\mathsf{T}}]_{\mathsf{BB}} \rangle + h(\mathbf{V}\mathbf{Z})$$

$$\stackrel{\textcircled{\tiny{2}}}{=} \ddot{c} + \frac{1}{2} \|\mathbf{V}\|_{\mathbf{Q}}^{2} + \langle \mathbf{V}, [\nabla f(\mathbf{X}^{t})(\mathbf{X}^{t})^{\mathsf{T}}]_{\mathsf{BB}} - \max(\mathbf{Q}\operatorname{vec}(\mathbf{I}_{k})) - \alpha \mathbf{I}_{k} \rangle + h(\mathbf{V}\mathbf{Z}) + \frac{1}{2} \|\mathbf{I}_{k}\|_{\mathbf{Q}}^{2},$$

where step ① uses Claim (c) of Lemma 2.2 that: $\frac{\alpha}{2} \|\mathbf{V} - \mathbf{I}_k\|_{\mathsf{F}}^2 = \alpha \langle \mathbf{I}_k, \mathbf{I}_k - \mathbf{V} \rangle$; step ② uses the definition of \mathbf{P} .

Part (b). We consider the case that \mathbf{Q} is chosen to be a diagonal matrix that $\mathbf{Q} = \varsigma \mathbf{I}_k$, where ς is defined in Equation (9). Using $\mathbf{V} \in \operatorname{St}(k,k)$, the term $\frac{1}{2} \|\mathbf{V}\|_{\mathbf{Q}}^2$ simplifies to a constant with $\frac{1}{2} \|\mathbf{V}\|_{\mathbf{Q}}^2 = \frac{\varsigma}{2} k$. We can deduce from (3):

$$\bar{\mathbf{V}}^t \in \arg\min_{\mathbf{V} \in \text{St}(k,k)} \mathcal{P}(\mathbf{V}) \triangleq \langle \mathbf{V}, \mathbf{P} \rangle + h(\mathbf{X}). \tag{34}$$

In particular, when $h(\mathbf{X}) = 0$, Problem (34) becomes the nearest orthogonality matrix problem and can be solved analytically, yielding a closed-form solution that:

$$\bar{\mathbf{V}}^t \in \arg\min_{\mathbf{V} \in \operatorname{St}(k,k)} \frac{1}{2} \|\mathbf{V} - (-\mathbf{P})\|_{\mathsf{F}}^2 = \mathbb{P}_{\mathcal{M}}(-\mathbf{P}) = -\mathbb{P}_{\mathcal{M}}(\mathbf{P}) = -\tilde{\mathbf{U}}\tilde{\mathbf{V}}^{\mathsf{T}}.$$

Here, $\mathbf{P} = \tilde{\mathbf{U}} \mathrm{Diag}(\mathbf{s}) \tilde{\mathbf{V}}^\mathsf{T}$ is the singular value decomposition of \mathbf{P} with $\tilde{\mathbf{U}}, \tilde{\mathbf{V}} \in \mathrm{St}(k, k), \mathbf{s} \in \mathbb{R}^k$, and $\mathbf{s} \geq \mathbf{0}$.

Notably, the multiplier for the orthogonality constraint $\mathbf{V}^\mathsf{T}\mathbf{V} = \mathbf{I}_k$ can be computed as: $\mathbf{\Lambda} = -\mathbf{P}^\mathsf{T}\bar{\mathbf{V}}^t \stackrel{@}{=} -[\tilde{\mathbf{U}}\mathrm{Diag}(\mathbf{s})\tilde{\mathbf{V}}^\mathsf{T}]^\mathsf{T} \cdot [-\tilde{\mathbf{U}}\tilde{\mathbf{V}}^\mathsf{T}] = \tilde{\mathbf{V}}\mathrm{Diag}(\mathbf{s})\tilde{\mathbf{U}}^\mathsf{T}\tilde{\mathbf{U}}\tilde{\mathbf{V}}^\mathsf{T} \stackrel{@}{=} \tilde{\mathbf{V}}\mathrm{Diag}(\mathbf{s})\tilde{\mathbf{V}}^\mathsf{T} \stackrel{@}{\succeq} \mathbf{0}$, where step \mathbb{Q} uses $\mathbf{P} = \tilde{\mathbf{U}}\mathrm{Diag}(\mathbf{s})\tilde{\mathbf{V}}^\mathsf{T}$ and $\bar{\mathbf{V}}^t = -\tilde{\mathbf{U}}\tilde{\mathbf{V}}^\mathsf{T}$; step \mathbb{Q} uses $\tilde{\mathbf{U}}^\mathsf{T}\tilde{\mathbf{U}} = \mathbf{I}_k$; step \mathbb{Q} uses $\mathbf{s} \geq 0$.

D.4 PROOF OF LEMMA 2.5

Proof. Any 2×2 matrix takes the form $\mathbf{V} = \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix} \right)$. The orthogonality constraint implies that $\mathbf{V} \in \operatorname{St}(2,2)$ meets the following three equations: $1 = a^2 + b^2$, $1 = c^2 + d^2$, 0 = ac + bd. Without loss of generality, we let $c = \sin(\theta)$ and $d = \cos(\theta)$ with $\theta \in \mathbb{R}$. Then we obtain either (i) $a = \cos(\theta)$, $b = -\sin(\theta)$ or (ii) $a = -\cos(\theta)$, $b = \sin(\theta)$. Therefore, we have the following Givens rotation matrix $\mathbf{V}_{\theta}^{\operatorname{rot}}$ and Jacobi reflection matrix $\mathbf{V}_{\theta}^{\operatorname{ref}}$:

$$\mathbf{V}_{\theta}^{\mathrm{rot}} \triangleq \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}, \ \mathbf{V}_{\theta}^{\mathrm{ref}} \triangleq \begin{bmatrix} -\cos(\theta) & \sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}.$$

Note that for any $a,b,c,d\in\mathbb{R}$, we have: $\det(\frac{a}{c}\frac{b}{d})=ad-bc$. Therefore, we obtain: $\det(\mathbf{V}^{\mathrm{rot}}_{\theta})=\cos^2(\theta)+\sin^2(\theta)=1$ and $\det(\mathbf{V}^{\mathrm{rot}}_{\theta})=-\cos^2(\theta)-\sin^2(\theta)=-1$ for any $\theta\in\mathbb{R}$.

П

E Proof for Section 3

```
function [Q,R] = JacobiGivensQR(X)
                                                                         2
n = size(X,1); Q = eye(n); R = X;
                                                                         3
for j=1:n
   for i=n:-1:(j+1)
                                                                         5
      B = [i-1;i]; V = Givens(R(i-1,j),R(i,j));
                                                                         6
      R(B,:) = V' *R(B,:); Q(:,B) = Q(:,B) *V;
      if (i==j+1 \&\& R(j,j)<0)
                                                                         7
                                                                         8
          V = [-1 \ 0; \ 0 \ -1]; % or <math>V = [-1 \ 0; \ 0 \ 1];
          R(B,:) = V' *R(B,:); Q(:,B) = Q(:,B) *V;
                                                                         9
                                                                         10
      end
                                                                         11
   end
                                                                         12
end
                                                                         13
if(R(n,n)<0)
    V = [1 \ 0; 0 \ -1]; R(B,:) = V' *R(B,:); Q(:,B) = Q(:,B) *V;
                                                                         14
                                                                         15
                                                                         16
function V = Givens(a,b)
                                                                         17
% Find a Givens rotation that V'*[a;b] = [r;0]
                                                                         18
                                                                         19
if (b==0)
                                                                         20
    c = 1; s = 0;
else
                                                                         21
    if (abs(b) > abs(a))
                                                                         22
                                                                         23
        tau = -a/b; s = 1/sqrt(1+tau^2); c = s*tau;
                                                                         24
                                                                         25
        tau = -b/a; c = 1/sqrt(1+tau^2); s = c*tau;
                                                                         26
    end
end
                                                                         27
                                                                         28
    [c s;-s c];
```

Listing 1: Matlab implementation for our **Jacobi-Givens-QR** algorithm.

E.1 Proof of Theorem 3.1

Proof. Part (a). First, recall the classical Givens-QR algorithm, which is detailed in Section 5.2.5 of (Golub & Van Loan, 2013)). This algorithm can decompose any matrix $\mathbf{X} \in \mathbb{R}^{n \times n}$ (not necessarily orthogonal) into the form $\mathbf{X} = \mathbf{Q}\mathbf{R}$, where \mathbf{Q} is an orthogonal matrix ($\mathbf{Q} \in \mathrm{St}(n,n)$) and \mathbf{R} is a lower triangular matrix with $\mathbf{R}_{ij} = 0$ for all i < j, achieved through $\mathrm{C}_n^2 = \frac{n(n-1)}{2}$ Givens rotation steps.

Combining the result from Lemma A.5, we can conclude that classical **Givens-QR** algorithm can decompose any orthogonal matrix into the form $\mathbf{X} = \mathbf{QR}$, where $\mathbf{Q} \in \mathrm{St}(n,n)$ and \mathbf{R} is diagonal matrix with $\mathbf{R}_{i,i} \in \{-1,+1\}$ for all $i \in [n]$.

We introduce a modification to the **Givens-QR** algorithm, resulting in our **Jacobi-Givens-QR** algorithm as presented in Listing 1. This algorithm can decompose any matrix $\mathbf{X} \in \operatorname{St}(n,n)$ into the form $\mathbf{X} = \mathbf{QR}$, where $\mathbf{Q} = \mathbf{X}$ and $\mathbf{R} = \mathbf{I}_n$, using a sequence of \mathbf{C}_n^k Givens rotation or Jacobi reflection steps.

Please take note of the following four important points in Listing 1.

- a) When we remove Lines 7-10 and Lines 13-15 from Listing 1, it essentially reverts to the classical **Givens-QR** algorithm. **Givens-QR** operates by selecting an appropriate Givens rotation matrix $\mathbf{V} = \begin{bmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{bmatrix}$ with a suitable rotation angle θ to zero-out the matrix element \mathbf{R}_{ij} systematically from left to right $(j=1 \to n)$ and bottom to top $(i=n \to (j+1))$ within every pair of neighboring columns.
- **b)** Lines 7-10 and Lines 13-15 can be viewed as correction steps to ensure that the entries $\mathbf{R}_{j,j} = 1$ for all j = n.
- c) Line 7-10 is executed for (n-2) times. In Line 7-10, when **Jacobi-Givens-QR** detects a negative entry $\mathbf{R}_{i-1,i-1}$ with i=j+1, it applies a rotation matrix $\mathbf{V} \triangleq \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$ to the two rows $\mathbf{B} = [i-1,i]$ to ensure that $\mathbf{R}_{i-1,i-1} = 1$.
- d) Line 13-15 is executed only once when $\det(\mathbf{X}) = -1$. In such cases, we have $\mathbf{R}_{\mathrm{BB}} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ and $\det(\mathbf{R}_{\mathrm{BB}}) = -1$, where $\mathbf{B} = [n-1,n]$ is the two indices for the final rotation or reflection step. To ensure that the resulting \mathbf{R}_{BB} is an identify matrix, **Jacobi-Givens-QR** employs a reflection matrix $\mathbf{V} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, leading to $\mathbf{V}^\mathsf{T}\mathbf{R}_{\mathrm{BB}} = \mathbf{I}_2$.

Therefore, we establish the conclusion that any orthogonal matrix $\mathbf{X} \in \mathrm{St}(n,n)$ can be expressed as $\mathbf{D} = \mathcal{W}_{C_n^k} ... \mathcal{W}_2 \mathcal{W}_1$, where $\mathcal{W}_i = \mathbf{U}_{\mathcal{B}_i} \mathcal{V}_i \mathbf{U}_{\mathcal{B}_i^c}^\mathsf{T} + \mathbf{U}_{\mathcal{B}_i^c} \mathbf{U}_{\mathcal{B}_i^c}^\mathsf{T}$, and $\mathcal{V}_i \in \mathrm{St}(2,2)$ is a suitable matrix associated with \mathcal{B}_i . Furthermore, if $\forall i, \, \mathcal{V}_i = \mathbf{I}_2$, we have $\forall i, \, \mathcal{W}_i = \mathbf{I}_n$, leading to $\mathbf{D} = \mathbf{I}_n$. This concludes the proof of the first part of this theorem.

Part (b). For any given $X \in St(n,r)$ and $X^0 \in St(n,r)$, we let:

$$\bar{\mathbf{D}} = \mathbb{P}_{\mathrm{St}(n,n)}(\mathbf{X}[\mathbf{X}^0]^\mathsf{T}),\tag{35}$$

where $\mathbb{P}_{\mathrm{St}(n,n)}(\mathbf{Y})$ denotes the nearest orthogonality matrix to the given matrix \mathbf{Y} .

Assume that the matrix $X[X^0]^T$ has the following singular value decomposition:

$$\mathbf{X}(\mathbf{X}^0)^\mathsf{T} = \mathbf{U}\mathrm{Diag}(\mathbf{z})\mathbf{V}^\mathsf{T}, \ \mathbf{z} \in \{0,1\}^n, \ \mathbf{U} \in \mathrm{St}(n,n), \ \mathbf{V} \in \mathrm{St}(n,n).$$

Therefore, we have the following equalities:

$$Diag(\mathbf{z}) = \mathbf{U}^{\mathsf{T}} \mathbf{X} [\mathbf{X}^{0}]^{\mathsf{T}} \mathbf{V}. \tag{36}$$

$$\bar{\mathbf{D}} = \mathbf{U}\mathbf{V}^{\mathsf{T}} \in \mathrm{St}(n,n).$$
 (37)

Furthermore, we derive the following results:

$$\begin{split} &\mathbf{z} \in \{0,1\}^n \\ &\Rightarrow \quad \mathrm{Diag}(\mathbf{z})^\mathsf{T} = \mathrm{Diag}(\mathbf{z})\mathrm{Diag}(\mathbf{z})^\mathsf{T} \\ &\Rightarrow \quad \mathbf{U}[\mathrm{Diag}(\mathbf{z})^\mathsf{T} - \mathrm{Diag}(\mathbf{z})\mathrm{Diag}(\mathbf{z})^\mathsf{T}]\mathbf{U}^\mathsf{T}\mathbf{X} = \mathbf{0} \\ &\stackrel{\oplus}{\Rightarrow} \quad \mathbf{U}[\mathbf{V}^\mathsf{T}\mathbf{X}^0\mathbf{X}^\mathsf{T}\mathbf{U} - \mathbf{U}^\mathsf{T}\mathbf{X}(\mathbf{X}^0)^\mathsf{T}\mathbf{V}\mathbf{V}^\mathsf{T}\mathbf{X}^0\mathbf{X}^\mathsf{T}\mathbf{U}]\mathbf{U}^\mathsf{T}\mathbf{X} = \mathbf{0} \\ &\Rightarrow \quad \mathbf{U}\mathbf{V}^\mathsf{T}\mathbf{X}^0\mathbf{X}^\mathsf{T}\mathbf{U}\mathbf{U}^\mathsf{T}\mathbf{X} - \mathbf{U}\mathbf{U}^\mathsf{T}\mathbf{X}(\mathbf{X}^0)^\mathsf{T}\mathbf{V}\mathbf{V}^\mathsf{T}\mathbf{X}^0\mathbf{X}^\mathsf{T}\mathbf{U}\mathbf{U}^\mathsf{T}\mathbf{X} = \mathbf{0} \\ &\stackrel{@}{\Rightarrow} \quad \mathbf{U}\mathbf{V}^\mathsf{T}\mathbf{X}^0 - \mathbf{X} = \mathbf{0} \\ &\stackrel{@}{\Rightarrow} \quad \bar{\mathbf{D}} \cdot \mathbf{X}^0 - \mathbf{X} = \mathbf{0}, \end{split}$$

where step ① uses (36); step ② uses $\mathbf{U}\mathbf{U}^\mathsf{T} = \mathbf{I}_n$, $\mathbf{V}\mathbf{V}^\mathsf{T} = \mathbf{I}_n$, $\mathbf{X}^\mathsf{T}\mathbf{X} = \mathbf{I}_r$, and $[\mathbf{X}^0]^\mathsf{T}\mathbf{X}^0 = \mathbf{I}_r$; step ③ uses (37). We conclude that, for any given $\mathbf{X} \in \mathrm{St}(n,r)$ and $\mathbf{X}^0 \in \mathrm{St}(n,r)$, we can always find a matrix $\bar{\mathbf{D}} \in \mathrm{St}(n,n)$ such that $\bar{\mathbf{D}}\mathbf{X}^0 = \mathbf{X}$.

Since the matrix $\bar{\mathbf{D}} \in \operatorname{St}(n,n)$ can be represented as $\bar{\mathbf{D}} = \mathcal{W}_{C_n^k}...\mathcal{W}_2\mathcal{W}_1$, where $\mathcal{W}_i = \mathbf{U}_{\mathcal{B}_i}\mathcal{V}_i\mathbf{U}_{\mathcal{B}_i}^\mathsf{T} + \mathbf{U}_{\mathcal{B}_i^c}\mathbf{U}_{\mathcal{B}_i^c}^\mathsf{T}$ for some suitable $\mathcal{V}_i \in \operatorname{St}(2,2)$ (as established in the first part of this

³Alternatively, one can use the reflection matrix $\mathbf{V} \triangleq \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$ instead of the rotation matrix $\mathbf{V} \triangleq \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$ to ensure that $\mathbf{R}_{i-1,i-1} = 1$.

theorem), we can conclude that any matrix $\mathbf{X} \in \operatorname{St}(n,r)$ can be expressed as $\mathbf{X} = \bar{\mathbf{D}}\mathbf{X}^0 =$ $\mathcal{W}_{\mathbf{C}_{\underline{c}}^{\underline{k}}}...\mathcal{W}_{2}\mathcal{W}_{1}\mathbf{X}^{0}.$

Proof for Theorem 3.6

 E.2

Proof. We use $\hat{\mathbf{X}}$, $\hat{\mathbf{X}}$, and $\hat{\mathbf{X}}$ to denote a global optimal point, a BS_k -point, and a critical point of Problem (1), respectively.

Setting the Riemannian subgradient of $\mathcal{K}(\mathbf{V}; \ddot{\mathbf{X}}, \mathbb{B})$ w.r.t. \mathbf{V} to zero, we have $\mathbf{0} \in \partial_{\mathcal{M}} \mathcal{K}(\mathbf{V}; \ddot{\mathbf{X}}, \mathbb{B}) =$ $\ddot{\mathbf{G}}(\mathbf{V}) \ominus \mathbf{V}[\ddot{\mathbf{G}}(\mathbf{V})]^{\mathsf{T}}\mathbf{V}$, where $\ddot{\mathbf{G}}(\mathbf{V}) = \alpha(\mathbf{V} - \mathbf{I}_k) + \mathbf{U}_{\mathsf{P}}^{\mathsf{T}}[\max(\mathbf{H}\text{vec}(\mathbf{X}^+ - \ddot{\mathbf{X}})) + \nabla f(\ddot{\mathbf{X}}) + \nabla f(\ddot{\mathbf{X}})]$ $\partial h(\mathbf{X}^+) | \ddot{\mathbf{X}}^\mathsf{T} \mathbf{U}_\mathsf{B}$ and $\mathbf{X}^+ = \ddot{\mathbf{X}} + \mathbf{U}_\mathsf{B} (\mathbf{V} - \mathbf{I}_k) \mathbf{U}_\mathsf{B}^\mathsf{T} \ddot{\mathbf{X}}$. Letting $\mathbf{V} = \mathbf{I}_k$, we have the following **necessary but not sufficient** condition for any BS_k-point:

$$\forall \mathbf{B} \in \{\mathcal{B}_i\}_{i=1}^{\mathbf{C}_n^k}, \ \mathbf{0} = \mathbf{U}_{\mathbf{B}}^{\mathsf{T}} (\mathbf{G} \ddot{\mathbf{X}}^{\mathsf{T}} - \ddot{\mathbf{X}} \mathbf{G}^{\mathsf{T}}) \mathbf{U}_{\mathbf{B}}, \text{ with } \mathbf{G} \in \nabla f(\ddot{\mathbf{X}}) + \partial h(\ddot{\mathbf{X}}).$$
(38)

Part (a). We now show that {critical points $\check{\mathbf{X}}$ } \supseteq {BS_k-points $\ddot{\mathbf{X}}$ } for all $k \ge 2$. We let $\mathbf{G} \in$ $\nabla f(\mathbf{X}) + \partial h(\mathbf{X})$. Using Lemma A.1, we have:

$$\mathbf{0}_{n,n} = \mathbf{G}\ddot{\mathbf{X}}^{\mathsf{T}} - \ddot{\mathbf{X}}\mathbf{G}^{\mathsf{T}} \quad \Rightarrow \quad (\mathbf{0}_{n,n} \cdot \ddot{\mathbf{X}}) = (\mathbf{G}\ddot{\mathbf{X}}^{\mathsf{T}} - \ddot{\mathbf{X}}\mathbf{G}^{\mathsf{T}})\ddot{\mathbf{X}}$$

$$\stackrel{\textcircled{0}}{\Rightarrow} \quad \mathbf{0}_{n,r} = \mathbf{G} - \ddot{\mathbf{X}}\mathbf{G}^{\mathsf{T}}\ddot{\mathbf{X}}, \qquad (39)$$

$$\Rightarrow \quad \ddot{\mathbf{X}}^{\mathsf{T}} \cdot \mathbf{0}_{n,r} = \ddot{\mathbf{X}}^{\mathsf{T}}(\mathbf{G} - \ddot{\mathbf{X}}\mathbf{G}^{\mathsf{T}}\ddot{\mathbf{X}})$$

$$\stackrel{\textcircled{2}}{\Rightarrow} \quad \mathbf{0}_{r,r} = \ddot{\mathbf{X}}^{\mathsf{T}}\mathbf{G} - \mathbf{G}^{\mathsf{T}}\ddot{\mathbf{X}}$$

$$\Rightarrow \quad \mathbf{0}_{n,n} = \ddot{\mathbf{X}}(\ddot{\mathbf{X}}^{\mathsf{T}}\mathbf{G} - \mathbf{G}^{\mathsf{T}}\ddot{\mathbf{X}})\ddot{\mathbf{X}}^{\mathsf{T}}$$

$$\stackrel{\textcircled{3}}{\Rightarrow} \quad \mathbf{0}_{n,n} = \ddot{\mathbf{X}}\underbrace{\ddot{\mathbf{X}}^{\mathsf{T}}\mathbf{G}\ddot{\mathbf{X}}^{\mathsf{T}}}_{\triangleq \mathbf{G}^{\mathsf{T}}} - \underbrace{\ddot{\mathbf{X}}\mathbf{G}^{\mathsf{T}}\ddot{\mathbf{X}}}_{\triangleq \mathbf{G}^{\mathsf{T}}}\ddot{\mathbf{X}}^{\mathsf{T}},$$

where steps ① and ② use $\ddot{\mathbf{X}}^\mathsf{T}\ddot{\mathbf{X}} = \mathbf{I}_r$; step ③ uses Equality (39) that $\mathbf{G} = \ddot{\mathbf{X}}\mathbf{G}^\mathsf{T}\ddot{\mathbf{X}}$. We conclude that the necessary condition in Equation (38) is equivalent to the optimality condition of critical points.

Part (b). We now show that $\{BS_2\text{-points }\ddot{\mathbf{X}}\} \supseteq \{\text{global optimal points }\bar{\mathbf{X}}\}$. We define $\mathcal{X}_{B}^{\star}(\mathbf{V}) \triangleq$ $\bar{\mathbf{X}} + \mathbf{U}_{\mathrm{B}}(\mathbf{V} - \mathbf{I}_k) \mathbf{U}_{\mathrm{B}}^{\mathsf{T}} \bar{\mathbf{X}}, \text{ and } \mathcal{K}(\mathbf{V}; \mathbf{X}, \mathbf{B}) \triangleq f(\mathbf{X}) + \langle \mathbf{V} - \mathbf{I}_k, [\nabla f(\mathbf{X})(\mathbf{X})^{\mathsf{T}}]_{\mathrm{BB}} \rangle + \frac{1}{2} \|\mathbf{V} - \mathbf{I}_k\|_{\mathbf{Q} + \alpha \mathbf{I}_k}^{2} + \frac{1}{2} \|$ $h(\mathbf{U}_{\mathbb{R}^c}^\mathsf{T}\mathbf{X}) + h(\mathbf{V}\mathbf{U}_{\mathbb{R}}^\mathsf{T}\mathbf{X})$. We let $\mathbf{V}_{(i)} \in \mathrm{St}(2,2)$ and $\mathcal{B}_i \in \{\mathcal{B}_i\}_{i=1}^{C_n^k}$. We derive:

$$\mathcal{K}(\mathbf{I}_{2}; \bar{\mathbf{X}}, \mathcal{B}_{i}), \forall \mathcal{B}_{i}$$

$$\stackrel{@}{=} F(\bar{\mathbf{X}}) = h(\bar{\mathbf{X}}) + f(\bar{\mathbf{X}})$$

$$\stackrel{@}{=} h(\mathbf{X}) + f(\mathbf{X}), \forall \mathbf{X} \in \operatorname{St}(n, r)$$

$$\stackrel{@}{\leq} h(\bar{\mathbf{X}} + \mathbf{U}_{\mathcal{B}_{i}}(\mathbf{V}_{(i)} - \mathbf{I}_{2})\mathbf{U}_{\mathcal{B}_{i}}^{\mathsf{T}}\bar{\mathbf{X}}) + f(\bar{\mathbf{X}} + \mathbf{U}_{\mathcal{B}_{i}}(\mathbf{V}_{(i)} - \mathbf{I}_{2})\mathbf{U}_{\mathcal{B}_{i}}^{\mathsf{T}}\bar{\mathbf{X}}), \forall \mathbf{V}_{(i)}, \forall \mathcal{B}_{i}$$

$$\stackrel{@}{=} h(\mathcal{X}_{\mathcal{B}_{i}}^{\star}(\mathbf{V}_{(i)})) + f(\mathcal{X}_{\mathcal{B}_{i}}^{\star}(\mathbf{V}_{(i)})), \forall \mathbf{V}_{(i)}, \forall \mathcal{B}_{i}$$

$$\stackrel{@}{=} \mathcal{K}(\mathbf{V}_{(i)}; \bar{\mathbf{X}}, \mathcal{B}_{i}), \forall \mathbf{V}_{(i)}, \forall \mathcal{B}_{i}$$

$$= \min_{\mathbf{V} \in \operatorname{St}(2,2)} \mathcal{K}(\mathbf{V}; \bar{\mathbf{X}}, \mathcal{B}_{i}), \forall \mathcal{B}_{i}, \tag{40}$$

where step ① uses the definition of $\mathcal{K}(\mathbf{V}; \mathbf{X}, \mathbf{B}) \triangleq f(\mathbf{X}) + \langle \mathbf{V} - \mathbf{I}_k, [\nabla f(\mathbf{X})(\mathbf{X})^\mathsf{T}]_{\mathbf{BB}} \rangle + \frac{1}{2} ||\mathbf{V} - \mathbf{V} - \mathbf{I}_k, [\nabla f(\mathbf{X})(\mathbf{X})^\mathsf{T}]_{\mathbf{BB}} \rangle + \frac{1}{2} ||\mathbf{V} - \mathbf{V} - \mathbf{I}_k, [\nabla f(\mathbf{X})(\mathbf{X})^\mathsf{T}]_{\mathbf{BB}} \rangle$ $\mathbf{I}_k \|_{\mathbf{Q} + \alpha \mathbf{I}_k}^2 + h(\mathbf{U}_{\mathbb{B}^c}^\mathsf{T} \mathbf{X}) + h(\mathbf{V} \mathbf{U}_{\mathbb{B}}^\mathsf{T} \mathbf{X});$ step ② uses the definition of $\bar{\mathbf{X}};$ step ③ uses the basis representation of orthogonal matrices when k=2, as shown in Theorem 3.1; step @ uses the definition of $\mathcal{X}_{\mathbb{R}}^*(\mathbf{V})$; step \mathfrak{S} uses the same strategy as in deriving Inequality (2). This leads to:

$$\mathbf{I}_2 \in \arg\min_{\mathbf{V} \in \mathrm{St}(2,2)} \ \mathcal{K}(\mathbf{V}; \bar{\mathbf{X}}, \mathcal{B}_i), \ \forall \mathcal{B}_i.$$

The inclusion above implies that $\{BS_2\text{-points }\ddot{\mathbf{X}}\} \supseteq \{\text{global optimal points }\bar{\mathbf{X}}\}.$

Part (c). We now show that $\{BS_k\text{-points }\ddot{\mathbf{X}}\}\supseteq \{BS_{k+1}\text{-points }\ddot{\mathbf{X}}\}$. It is evident that the subproblem of finding $BS_k\text{-points}$ is encompassed within that of finding $BS_{k+1}\text{-points}$ stationary point. Thus, we conclude that the optimality of the latter is stronger.

Part (d). The inclusion {critical points $\check{\mathbf{X}}$ } \subseteq {BS_k-points $\ddot{\mathbf{X}}$ } may not always hold true. This can be illustrated through simple examples of 2×2 optimization problems under orthogonality constraints (see Appendix Section C.1 for more details). Lastly, it is also evident that the inclusions {BS₂-points $\ddot{\mathbf{X}}$ } \subseteq {global optimal points $\ddot{\mathbf{X}}$ } and {BS_k-points $\ddot{\mathbf{X}}$ } \subseteq {BS_{k+1}-points $\ddot{\mathbf{X}}$ } may not always hold true.

F PROOF FOR SECTION 4

F.1 Proof for Theorem 4.2

Proof. We define $\mathcal{K}(\mathbf{V}; \mathbf{X}^t, \mathbf{B}) \triangleq \frac{1}{2} \|\mathbf{V} - \mathbf{I}_k\|_{\mathbf{Q} + \alpha \mathbf{I}_k}^2 + h(\mathbf{V}\mathbf{Z}) + \langle \mathbf{V}, [\nabla f(\mathbf{X}^t)(\mathbf{X}^t)^\mathsf{T}]_{\mathbf{B}\mathbf{B}} \rangle + \ddot{c}$, where $\mathbf{Z} \triangleq \mathbf{U}_{\mathbf{B}}^\mathsf{T} \mathbf{X}^t$ and $\ddot{c} = h(\mathbf{U}_{\mathbf{B}^c}^\mathsf{T} \mathbf{X}^t) + f(\mathbf{X}^t) - \langle \mathbf{I}_k, [\nabla f(\mathbf{X}^t)(\mathbf{X}^t)^\mathsf{T}]_{\mathbf{B}\mathbf{B}} \rangle$ is a constant.

We define $\tilde{c} \triangleq \frac{2}{\alpha} \cdot (F(\mathbf{X}^0) - F(\mathbf{X}^\infty)).$

Part (a). First, we have the following equalities:

$$h(\mathbf{X}^{t+1}) - h(\mathbf{X}^{t}) \stackrel{@}{=} h(\mathbf{U}_{\mathsf{B}} \bar{\mathbf{V}}^{t} \mathbf{U}_{\mathsf{B}}^{\mathsf{T}} \mathbf{X}^{t} + \mathbf{U}_{\mathsf{B}^{c}} \mathbf{U}_{\mathsf{B}^{c}}^{\mathsf{T}} \mathbf{X}^{t}) - h(\mathbf{U}_{\mathsf{B}} \mathbf{U}_{\mathsf{B}}^{\mathsf{T}} \mathbf{X}^{t} + \mathbf{U}_{\mathsf{B}^{c}} \mathbf{U}_{\mathsf{B}^{c}}^{\mathsf{T}} \mathbf{X}^{t})$$

$$\stackrel{@}{=} h(\mathbf{U}_{\mathsf{B}} \bar{\mathbf{V}}^{t} \mathbf{U}_{\mathsf{B}}^{\mathsf{T}} \mathbf{X}^{t}) + h(\mathbf{U}_{\mathsf{B}^{c}} \mathbf{U}_{\mathsf{B}^{c}}^{\mathsf{T}} \mathbf{X}^{t}) - h(\mathbf{U}_{\mathsf{B}} \mathbf{U}_{\mathsf{B}^{c}}^{\mathsf{T}} \mathbf{X}^{t}) - h(\mathbf{U}_{\mathsf{B}^{c}} \mathbf{U}_{\mathsf{B}^{c}}^{\mathsf{T}} \mathbf{X}^{t}) - h(\mathbf{U}_{\mathsf{B}^{c}} \mathbf{U}_{\mathsf{B}^{c}}^{\mathsf{T}} \mathbf{X}^{t})$$

$$\stackrel{@}{=} h(\bar{\mathbf{V}}^{t} \mathbf{U}_{\mathsf{B}}^{\mathsf{T}} \mathbf{X}^{t}) - h(\mathbf{U}_{\mathsf{B}^{c}}^{\mathsf{T}} \mathbf{X}^{t}), \tag{41}$$

where step ① uses $\mathbf{X}^{t+1} = \mathbf{U}_{\mathsf{B}} \mathbf{V} \mathbf{U}_{\mathsf{B}}^{\mathsf{T}} \mathbf{X}^t + \mathbf{U}_{\mathsf{B}^c} \mathbf{U}_{\mathsf{B}^c}^{\mathsf{T}} \mathbf{X}^t$ as in (4) and $\mathbf{I}_k = \mathbf{U}_{\mathsf{B}} \mathbf{U}_{\mathsf{B}}^{\mathsf{T}} + \mathbf{U}_{\mathsf{B}^c} \mathbf{U}_{\mathsf{B}^c}^{\mathsf{T}}$; step ② and step ③ use the coordinate-wise separable structure of $h(\cdot)$.

Second, since $\bar{\mathbf{V}}^t \in \arg\min_{\mathbf{V} \in \mathrm{St}(k,k)} \mathcal{K}(\mathbf{V};\mathbf{X}^t,\mathsf{B})$, it follows that $\mathcal{K}(\bar{\mathbf{V}}^t;\mathbf{X}^t,\mathsf{B}) \leq \mathcal{K}(\mathbf{I}_k;\mathbf{X}^t,\mathsf{B})$. This further leads to:

$$h(\bar{\mathbf{V}}^t \mathbf{U}_{\mathrm{B}}^{\mathsf{T}} \mathbf{X}^t) + \frac{1}{2} \|\bar{\mathbf{V}}^t - \mathbf{I}_k\|_{\mathbf{Q} + \alpha \mathbf{I}_k}^2 + \langle \bar{\mathbf{V}}^t - \mathbf{I}_k, [\nabla f(\mathbf{X}^t)(\mathbf{X}^t)^{\mathsf{T}}]_{\mathrm{BB}} \rangle \le h(\mathbf{U}_{\mathrm{B}}^{\mathsf{T}} \mathbf{X}^t). \tag{42}$$

Third, we denote $\mathbf{X}^{t+1} = \mathcal{X}_{\mathrm{B}}^t(\bar{\mathbf{V}}^t)$ and derive:

$$f(\mathbf{X}^{t+1}) - f(\mathbf{X}^{t}) \stackrel{\text{\tiny (U)}}{\leq} \langle \mathcal{X}_{\mathbb{B}}^{t}(\bar{\mathbf{V}}^{t}) - \mathbf{X}^{t}, \nabla f(\mathbf{X}^{t}) \rangle + \frac{1}{2} \|\mathcal{X}_{\mathbb{B}}^{t}(\bar{\mathbf{V}}^{t}) - \mathbf{X}^{t}\|_{\mathbf{H}}^{2}$$

$$\stackrel{\text{\tiny (2)}}{=} \langle \mathbf{U}_{\mathbb{B}}(\bar{\mathbf{V}}^{t} - \mathbf{I}_{k})\mathbf{U}_{\mathbb{B}}^{\mathsf{T}}\mathbf{X}^{t}, \nabla f(\mathbf{X}^{t}) \rangle + \frac{1}{2} \|\bar{\mathbf{V}}^{t} - \mathbf{I}_{k}\|_{\mathbf{Q}}^{2}$$

$$\stackrel{\text{\tiny (3)}}{\leq} \langle \bar{\mathbf{V}}^{t} - \mathbf{I}_{k}, [\nabla f(\mathbf{X}^{t})(\mathbf{X}^{t})^{\mathsf{T}}]_{\mathbb{B}\mathbb{B}} \rangle + \frac{1}{2} \|\bar{\mathbf{V}}^{t} - \mathbf{I}_{k}\|_{\mathbf{Q}}^{2}, \tag{43}$$

where step ① uses Inequality (2); step ② uses Claim (a) of Lemma 2.2; step ③ uses $\mathbf{Q} \geq \mathbf{Q}$.

Adding (41), (42), and (43) together, we obtain the following sufficient decrease condition:

$$F(\mathbf{X}^{t+1}) - F(\mathbf{X}^t) \le -\frac{\alpha}{2} \|\bar{\mathbf{V}}^t - \mathbf{I}_k\|_{\mathsf{F}}^2 \le -\frac{\alpha}{2} \|\mathbf{X}^{t+1} - \mathbf{X}^t\|_{\mathsf{F}}^2, \tag{44}$$

where step ① uses Claim (c) of Lemma 2.2.

Part (b). We assume that \mathbb{B}^t is selected from $\{\mathcal{B}_i\}_{i=1}^{C_n^k}$ randomly and uniformly.

Taking the expectation for Inequality (44), we obtain a lower bound on the expected progress made by each iteration:

$$\mathbb{E}_{\mathcal{E}^t}[F(\mathbf{X}^{t+1})] - F(\mathbf{X}^t) \le -\mathbb{E}_{\mathcal{E}^t}\left[\frac{\alpha}{2} \|\bar{\mathbf{V}}^t - \mathbf{I}_k\|_{\mathsf{F}}^2\right].$$

Telescoping the inequality above over t = 0, 1, ..., T, we have:

$$\mathbb{E}_{\boldsymbol{\xi}^T}[\tfrac{\alpha}{2} \sum_{t=0}^T \|\bar{\mathbf{V}}^t - \mathbf{I}_k\|_{\mathsf{F}}^2] \leq \mathbb{E}_{\boldsymbol{\xi}^T}[F(\mathbf{X}^0) - F(\mathbf{X}^{T+1})] \leq \mathbb{E}_{\boldsymbol{\xi}^T}[F(\mathbf{X}^0) - F(\mathbf{X}^\infty)],$$

where \mathbf{X}^{∞} denotes the limit point of Algorithm 1. As a result, there exists an index \bar{t} with $0 \leq \bar{t} \leq T$ such that

 $\mathbb{E}_{\xi^T}[\|\bar{\mathbf{V}}^{\bar{t}} - \mathbf{I}_k\|_{\mathsf{F}}^2] \le \frac{2}{\alpha(T+1)}[F(\mathbf{X}^0) - F(\mathbf{X}^\infty)] = \frac{\tilde{c}}{T+1}.$ (45)

Furthermore, for any t, $\bar{\mathbf{V}}^t$ is the optimal solution of the following minimization problem at \mathbf{X}^t : $\bar{\mathbf{V}}^t \in \arg\min_{\mathbf{V}} \mathcal{K}(\mathbf{V}; \mathbf{X}^t, \mathbf{B}^t)$. Since $\bar{\mathbf{V}}^t$ is a random output matrix that depends on the observed realization of the random variable \mathbf{B}^t , we directly obtain the following equality:

$$\frac{1}{C^k} \sum_{i=1}^{C^k} \operatorname{dist}(\mathbf{I}_k, \arg \min_{\mathbf{V}} \mathcal{K}(\mathbf{V}; \mathbf{X}^t, \mathcal{B}_i))^2 = \mathbb{E}_{\xi^t}[\|\bar{\mathbf{V}}^t - \mathbf{I}_k\|_{\mathsf{F}}^2]. \tag{46}$$

Combining (45) and (46), we conclude that there exists an index \bar{t} with $\bar{t} \in [0,T]$ such that the associated solution $\mathbf{X}^{\bar{t}}$ qualifies as an ϵ -BS $_k$ -point of Problem (1), provided that T is sufficiently large such that $\frac{\bar{c}}{T+1} \leq \epsilon$. We conclude that OBCD finds an ϵ -BS $_k$ -point of Problem (1) in at most T iterations deterministically, where $T \geq \lceil \frac{\bar{c}}{\epsilon} - 1 \rceil$.

F.2 PROOF OF LEMMA 4.4

 Proof. For notation simplicity, we define: $\|\partial F(\mathbf{X})\|_{\mathsf{F}} = \inf_{\mathbf{Y} \in \partial F(\mathbf{X})} \|\mathbf{Y}\|_{\mathsf{F}} = \operatorname{dist}(\mathbf{0}, \partial F(\mathbf{X})).$

We define $\mathbb{A} \ominus \mathbb{B}$ as the element-wise subtraction between sets \mathbb{A} and \mathbb{B} .

We let $\mathbb{H}^{t+1} \in \partial h(\mathbf{X}^{t+1})$, and define:

$$\Omega_0 \triangleq \mathbf{U}_{\mathbf{B}^t}^{\mathsf{T}} [\nabla f(\mathbf{X}^{t+1}) + \mathbf{H}^{t+1}] [\mathbf{X}^{t+1}]^{\mathsf{T}} \mathbf{U}_{\mathbf{B}^t} \in \mathbb{R}^{k \times k}, \tag{47}$$

$$\Omega_1 \triangleq \mathbf{U}_{\mathbf{B}^t}^{\mathsf{T}} [\nabla f(\mathbf{X}^{t+1}) + \mathbf{H}^{t+1}] [\mathbf{X}^t]^{\mathsf{T}} \mathbf{U}_{\mathbf{B}^t} \in \mathbb{R}^{k \times k}, \tag{48}$$

$$\Omega_2 \triangleq \mathbf{U}_{\mathrm{B}^t}^{\mathsf{T}} [\nabla f(\mathbf{X}^t) - \nabla f(\mathbf{X}^{t+1})] [\mathbf{X}^t]^{\mathsf{T}} \mathbf{U}_{\mathrm{B}^t} \in \mathbb{R}^{k \times k}. \tag{49}$$

Part (a). First, using the optimality of $\bar{\mathbf{V}}^t$ for the subproblem, we have:

$$\begin{aligned} \mathbf{0}_{k,k} &= \tilde{\mathbf{G}} - \bar{\mathbf{V}}^t \tilde{\mathbf{G}}^\mathsf{T} \bar{\mathbf{V}}^t \\ \text{where } \tilde{\mathbf{G}} &= \underbrace{\max((\mathbf{Q} + \alpha \mathbf{I}_k) \text{vec}(\bar{\mathbf{V}}^t - \mathbf{I}_k))}_{\triangleq \Upsilon_1} + \underbrace{\mathbf{U}_{\mathbb{B}^t}^\mathsf{T} [\nabla f(\mathbf{X}^t) + \mathbb{H}^{t+1}] (\mathbf{X}^t)^\mathsf{T} \mathbf{U}_{\mathbb{B}^t}}_{\triangleq \Upsilon_2}. \end{aligned}$$

Using the relation that $\tilde{\mathbf{G}} = \Upsilon_1 + \Upsilon_2$, we obtain the following results from the above equality:

$$\mathbf{0}_{k,k} = (\Upsilon_1 + \Upsilon_2) - \bar{\mathbf{V}}^t (\Upsilon_1 + \Upsilon_2)^\mathsf{T} \bar{\mathbf{V}}^t$$

$$\stackrel{\textcircled{1}}{\Rightarrow} \mathbf{0}_{k,k} = \Upsilon_1 + \Omega_1 + \Omega_2 - \bar{\mathbf{V}}^t (\Upsilon_1 + \Omega_1 + \Omega_2)^\mathsf{T} \bar{\mathbf{V}}^t$$

$$\Rightarrow \Omega_1 = \bar{\mathbf{V}}^t (\Upsilon_1 + \Omega_1 + \Omega_2)^\mathsf{T} \bar{\mathbf{V}}^t - \Upsilon_1 - \Omega_2, \tag{50}$$

where step ① uses $\Upsilon_2 = \Omega_1 + \Omega_2$.

Second, since both \mathbb{B}^t and \mathbb{B}^{t+1} are randomly and dependently selected from $\{\mathcal{B}_i\}_{i=1}^{\mathbb{C}^k}$ with replacement, each with an equal probability of $\frac{1}{\mathbb{C}^k}$, for any $\tilde{\mathbf{A}} \in \mathbb{R}^{n \times n}$, we have:

$$\mathbb{E}_{\mathbb{B}^{t+1}}[\|\mathbf{U}_{\mathbb{B}^{t+1}}^\mathsf{T}\tilde{\mathbf{A}}\mathbf{U}_{\mathbb{B}^{t+1}}\|_{\mathsf{F}}^2 = \tfrac{1}{C^k}\sum_{i=1}^{C_n^k}\|\mathbf{U}_{\mathcal{B}_i}^\mathsf{T}\tilde{\mathbf{A}}\mathbf{U}_{\mathcal{B}_i}\|_{\mathsf{F}}^2 = \mathbb{E}_{\mathbb{B}^t}\|\mathbf{U}_{\mathbb{B}^t}^\mathsf{T}\tilde{\mathbf{A}}\mathbf{U}_{\mathbb{B}^t}\|_{\mathsf{F}}^2.$$

Using the definition $\xi^t \triangleq (B^1, B^2, \dots, B^t)$, we have:

$$\mathbb{E}_{\xi^{t+1}}[\|\mathbf{U}_{\mathsf{B}^{t+1}}^{\mathsf{T}}\tilde{\mathbf{A}}\mathbf{U}_{\mathsf{B}^{t+1}}\|_{\mathsf{F}}^{2} = \mathbb{E}_{\xi^{t}}\|\mathbf{U}_{\mathsf{B}^{t}}^{\mathsf{T}}\tilde{\mathbf{A}}\mathbf{U}_{\mathsf{B}^{t}}\|_{\mathsf{F}}^{2}.$$
(51)

Third, we derive the following results:

$$\mathbb{E}_{\xi^{t+1}}[\operatorname{dist}(\mathbf{0}, \partial_{\mathcal{M}}\mathcal{K}(\mathbf{I}_{k}; \mathbf{X}^{t+1}, \mathbf{B}^{t+1}))] = \mathbb{E}_{\xi^{t+1}}[\|\partial_{\mathcal{M}}\mathcal{K}(\mathbf{I}_{k}; \mathbf{X}^{t+1}, \mathbf{B}^{t+1})\|_{\mathsf{F}}]$$

$$\stackrel{@}{=} \mathbb{E}_{\xi^{t+1}}[\|\mathbf{U}_{\mathsf{B}^{t+1}}^{\mathsf{T}} \{\partial F(\mathbf{X}^{t+1})[\mathbf{X}^{t+1}]^{\mathsf{T}} \ominus \mathbf{X}^{t+1}[\partial F(\mathbf{X}^{t+1})]^{\mathsf{T}}\} \mathbf{U}_{\mathsf{B}^{t+1}}\|_{\mathsf{F}}]$$

$$\stackrel{@}{=} \mathbb{E}_{\xi^{t}}[\|\mathbf{U}_{\mathsf{B}^{t}}^{\mathsf{T}} \{\partial F(\mathbf{X}^{t+1})[\mathbf{X}^{t+1}]^{\mathsf{T}} \ominus \mathbf{X}^{t+1}[\partial F(\mathbf{X}^{t+1})]^{\mathsf{T}}\} \mathbf{U}_{\mathsf{B}^{t}}\|_{\mathsf{F}}]$$

$$\stackrel{@}{\leq} \mathbb{E}_{\xi^{t}}[\|\Omega_{0} - \Omega_{0}^{\mathsf{T}}\|_{\mathsf{F}}]$$

$$\stackrel{@}{\leq} 2\mathbb{E}_{\xi^{t}}[\|\Omega_{0} - \Omega_{1}\|_{\mathsf{F}}] + \mathbb{E}_{\xi^{t}}[\|\Omega_{1} - \Omega_{1}^{\mathsf{T}}\|_{\mathsf{F}}]$$

$$\stackrel{@}{=} 2\mathbb{E}_{\xi^{t}}[\|\Omega_{0} - \Omega_{1}\|_{\mathsf{F}}] + \mathbb{E}_{\xi^{t}}[\|\bar{\mathbf{V}}^{t}(\Upsilon_{1} + \Omega_{1} + \Omega_{2})^{\mathsf{T}}\bar{\mathbf{V}}^{t} - \Upsilon_{1} - \Omega_{2} - \Omega_{1}^{\mathsf{T}}\|_{\mathsf{F}}]$$

$$\stackrel{@}{=} 2\mathbb{E}_{\xi^{t}}[\|\Omega_{0} - \Omega_{1}\|_{\mathsf{F}}] + \mathbb{E}_{\xi^{t}}[\|\bar{\mathbf{V}}^{t}\Upsilon_{1}^{\mathsf{T}}\bar{\mathbf{V}}^{t} - \Upsilon_{1}\|_{\mathsf{F}}] + \mathbb{E}_{\xi^{t}}[\|\bar{\mathbf{V}}^{t}\Omega_{1}^{\mathsf{T}}\bar{\mathbf{V}}^{t} - \Omega_{1}^{\mathsf{T}}\|_{\mathsf{F}}]$$

$$+ \mathbb{E}_{\xi^{t}}[\|\bar{\mathbf{V}}^{t}\Omega_{2}^{\mathsf{T}}\bar{\mathbf{V}}^{t} - \Omega_{2}\|_{\mathsf{F}}]$$
(52)

where step ① uses the definition of $\partial_{\mathcal{M}}\mathcal{K}(\mathbf{V};\mathbf{X}^{t+1},\mathbb{B}^{t+1})$ at the point $\mathbf{V}=\mathbf{I}_k$; step ② uses Equality (51) with $\tilde{\mathbf{A}}=\partial F(\mathbf{X}^{t+1})(\mathbf{X}^{t+1})^{\mathsf{T}}\ominus\mathbf{X}^{t+1}(\partial F(\mathbf{X}^{t+1}))^{\mathsf{T}}$; step ③ uses the definition of Ω_0 in Equation (47); step ④ uses Lemma A.2; step ⑤ uses Equality (50); step ⑥ uses the triangle inequality.

We now establish individual bounds for each term in Inequality (52). For the first term $2\mathbb{E}_{\xi^t}[\|\Omega_0 - \Omega_1\|_{\mathsf{F}}]$ in (52), we have:

$$2\mathbb{E}_{\xi^{t}}[\|\Omega_{0} - \Omega_{1}\|_{\mathsf{F}}]$$

$$\leq 2\mathbb{E}_{\xi^{t}}[\|\mathbf{U}_{\mathsf{B}^{t}}^{\mathsf{T}}[\nabla f(\mathbf{X}^{t+1}) + \mathbb{H}^{t+1}][\mathbf{X}^{t+1} - \mathbf{X}^{t}]^{\mathsf{T}}\mathbf{U}_{\mathsf{B}^{t}}\|_{\mathsf{F}}]$$

$$\stackrel{@}{=} 2\mathbb{E}_{\xi^{t}}[\|\mathbf{U}_{\mathsf{B}^{t}}^{\mathsf{T}}[\nabla f(\mathbf{X}^{t+1}) + \mathbb{H}^{t+1}][\mathbf{U}_{\mathsf{B}}(\bar{\mathbf{V}}^{t} - \mathbf{I}_{k})\mathbf{U}_{\mathsf{B}^{t}}\mathbf{X}^{t}]^{\mathsf{T}}\mathbf{U}_{\mathsf{B}^{t}}\|_{\mathsf{F}}]$$

$$\stackrel{@}{\leq} 2(l_{f} + l_{h})\mathbb{E}_{\xi^{t}}[\|\bar{\mathbf{V}}^{t} - \mathbf{I}_{k}\|_{\mathsf{F}}], \tag{53}$$

where step ① uses $\mathbf{X}^{t+1} = \mathbf{X}^t + \mathbf{U}_{\mathrm{B}}(\bar{\mathbf{V}}^t - \mathbf{I}_k)\mathbf{U}_{\mathrm{B}}^{\mathsf{T}}\mathbf{X}^t$; step ② uses the inequality $\|\mathbf{X}\mathbf{Y}\|_{\mathsf{F}} \leq \|\mathbf{X}\|_{\mathsf{F}}\|\mathbf{Y}\|_{\mathsf{sp}}$ for all \mathbf{X} and \mathbf{Y} repeatedly, and the fact that $\forall \mathbf{X}, \|\nabla f(\mathbf{X})\|_{\mathsf{sp}} \leq l_f, \|\partial h(\mathbf{X})\|_{\mathsf{sp}} \leq l_h$.

For the second term $\mathbb{E}_{\varepsilon^t}[\|\bar{\mathbf{V}}^t \Upsilon_1^\mathsf{T} \bar{\mathbf{V}}^t - \Upsilon_1\|_\mathsf{F}]$ in (52), we have::

$$\mathbb{E}_{\xi^{t}}[\|\bar{\mathbf{V}}^{t}\boldsymbol{\Upsilon}_{1}^{\mathsf{T}}\bar{\mathbf{V}}^{t} - \boldsymbol{\Upsilon}_{1}\|_{\mathsf{F}}] \\
\stackrel{\textcircled{0}}{\leq} \mathbb{E}_{\xi^{t}}[\|\bar{\mathbf{V}}^{t}\boldsymbol{\Upsilon}_{1}^{\mathsf{T}}\bar{\mathbf{V}}^{t}\|_{\mathsf{F}}] + \mathbb{E}_{\xi^{t}}[\|\boldsymbol{\Upsilon}_{1}\|_{\mathsf{F}}] \\
\stackrel{\textcircled{2}}{\leq} 2\mathbb{E}_{\xi^{t}}[\|\boldsymbol{\Upsilon}_{1}\|_{\mathsf{F}}] \\
\stackrel{\textcircled{3}}{=} 2\mathbb{E}_{\xi^{t}}[\|\mathrm{mat}((\mathbf{Q} + \alpha\mathbf{I}_{k})\mathrm{vec}(\bar{\mathbf{V}}^{t} - \mathbf{I}_{k}))\|_{\mathsf{F}}] \\
\leq 2\|\mathbf{Q} + \alpha\mathbf{I}_{k}\|_{\mathsf{sp}} \cdot \mathbb{E}_{\xi^{t}}[\|\bar{\mathbf{V}}^{t} - \mathbf{I}_{k})\|_{\mathsf{F}}] \\
\stackrel{\textcircled{4}}{\leq} 2(L_{f} + \alpha) \cdot \mathbb{E}_{\xi^{t}}[\|\bar{\mathbf{V}}^{t} - \mathbf{I}_{k})\|_{\mathsf{F}}] \tag{54}$$

where step ① uses the triangle inequality; step ② uses the inequality $\|\mathbf{XY}\|_{\mathsf{F}} \leq \|\mathbf{X}\|_{\mathsf{F}} \|\mathbf{Y}\|_{\mathsf{sp}}$ for all \mathbf{X} and \mathbf{Y} ; step ③ uses the definition of Ω_1 in (48); step ④ uses the fact that $\|\mathbf{Q}\|_{\mathsf{sp}} \leq L_f$.

For the third term $\mathbb{E}_{\mathcal{E}^t}[\|\bar{\mathbf{V}}^t\Omega_1^\mathsf{T}\bar{\mathbf{V}}^t - \Omega_1^\mathsf{T}\|_\mathsf{F}]$ in (52), we have:

$$\mathbb{E}_{\xi^{t}}[\|\bar{\mathbf{V}}^{t}\Omega_{1}^{\mathsf{T}}\bar{\mathbf{V}}^{t} - \Omega_{1}^{\mathsf{T}}\|_{\mathsf{F}}]$$

$$\stackrel{\textcircled{1}}{=} \mathbb{E}_{\xi^{t}}[\|\bar{\mathbf{V}}^{t}\Omega_{1}^{\mathsf{T}}(\bar{\mathbf{V}}^{t} - \mathbf{I}_{k}) + (\bar{\mathbf{V}}^{t} - \mathbf{I}_{k})\Omega_{1}^{\mathsf{T}}\|_{\mathsf{F}}]$$

$$\stackrel{\textcircled{2}}{\leq} 2\mathbb{E}_{\xi^{t}}[\|\Omega_{1}\|_{\mathsf{sp}} \cdot \|(\bar{\mathbf{V}}^{t} - \mathbf{I}_{k})\|_{\mathsf{F}}]$$

$$\stackrel{\textcircled{3}}{\leq} 2\mathbb{E}_{\xi^{t}}[\|\nabla f(\mathbf{X}^{t+1}) + \mathbb{H}^{t+1}\|_{\mathsf{sp}} \cdot \|(\bar{\mathbf{V}}^{t} - \mathbf{I}_{k})\|_{\mathsf{F}}]$$

$$\stackrel{\textcircled{4}}{\leq} 2(l_{f} + l_{h})\mathbb{E}_{\xi^{t}}[\|(\bar{\mathbf{V}}^{t} - \mathbf{I}_{k})\|_{\mathsf{F}}]$$

$$(55)$$

where step ① uses the fact that $-\bar{\mathbf{V}}^t\Omega_1^\mathsf{T}\mathbf{I}_k + \bar{\mathbf{V}}^t\Omega_1^\mathsf{T} = \mathbf{0}$; step ② uses the norm inequality; step ③ uses the fact that $\|\Omega_1\|_{\mathsf{sp}} = \|\mathbf{U}_{\mathbb{B}^t}^\mathsf{T}[\nabla f(\mathbf{X}^{t+1}) + \mathbb{H}^{t+1}][\mathbf{X}^t]^\mathsf{T}\mathbf{U}_{\mathbb{B}^t}\|_{\mathsf{sp}} \leq \|\nabla f(\mathbf{X}^{t+1}) + \mathbb{H}^{t+1}\|_{\mathsf{sp}}$ which can

be derived using the norm inequality; step 4 uses the fact that $\forall \mathbf{X}, \|\nabla f(\mathbf{X})\|_{\mathsf{sp}} \leq l_f, \|\partial h(\mathbf{X})\|_{\mathsf{sp}} \leq l_h$.

For the fourth term $\mathbb{E}_{\xi^t}[\|\bar{\mathbf{V}}^t\Omega_2^\mathsf{T}\bar{\mathbf{V}}^t - \Omega_2\|_\mathsf{F}]$ in (52), we have:

$$\mathbb{E}_{\xi^{t}}[\|\bar{\mathbf{V}}^{t}\Omega_{2}^{\mathsf{T}}\bar{\mathbf{V}}^{t} - \Omega_{2}\|_{\mathsf{F}}] \\
\leq \mathbb{E}_{\xi^{t}}[\|\bar{\mathbf{V}}^{t}\Omega_{2}^{\mathsf{T}}\bar{\mathbf{V}}^{t}\|_{\mathsf{F}}] + \mathbb{E}[\|\Omega_{2}\|_{\mathsf{F}}] \\
\leq 2\mathbb{E}_{\xi^{t}}[\|\Omega_{2}\|_{\mathsf{F}}] \\
\stackrel{@}{=} 2\mathbb{E}_{\xi^{t}}[\|U_{\mathbb{B}^{t}}^{\mathsf{T}}[\nabla f(\mathbf{X}^{t}) - \nabla f(\mathbf{X}^{t+1})][\mathbf{X}^{t}]^{\mathsf{T}}\mathbf{U}_{\mathbb{B}^{t}}\|_{\mathsf{F}}] \\
\stackrel{@}{=} 2\mathbb{E}_{\xi^{t}}[\|\nabla f(\mathbf{X}^{t}) - \nabla f(\mathbf{X}^{t+1})\|_{\mathsf{F}}] \\
\stackrel{@}{=} 2L_{f}\mathbb{E}_{\xi^{t}}[\|\mathbf{X}^{t} - \mathbf{X}^{t+1}\|_{\mathsf{F}}] \\
\stackrel{@}{=} 2L_{f}\mathbb{E}_{\xi^{t}}[\|\bar{\mathbf{V}}^{t} - \mathbf{I}_{k}\|_{\mathsf{F}}], \tag{56}$$

where step ① uses the triangle inequality; step ② uses the norm inequality; step ③ uses the definition of $\Omega_2 = \mathrm{U}_{\mathrm{B}^t}^{\mathsf{T}}[\nabla f(\mathbf{X}^t) - \nabla f(\mathbf{X}^{t+1})][\mathbf{X}^t]^{\mathsf{T}}\mathrm{U}_{\mathrm{B}^t}$ in (49); step ④ uses the norm inequality; step ⑤ uses the fact that $\nabla f(\mathbf{X})$ is L_f -Lipschitz continuous; step ⑥ uses Claim (\mathbf{c}) of Lemma 2.2.

In view of (53), (54), (55), (56), and (52), we have:

$$\mathbb{E}_{\xi^{t+1}}[\|\partial_{\mathcal{M}}\mathcal{K}(\mathbf{I}_k;\mathbf{X}^{t+1},\mathbf{B}^{t+1})\|_{\mathsf{F}}] \leq \underbrace{(c_1+c_2+c_3+c_4)}_{\triangleq_{\phi}} \cdot \mathbb{E}_{\xi^t}[\|\bar{\mathbf{V}}^t - \mathbf{I}_k\|_{\mathsf{F}}],$$

where $c_1 = 2(l_f + l_h)$, $c_2 = 2(L_f + \alpha)$, $c_3 = 2(l_f + l_h)$, and $c_4 = 2L_f$.

Part (b). we show that $\mathbb{E}_{\xi^t}[\operatorname{dist}(\mathbf{0}, \partial_{\mathcal{M}} F(\mathbf{X}^t))] \leq \gamma \cdot \mathbb{E}_{\xi^t}[\operatorname{dist}(\mathbf{0}, \partial_{\mathcal{M}} \mathcal{K}(\mathbf{I}_k; \mathbf{X}^t, \mathsf{B}^t))]$, where $\gamma \triangleq (C_n^k/C_{n-2}^{k-2})^{1/2}$. For all $\mathbf{D}^t \triangleq \partial F(\mathbf{X}^t)[\mathbf{X}^t]^\mathsf{T} \ominus \mathbf{X}^t[\partial F(\mathbf{X}^t)]^\mathsf{T}$, we obtain:

$$\|\mathbf{D}^{t}\|_{\mathsf{F}}^{2} = \sum_{i} \sum_{j \neq i} (\mathbf{D}_{ij}^{t})^{2} + \sum_{i} \sum_{j=i} (\mathbf{D}_{ij}^{t})^{2}$$

$$\stackrel{@}{=} \sum_{i} \sum_{j \neq i} (\mathbf{D}_{ij}^{t})^{2}$$

$$\stackrel{@}{=} \frac{1}{C_{n-2}^{k-2}} \sum_{i=1}^{C_{n}^{k}} \|\mathbf{U}_{\mathcal{B}_{i}}^{\mathsf{T}} \mathbf{D}^{t} \mathbf{U}_{\mathcal{B}_{i}}\|_{\mathsf{F}}^{2}$$

$$\stackrel{@}{=} \frac{1}{C_{n-2}^{k-2}} \cdot C_{n}^{k} \mathbb{E}_{\mathsf{B}^{t}} [\|\mathbf{U}_{\mathsf{B}^{t}}^{\mathsf{T}} \mathbf{D}^{t} \mathbf{U}_{\mathsf{B}^{t}}\|_{\mathsf{F}}^{2}]$$

$$\stackrel{@}{=} \gamma^{2} \mathbb{E}_{\mathsf{B}^{t}} [\|\mathbf{U}_{\mathsf{D}^{t}}^{\mathsf{T}} \mathbf{D}^{t} \mathbf{U}_{\mathsf{B}^{t}}\|_{\mathsf{F}}^{2}], \tag{57}$$

where step ① uses the fact that $\mathbf{D}_{ii}^t = 0$ for all $i \in [n]$; step ② uses Claim (\boldsymbol{a}) of this lemma with $\mathbf{D}_{ii}^t = 0$ for all $i \in [n]$; step ③ uses $\mathbb{E}_{\mathbb{B}^t}[\|\mathbf{U}_{\mathbb{B}^t}^\mathsf{T}\mathbf{W}\mathbf{U}_{\mathbb{B}^t}\|_{\mathsf{F}}^2] = \frac{1}{\mathbb{C}_n^k} \sum_{i=1}^{\mathbb{C}_n^k} \|\mathbf{U}_{\mathcal{B}_i}^\mathsf{T}\mathbf{W}\mathbf{U}_{\mathcal{B}_i}\|_{\mathsf{F}}^2$ as \mathbb{B}^t are chosen from $\{\mathcal{B}_i\}_{i=1}^{\mathbb{C}_n^k}$ randomly and uniformly; ④ uses the definition of γ . We further derive:

$$\mathbb{E}_{\xi^{t}} \| \partial_{\mathcal{M}} F(\mathbf{X}^{t}) \|_{\mathsf{F}} \stackrel{@}{=} \| \partial F(\mathbf{X}^{t}) \ominus \mathbf{X}^{t} [\partial F(\mathbf{X}^{t})]^{\mathsf{T}} \mathbf{X}^{t} \|_{\mathsf{F}}$$

$$\stackrel{@}{=} \| \partial F(\mathbf{X}^{t}) [\mathbf{X}^{t}]^{\mathsf{T}} \mathbf{X}^{t} \ominus \mathbf{X}^{t} [\partial F(\mathbf{X}^{t})]^{\mathsf{T}} \mathbf{X}^{t} \|_{\mathsf{F}}$$

$$\stackrel{@}{\leq} \| \partial F(\mathbf{X}^{t}) [\mathbf{X}^{t}]^{\mathsf{T}} \ominus \mathbf{X}^{t} [\partial F(\mathbf{X}^{t})]^{\mathsf{T}} \|_{\mathsf{F}}$$

$$\stackrel{@}{=} \gamma \mathbb{E}_{\mathsf{B}^{t}} [\| \mathbf{U}_{\mathsf{B}^{t}}^{\mathsf{T}} \{ \partial F(\mathbf{X}^{t}) [\mathbf{X}^{t}]^{\mathsf{T}} \ominus \mathbf{X}^{t} [\partial F(\mathbf{X}^{t})]^{\mathsf{T}} \} \mathbf{U}_{\mathsf{B}^{t}} \|_{\mathsf{F}}]$$

$$\stackrel{@}{=} \gamma \| \partial_{\mathcal{M}} \mathcal{K}(\mathbf{I}_{k}; \mathbf{X}^{t}, \mathsf{B}^{t}) \|_{\mathsf{F}}$$

$$(58)$$

where step ① uses the definition of $\partial_{\mathcal{M}}F(\mathbf{X}^t)$); step ② uses $[\mathbf{X}^t]^\mathsf{T}\mathbf{X}^t = \mathbf{I}_k$; step ③ uses the inequality that $\|\mathbf{A}\mathbf{X}\|_\mathsf{F}^2 \le \|\mathbf{A}\|_\mathsf{F}^2$ for all $\mathbf{X} \in \mathrm{St}(n,r)$; step ④ uses Equality (57); step ⑤ uses the definition of $\partial_{\mathcal{M}}\mathcal{K}(\mathbf{I}_k; \mathbf{X}^t, \mathbb{B}^t)$.

F.3 Proof of Theorem 4.6

 Proof. We derive the following results:

$$\mathbb{E}_{\xi^{T}}[\operatorname{dist}^{2}(\mathbf{0}, \partial_{\mathcal{M}} F(\mathbf{X}^{T+1}))] \stackrel{\widehat{\underline{}}}{=} \gamma^{2} \cdot \mathbb{E}_{\xi^{T+1}}[\operatorname{dist}^{2}(\mathbf{0}, \partial_{\mathcal{M}} \mathcal{K}(\mathbf{I}_{k}; \mathbf{X}^{T+1}, \mathbf{B}^{T+1}))] \\
\stackrel{\widehat{\underline{}}{\leq}}{\leq} \gamma^{2} \cdot \phi^{2} \cdot \mathbb{E}_{\xi^{T}}[\|\bar{\mathbf{V}}^{T} - \mathbf{I}_{k}\|_{\mathsf{F}}^{2}] \\
\stackrel{\widehat{\underline{}}{\leq}}{\leq} \gamma^{2} \cdot \phi^{2} \cdot \frac{\bar{c}}{T+1},$$

where step ① uses Lemma 4.4(b); step ② uses Lemma 4.4(a); step ③ uses Inequality (45).

Therefore, we conclude that there exists an index \bar{t} with $\bar{t} \in [0,T]$ such that the associated solution $\mathbf{X}^{\bar{t}}$ qualifies as an ϵ -critical point of Problem (1) satisfying $\mathbb{E}_{\xi^{\bar{t}}}[\mathrm{dist}^2(\mathbf{0},\partial_{\mathcal{M}}F(\mathbf{X}^{\bar{t}+1}))] \leq \epsilon$, provided that T is sufficiently large to ensure $\gamma^2 \cdot \phi^2 \cdot \frac{\tilde{c}}{T+1} \leq \epsilon$.

F.4 Proof of Theorem 4.9

Proof. Initially, given $F_{\iota}(\mathbf{X}) \triangleq F(\mathbf{X}) + \iota_{\mathcal{M}}(\mathbf{X})$ is a KL function by our assumption, we can conclude, from Proposition 4.8, that:

$$\frac{1}{\varphi'(F_{\iota}(\mathbf{X}^{t}) - F_{\iota}(\mathbf{X}^{\infty}))} \le \operatorname{dist}(0, \partial F_{\iota}(\mathbf{X}^{t})). \tag{59}$$

Since $\varphi(\cdot)$ is a concave desingularization function, we have: $\varphi(b) + (a-b)\varphi'(a) \leq \varphi(a)$. Applying the inequality above with $a = F(\mathbf{X}^t) - F(\mathbf{X}^\infty)$ and $b = F(\mathbf{X}^{t+1}) - F(\mathbf{X}^\infty)$, we have:

$$(F(\mathbf{X}^t) - F(\mathbf{X}^{t+1}))\varphi'(F(\mathbf{X}^t) - F(\mathbf{X}^{\infty})) \le \underbrace{\varphi(F(\mathbf{X}^t) - F(\mathbf{X}^{\infty}))}_{\triangleq \varphi^t} - \varphi(F(\mathbf{X}^{t+1}) - F(\mathbf{X}^{\infty})). (60)$$

Part (a). We derive the following inequalities:

$$(E_{t+1})^{2} \triangleq \mathbb{E}_{\xi^{t}}[\|\bar{\mathbf{V}}^{t} - \mathbf{I}_{k}\|_{\mathsf{F}}^{2}] \stackrel{\circ}{\leq} \frac{2}{\alpha} \cdot \mathbb{E}_{\xi^{t}}[F(\mathbf{X}^{t}) - F(\mathbf{X}^{t+1})]$$

$$\stackrel{\circ}{\leq} \frac{2}{\alpha} \cdot \mathbb{E}_{\xi^{t}}[(\varphi^{t} - \varphi^{t+1}) \cdot \frac{1}{\varphi'(F(\mathbf{X}^{t}) - F(\mathbf{X}^{\infty}))}]$$

$$\stackrel{\circ}{\leq} \frac{2}{\alpha} \cdot \mathbb{E}_{\xi^{t}}[(\varphi^{t} - \varphi^{t+1}) \cdot \operatorname{dist}(0, \partial F_{t}(\mathbf{X}^{t}))]$$

$$\stackrel{\circ}{\leq} \frac{2}{\alpha} \cdot \mathbb{E}_{\xi^{t}}[(\varphi^{t} - \varphi^{t+1}) \cdot \|\partial_{\mathcal{M}}F(\mathbf{X}^{t})\|_{\mathsf{F}}]$$

$$\stackrel{\circ}{\leq} \frac{2}{\alpha} \cdot \mathbb{E}_{\xi^{t}}[(\varphi^{t} - \varphi^{t+1})\gamma\|\partial_{\mathcal{M}}\mathcal{K}(\mathbf{I}_{k}; \mathbf{X}^{t}, \mathbf{B}^{t})\|_{\mathsf{F}}]$$

$$\stackrel{\circ}{\leq} \frac{2}{\alpha} \cdot \mathbb{E}_{\xi^{t-1}}[(\varphi^{t} - \varphi^{t+1})\gamma\phi\|\bar{\mathbf{V}}^{t-1} - \mathbf{I}_{k}\|_{\mathsf{F}}]$$

$$\stackrel{\circ}{=} \frac{2}{\alpha} \cdot \gamma\phi \cdot (\varphi^{t} - \varphi^{t+1}) \cdot E_{t},$$

where step ① uses the sufficient decrease condition as shown in Theorem 4.2; step ② uses Inequality (60); step ③ uses Inequality (59); step ④ uses Lemma A.7; step ⑤ uses Inequality (58); step ⑥ uses Lemma 4.4; step ⑦ uses the definitions of $\{\kappa, \varphi^t, E_t\}$.

Part (b). Applying Lemma A.10 with $p^t = \kappa \varphi^t$ with $p^t \ge p^{t+1}$, for all $i \ge 1$, we have:

$$\sum_{j=i}^{\infty} E_{j+1} \le E_i + 2p^i.$$

Using the definition of $D_t \triangleq \sum_{i=t}^{\infty} E_{j+1}$ and letting i = t, we obtain:

$$D_t \le E_t + 2p^t \stackrel{\text{①}}{=} E_t + 2\kappa\varphi^t \stackrel{\text{②}}{\le} E_t + 2\kappa\varphi^1 \stackrel{\text{③}}{\le} 2\sqrt{k} + 2\kappa\varphi^1,$$

where step ① uses $p^t = \kappa \varphi^t$; step ② uses $\varphi^t \leq \varphi^1$; step ③ uses $E_t \triangleq \mathbb{E}_{\xi^{t-1}}[\|\bar{\mathbf{V}}^{t-1} - \mathbf{I}_k\|_{\mathsf{F}}] \leq \mathbb{E}_{\xi^{t-1}}[\|\bar{\mathbf{V}}^{t-1}\|_{\mathsf{F}}] + \|\mathbf{I}_k\|_{\mathsf{F}} \leq \sqrt{k} + \sqrt{k}$. We conclude that $D_t \triangleq \sum_{j=t}^{\infty} E_{j+1}$ is always upper-bounded.

Using the fact that $\|\mathbf{X}^{t+1} - \mathbf{X}^t\|_{\mathsf{F}}^2 \leq \|\bar{\mathbf{V}}^t - \mathbf{I}_k\|_{\mathsf{F}}^2$ as shown in Lemma 2.2(c), we conclude that $\sum_{i=1}^{\infty} \mathbb{E}_{\xi^i}[\|\mathbf{X}^{i+1} - \mathbf{X}^i\|_{\mathsf{F}}]$ is also always upper-bounded.

F.5 Proof of Theorem 4.10

Proof. We define $\varphi^t \triangleq \varphi(s^t)$, where $s^t \triangleq F(\mathbf{X}^t) - F(\mathbf{X}^{\infty})$.

We define $E_{t+1} \triangleq \mathbb{E}_{\xi^t}[\|\bar{\mathbf{V}}^t - \mathbf{I}_k\|_{\mathsf{F}}]$, and $D_i = \sum_{i=1}^{\infty} E_{i+1}$.

First, we have:

$$\begin{split} \|\mathbf{X}^T - \mathbf{X}^{\infty}\|_{\mathsf{F}} & \stackrel{@}{\leq} & \sum_{j=T}^{\infty} \|\mathbf{X}^j - \mathbf{X}^{j+1}\|_{\mathsf{F}} \\ & \stackrel{@}{\leq} & \sum_{j=T}^{\infty} \|\bar{\mathbf{V}}^j - \mathbf{I}_k\|_{\mathsf{F}} \\ & \stackrel{@}{=} & \sum_{j=T}^{\infty} E_{j+1} \\ & \stackrel{@}{=} & D_T, \end{split}$$

where step ① uses the triangle inequality; step ② uses $\|\mathbf{X}^{t+1} - \mathbf{X}^t\|_{\mathsf{F}}^2 \leq \|\bar{\mathbf{V}}^t - \mathbf{I}_k\|_{\mathsf{F}}^2$, as shown in Lemma 2.2(c); step ③ uses the definition of E_{t+1} ; step ④ uses the definition of D_T . Therefore, it suffices to establish the convergence rate of D_T .

Second, we obtain the following results:

ring results:
$$\frac{1}{\varphi'(s^t)} \stackrel{\textcircled{0}}{\leq} \|\operatorname{dist}(\mathbf{0}, \partial F_{\iota}(\mathbf{X}^t))\|_{\mathsf{F}}$$

$$\stackrel{\textcircled{2}}{\leq} \|\partial_{\mathcal{M}}F(\mathbf{X}^t)\|_{\mathsf{F}}$$

$$\stackrel{\textcircled{3}}{\leq} \mathbb{E}_{\xi^t}[\gamma\|\partial_{\mathcal{M}}\mathcal{K}(\mathbf{I}_k; \mathbf{X}^t, \mathsf{B}^t)\|_{\mathsf{F}}$$

$$\stackrel{\textcircled{4}}{\leq} \mathbb{E}_{\xi^t}[\gamma\phi\|\bar{\mathbf{V}}^{t-1} - \mathbf{I}_k\|_{\mathsf{F}}$$

$$\stackrel{\textcircled{5}}{\leq} \gamma\phi E_t,$$
resition 4.8 that dist $(\mathbf{0}, \partial F_{\iota}(\mathbf{X}'))\varphi'(F_{\iota}(\mathbf{X}'))\varphi$

where step ① uses uses Proposition 4.8 that $\operatorname{dist}(\mathbf{0}, \partial F_{\iota}(\mathbf{X}'))\varphi'(F_{\iota}(\mathbf{X}') - F_{\iota}(\mathbf{X}^{\infty})) \geq 1$; step ② uses Lemma A.7; step ③ uses Inequality (58); step ④ uses the Riemannian subgradient lower bound for the iterates gap in Lemma 4.4; step ⑤ uses the definition of $E_t \triangleq \mathbb{E}_{\mathcal{E}^{t-1}}[\|\hat{\mathbf{V}}^{t-1} - \mathbf{I}_k\|_{\mathbf{F}}^2]$.

Third, using the definition of D_t , we derive:

$$D_{t} \triangleq \sum_{i=t}^{\infty} E_{i+1}$$

$$\stackrel{\textcircled{0}}{\leq} E_{t} + 2\kappa \varphi^{t}$$

$$\stackrel{\textcircled{2}}{=} E_{t} + 2\kappa c \cdot \left\{ [s^{t}]^{\sigma} \right\}^{\frac{1-\sigma}{\sigma}}$$

$$\stackrel{\textcircled{3}}{=} E_{t} + 2\kappa c \cdot \left\{ c(1-\sigma) \cdot \frac{1}{\varphi'(s^{t})} \right\}^{\frac{1-\sigma}{\sigma}}$$

$$\stackrel{\textcircled{4}}{=} E_{t} + 2\kappa c \cdot \left\{ c(1-\sigma) \cdot \gamma \phi E_{t} \right\}^{\frac{1-\sigma}{\sigma}}$$

$$\stackrel{\textcircled{5}}{=} D_{t-1} - D_{t} + 2\kappa c \cdot \left\{ c(1-\sigma) \cdot \gamma \phi(D_{t-1} - D_{t}) \right\}^{\frac{1-\sigma}{\sigma}}$$

$$= D_{t-1} - D_{t} + \underbrace{2\kappa c \cdot \left[c(1-\sigma)\gamma \phi \right]^{\frac{1-\sigma}{\sigma}}}_{\triangleq ::} \cdot \left\{ D_{t-1} - D_{t} \right\}^{\frac{1-\sigma}{\sigma}}, \tag{61}$$

where step ① uses $\sum_{i=t}^{\infty} E_{i+1} \leq E_t + 2\kappa \varphi^t$, as shown in Theorem 4.9(\boldsymbol{b}); step ② uses the definitions that $\varphi^t \triangleq \varphi(s^t)$, and $\varphi(s) = cs^{1-\sigma}$; step ③ uses $\varphi'(s) = c(1-\sigma) \cdot [s]^{-\sigma}$, leading to $[s^t]^{\sigma} = c(1-\sigma) \cdot \frac{1}{\varphi'(s^t)}$; step ④ uses Inequality (61); step ⑤ uses the fact that $E_t = D_{t-1} - D_t$.

We consider three cases for $\sigma \in [0, 1)$.

 Part (a). We consider $\sigma = 0$. We have from Inequality (61):

$$0 \leq -\frac{1}{\varphi'(s^{t})} + \gamma \phi E_{t}$$

$$\stackrel{@}{=} -\frac{1}{c(1-\sigma)\cdot[s^{t}]^{-\sigma}} + \gamma \phi E_{t}$$

$$\stackrel{@}{=} -\frac{1}{c} + \gamma \phi E_{t}, \tag{62}$$

where step ① uses $\varphi'(s) = c(1-\sigma) \cdot [s]^{-\sigma}$; step ② uses $\sigma = 0$ and $E_t = D_{t-1} - D_t$.

Since $E_t \to 0$, and $\gamma, \phi, c > 0$, Inequality (62) results in a contradiction $E_t \ge \frac{1}{c\gamma\phi} > 0$. Therefore, there exists t' such that $D_t = 0$ for all t > t', ensuring that the algorithm terminates in a finite number of steps.

Part (b). We consider $\sigma \in (0, \frac{1}{2}]$. We let $t' \triangleq \{i \mid D_{i-1} - D_i \leq 1\}$. For all $t \geq t'$, we have from Inequality (61):

$$D_{t} \leq D_{t-1} - D_{t} + (D_{t-1} - D_{t})^{\frac{1-\sigma}{\sigma}} \cdot \ddot{\kappa}$$

$$\leq D_{t-1} - D_{t} + (D_{t-1} - D_{t}) \cdot \ddot{\kappa}$$

$$\leq D_{t-1} \cdot \frac{\ddot{\kappa}+1}{\ddot{\kappa}+2}, \tag{63}$$

where step ① uses the fact that $x^{(1-\sigma)/\sigma} \le x$ for all $\sigma \in (0, \frac{1}{2}]$, and $x = D_{t-1} - D_t \in [0, 1]$. Therefore, we have:

$$D_T \le D_1 \cdot \left(\frac{\ddot{\kappa}+1}{\ddot{\kappa}+2}\right)^{T-1}.$$

Part (c). We consider $\sigma \in (\frac{1}{2}, 1)$. We define $w \triangleq \frac{1-\sigma}{\sigma} \in (0, 1)$, and $\tau \triangleq 1/w - 1 \in (0, \infty)$.

We let R be any positive constant such that $E_t \leq R$ for all $t \geq 1$.

For all $t \ge 2$, we have from Inequality (61):

$$D_{t} \leq D_{t-1} - D_{t} + \ddot{\kappa} \cdot (D_{t-1} - D_{t})^{\frac{1-\sigma}{\sigma}}$$

$$\stackrel{\textcircled{1}}{=} \ddot{\kappa} (D_{t-1} - D_{t})^{w} + (D_{t-1} - D_{t})^{w} \cdot (E_{t})^{1-w}$$

$$\stackrel{\textcircled{2}}{\leq} \ddot{\kappa} (D_{t-1} - D_{t})^{w} + (D_{t-1} - D_{t})^{w} \cdot R^{1-w}$$

$$= (D_{t-1} - D_{t})^{w} \cdot \underbrace{(\ddot{\kappa} + R^{1-w})}_{\underline{\Delta}_{\dot{\kappa}}},$$

where step ① uses the definition of w and the fact that $D_{t-1} - D_t = E_t$; step ② uses the fact that $\max_{x \in (0,R]} x^{1-w} \le R^{1-w}$ if $w \in (0,1)$ and R > 0. We further obtain:

$$\underbrace{[D_t]^{1/w}}_{=[D_t]^{\tau+1}} \le (D_{t-1} - D_t) \cdot \dot{\kappa}^{1/w}.$$

Applying Lemma A.11 with $a = \dot{\kappa}^{1/w}$, we have:

$$D_T \le \mathcal{O}(T^{-1/\tau}) \stackrel{\textcircled{0}}{=} \mathcal{O}(T^{-\frac{1}{1/w-1}}) \stackrel{\textcircled{2}}{=} \mathcal{O}(T^{-\frac{1}{\frac{\sigma}{1-\sigma}-1}}) = \mathcal{O}(T^{-\frac{1-\sigma}{2\sigma-1}}).$$

where step ① uses $\tau \triangleq 1/w - 1$; step ② uses $w \triangleq \frac{1-\sigma}{\sigma}$.

G ADDITIONAL EXPERIMENT DETAILS AND RESULTS

In this section, we present additional experiment details and results on the ℓ_0 norm-based SPCA.

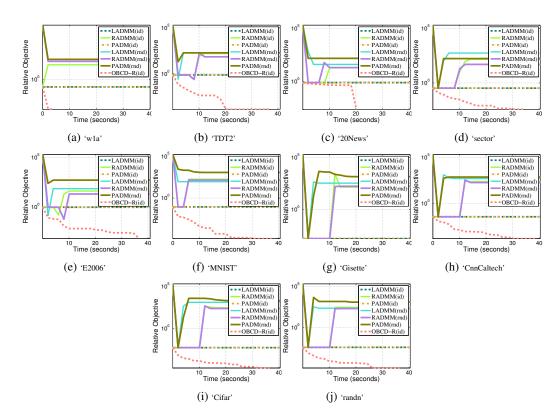


Figure 3: The convergence curve for solving L_0 norm-based SPCA with $\lambda = 10$.

G.1 DATA SETS

To generate the data matrix \mathbf{A} , we consider 10 publicly available real-world or randomly generated data sets: 'w1a', 'TDT2', '20News', 'sector', 'E2006', 'MNIST', 'Gisette', 'Caltech', 'Cifar', 'randn'. We randomly select a subset of examples from the original data set. The size of $\mathbf{A} \in \mathbb{R}^{m \times n}$ is chosen from the following set $(m,n) \in \{(2477,300), (500,1000), (8000,1000), (6412,1000), (2000,1000), (60000,784), (3000,1000), (1000,1000), (500,1000)\}.$ We scale the matrix \mathbf{A} to have unit Frobenius norm by setting $\mathbf{A} = \frac{\mathbf{A}}{\|\mathbf{A}\|_{\mathrm{F}}}$.

G.2 ADDITIONAL EXPERIMENT RESULTS

Figures 3, 4, 5, and 6 show the convergence curves of the compared methods for solving L_0 -norm-based SPCA with $\lambda \in \{10, 50, 100, 500\}$, respectively. The results confirm that the proposed **OBCD** consistently achieves lower objective values than other methods, reinforcing the conclusions presented in the main paper.

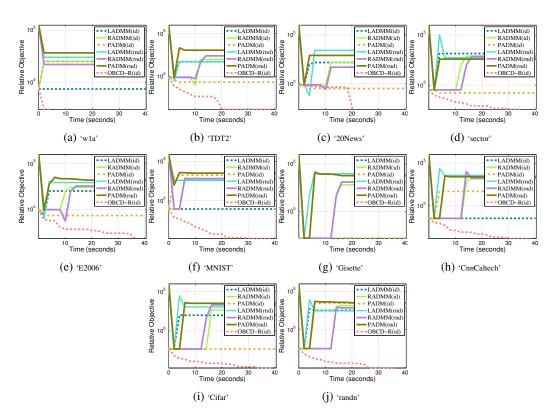


Figure 4: The convergence curve for solving L_0 norm-based SPCA with $\lambda = 50$.

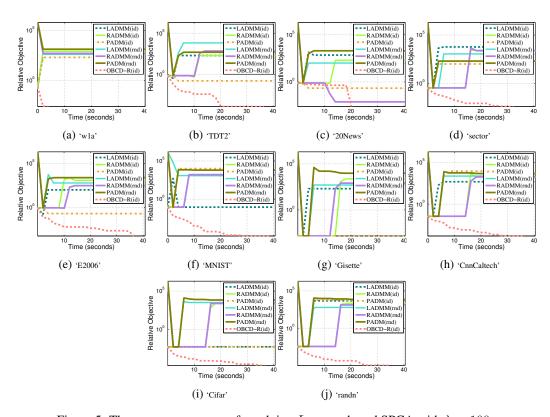


Figure 5: The convergence curve for solving L_0 norm-based SPCA with $\lambda = 100$.

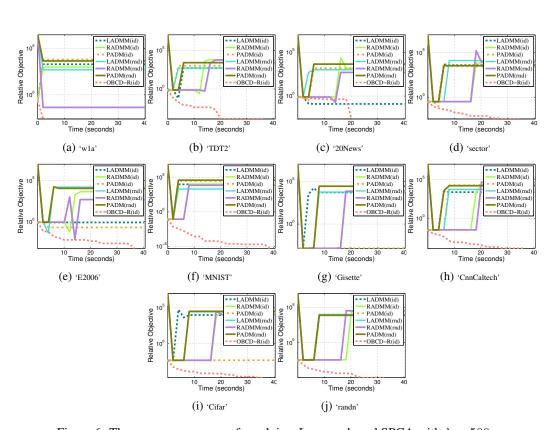


Figure 6: The convergence curve for solving L_0 norm-based SPCA with $\lambda = 500$.