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

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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 ('$\triangleq$' 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. ($\mathbb{A}$sm-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 differentiable and $\mathbf{H}$-smooth with $\mathbf{H} \in \mathbb{R}^{nr\times nr}$ such that:

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

where $\|\mathbf{H}\|_{\mathsf{sp}} \leq L_f$ for some constant $L_f > 0$ and $\|\mathbf{X}\|^2_{\mathbf{H}} \triangleq \mathrm{vec}(\mathbf{X})^\mathsf{T}\mathbf{H}\mathrm{vec}(\mathbf{X})$ [1]. Here, $\|\mathbf{H}\|_{\mathsf{sp}}$ 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). ($\mathbb{A}$sm-ii) The function $h(\mathbf{X}) : \mathbb{R}^{n\times r} \mapsto \mathbb{R}$ is proper, 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 $h(\mathbf{X}) = \|\mathbf{X}\|_p$ with $p \in \{0, 1\}$, the capped-ℓ_1 function $h(\mathbf{X}) = \sum_{i,j} \max(|\mathbf{X}_{ij}|, \tau)$ with $\tau > 0$, and the indicator function for non-negativity constraints $h(\mathbf{X}) = \iota_{\geq 0}(\mathbf{X})$. ($\mathbb{A}$sm-iii) The following small-sized subproblem can be solved exactly and efficiently:

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

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 $h(\mathbf{V}\mathbf{Z}) \triangleq \sum_{i,j} h([\mathbf{V}\mathbf{Z}]_{ij})$, given the coordinate-wise separability of $h(\cdot)$. This assumption is analogous to the "prox-friendly" condition in (variable-metric) proximal gradient methods

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

(Beck & Teboulle, 2009; Raguet et al., 2013), but instead of a standard proximal operator for *a single nonsmooth term* in the *full* space, our subproblem jointly handles *two nonsmooth components* (the function $h(\cdot)$ and the orthogonality constraint) in a low-dimensional $k \times k$ space.

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., 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 cast as instances of Problem (1). Below, we present two representative examples: L_0-regularized sparse PCA and L_1-regularized sparse PCA. An additional example on nonnegative PCA is provided in Appendix Section G.1.

► **L_0-Regularized Sparse PCA**. L_0-regularized 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-Regularized Sparse PCA**. 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-regularized 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 grouped into four 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. ***(iv)*** Landing methods (Ablin & Peyré, 2022; Vary et al.; Ablin et al., 2024). These methods avoid explicit retractions by working in the ambient Euclidean space while adding a penalty that attracts iterates toward the orthogonal manifold. Each update combines a descent direction for the objective with a corrective term that reduces constraint violation, and, with appropriate step sizes, the iterates converge to points that are nearly orthogonal and nearly stationary for the original problem.

► **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; Lyu & Li, 2025). 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 Penalty-based Splitting Method (PSM) (Yuan, 2024; Chen, 2012).

► **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 coordinate-wise nonsmooth problems with $k \geq 2$ 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 methods typically suffer from one or more of the following limitations: ***(i)*** they rely on full gradient information, incurring high computational costs per iteration; ***(ii)*** they do not accommodate coordinate-wise nonsmooth composite objectives; ***(iii)*** they lack true descent properties and are often infeasible methods what only attain feasibility only at the limit; ***(iv)*** they often lack rigorous last-iterate convergence guarantees; ***(v)*** they provide only weak optimality results at critical points. ★ In contrast, our methods overcome these limitations by using a tailored block coordinate descent framework for efficient composite optimization on the Stiefel manifold, with 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 $\mathcal{M} \triangleq \mathrm{St}(n, r)$. Matlab-style colon notation is used to describe submatrices. For a matrix $\mathbf{X} \in \mathbb{R}^{n\times r}$, let $\mathrm{vec}(\mathbf{X}) \in \mathbb{R}^{nr\times 1}$ denote the vector formed by stacking its columns, and let $\mathrm{mat}(\mathbf{x}) \in \mathbb{R}^{n\times r}$ denote the inverse operator, such that $\mathrm{mat}(\mathrm{vec}(\mathbf{X})) = \mathbf{X}$. 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.

2 The Proposed **OBCD** Algorithm

In this section, we introduce **OBCD**, a Block Coordinate Descent algorithm for solving coordinate-wise 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.

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

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 $\mathtt{B}$ and $\mathtt{B}^c$, where $\mathtt{B}$ is the working set with $|\mathtt{B}| = k$ and $\mathtt{B}^c = \{1, 2, ..., n\} \setminus \mathtt{B}$. To simplify notation, we use $\mathtt{B}$ instead of $\mathtt{B}^t$, as t can be inferred from the context. We only update k rows of the variable $\mathbf{X}$ via $\mathbf{X}^{t+1}(\mathtt{B}, :) \Leftarrow \mathbf{V}\mathbf{X}^t(\mathtt{B}, :)$ for some appropriate matrix $\mathbf{V} \in \mathbb{R}^{k\times k}$. The following equivalent expressions hold:

$$\mathbf{X}^{t+1}(\mathtt{B}, :) = \mathbf{V}\mathbf{X}^t(\mathtt{B}, :) \quad \Leftrightarrow \quad \mathbf{X}^{t+1} = (\mathrm{U}_{\mathtt{B}}\mathbf{V}\mathrm{U}_{\mathtt{B}}^{\mathsf{T}} + \mathrm{U}_{\mathtt{B}^c}\mathrm{U}_{\mathtt{B}^c}^{\mathsf{T}})\mathbf{X}^t \tag{4}$$

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

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

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

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

Lemma 2.1. *(Proof in Appendix D.1) We let $\mathtt{B} \in \{\mathcal{B}_i\}_{i=1}^{\mathrm{C}_n^k}$, where the set $\{\mathcal{B}_1, \mathcal{B}_2, ..., \mathcal{B}_{\mathrm{C}_n^k}\}$ denotes all possible combinations of the index vectors choosing k items from n without repetition. We let $\mathbf{V} \in \mathrm{St}(k, k)$. We define $\mathbf{X}^+ \triangleq \mathcal{X}_{\mathtt{B}}(\mathbf{V}) \triangleq \mathbf{X} + \mathrm{U}_{\mathtt{B}}(\mathbf{V} - \mathbf{I}_k)\mathrm{U}_{\mathtt{B}}^{\mathsf{T}}\mathbf{X}$. **(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 $\mathbf{X} \in \mathrm{St}(n, r)$, then $\mathbf{X}^+ \in \mathrm{St}(n, r)$.*

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

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

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

The following lemma offers important properties for the update rule $\mathbf{X}^+ = \mathbf{X} + \mathrm{U}_{\mathtt{B}}(\mathbf{V} - \mathbf{I}_k)\mathrm{U}_{\mathtt{B}}^{\mathsf{T}}\mathbf{X}$.

Lemma 2.2. *(Proof in Appendix D.2) We define $\mathbf{X}^+ = \mathbf{X} + \mathrm{U}_{\mathtt{B}}(\mathbf{V} - \mathbf{I}_k)\mathrm{U}_{\mathtt{B}}^{\mathsf{T}}\mathbf{X}$. For any $\mathbf{X} \in \mathrm{St}(n, r)$, $\mathbf{V} \in \mathrm{St}(k, k)$, $\mathtt{B} \in \{\mathcal{B}_i\}_{i=1}^{\mathrm{C}_n^k}$, and symmetric matrix $\mathbf{H} \in \mathbb{R}^{nr\times nr}$, we have: **(a)** $\frac{1}{2}\|\mathbf{X}^+ - \mathbf{X}\|_{\mathbf{H}}^2 = \frac{1}{2}\|\mathbf{V} - \mathbf{I}_k\|_{\underline{\mathbf{Q}}}^2$, where $\underline{\mathbf{Q}} \triangleq (\mathbf{Z}^{\mathsf{T}} \otimes \mathrm{U}_{\mathtt{B}})^{\mathsf{T}}\mathbf{H}(\mathbf{Z}^{\mathsf{T}} \otimes \mathrm{U}_{\mathtt{B}})$, $\mathbf{Z} \triangleq \mathrm{U}_{\mathtt{B}}^{\mathsf{T}}\mathbf{X} \in \mathbb{R}^{k\times r}$, and $\mathbf{X} \otimes \mathbf{Y}$ is the Kronecker product of $\mathbf{X}$ and $\mathbf{Y}$. **(b)** $\frac{1}{2}\|\mathbf{X}^+ - \mathbf{X}\|_{\mathsf{F}}^2 = \langle \mathbf{I}_k - \mathbf{V}, \mathrm{U}_{\mathtt{B}}^{\mathsf{T}}\mathbf{X}\mathbf{X}^{\mathsf{T}}\mathrm{U}_{\mathtt{B}}\rangle$. **(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 $\mathtt{B}^t$ 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 $F(\mathcal{X}_{\mathtt{B}}^t(\mathbf{V}))$ in Problem (7). Initially, for any $\mathbf{X}^t \in \mathrm{St}(n, r)$ and $\mathbf{V} \in \mathrm{St}(k, k)$, we establish following inequalities: $f(\mathcal{X}_{\mathtt{B}}^t(\mathbf{V})) - f(\mathbf{X}^t) \overset{①}{\leq} \langle \mathcal{X}_{\mathtt{B}}^t(\mathbf{V}) - \mathbf{X}^t, \nabla f(\mathbf{X}^t)\rangle + \frac{1}{2}\|\mathcal{X}_{\mathtt{B}}^t(\mathbf{V}) - \mathbf{X}^t\|_{\mathbf{H}}^2 \overset{②}{=} \langle \mathrm{U}_{\mathtt{B}}(\mathbf{V} - \mathbf{I}_k)\mathrm{U}_{\mathtt{B}}^{\mathsf{T}}\mathbf{X}^t, \nabla f(\mathbf{X}^t)\rangle + \frac{1}{2}\|\mathbf{V} - \mathbf{I}_k\|_{\underline{\mathbf{Q}}}^2 \overset{③}{\leq} \langle \mathbf{V} - \mathbf{I}_k, [\nabla f(\mathbf{X}^t)(\mathbf{X}^t)^{\mathsf{T}}]_{\mathtt{BB}}\rangle + \frac{1}{2}\|\mathbf{V} - \mathbf{I}_k\|_{\mathbf{Q}+\alpha\mathbf{I}}^2$, where step ① uses Inequality (2); step ② uses Lemma 2.2(a); step ③ uses $\alpha > 0$ and $\underline{\mathbf{Q}} \preceq \mathbf{Q}$, which can be ensured by choosing $\mathbf{Q}$ using one of the following methods:

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

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

where $\mathbf{Z} \triangleq \mathrm{U}_{\mathtt{B}}^{\mathsf{T}}\mathbf{X}^t$. 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 $\mathcal{K}(\mathbf{V}; \mathbf{X}^t, \mathtt{B})$ that majorizes $F(\mathcal{X}_{\mathtt{B}}^t(\mathbf{V})) = f(\mathcal{X}_{\mathtt{B}}^t(\mathbf{V})) + h(\mathcal{X}_{\mathtt{B}}^t(\mathbf{V}))$:

$$\begin{aligned} F(\mathcal{X}_{\mathtt{B}}^t(\mathbf{V})) &\leq f(\mathbf{X}^t) + \langle \mathbf{V} - \mathbf{I}_k, [\nabla f(\mathbf{X}^t)(\mathbf{X}^t)^{\mathsf{T}}]_{\mathtt{BB}}\rangle + \tfrac{1}{2}\|\mathbf{V} - \mathbf{I}_k\|_{\mathbf{Q}+\alpha\mathbf{I}}^2 + h(\mathbf{V}\mathrm{U}_{\mathtt{B}}^{\mathsf{T}}\mathbf{X}^t) \\ &\leq \mathcal{K}(\mathbf{V}; \mathbf{X}^t, \mathtt{B}) \triangleq \tfrac{1}{2}\|\mathbf{V} - \mathbf{I}_k\|_{\mathbf{Q}+\alpha\mathbf{I}}^2 + \langle \mathbf{V}, [\nabla f(\mathbf{X}^t)(\mathbf{X}^t)^{\mathsf{T}}]_{\mathtt{BB}}\rangle + h(\mathbf{V}\mathrm{U}_{\mathtt{B}}^{\mathsf{T}}\mathbf{X}^t) + \ddot{c}, \end{aligned} \tag{10}$$

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

1: **Input:** proximal parameter $\alpha > 0$, initial feasible point $\mathbf{X}^0$, block size $k \geq 2$, $t = 0$.
2: **for** $t = 0$ **to** T **do**
3: (**S1**) Select working set $\mathtt{B}^t \in \{1, \ldots, n\}^k$. Let $\mathtt{B} = \mathtt{B}^t$ and $\mathtt{B}^c = \{1, \ldots, n\} \setminus \mathtt{B}$.
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

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

Alternatively, find a local solution $\bar{\mathbf{V}}^t$ such that $\mathcal{K}(\bar{\mathbf{V}}^t; \mathbf{X}^t, \mathtt{B}) \leq \mathcal{K}(\mathbf{I}_k; \mathbf{X}^t, \mathtt{B})$.
6: (**S4**) $\mathbf{X}^{t+1}(\mathtt{B}, :) \leftarrow \bar{\mathbf{V}}^t \, \mathbf{X}^t(\mathtt{B}, :)$
7: **end for**

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

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

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 gradient of $\nabla f(\mathbf{X}^t)$ and the solution $\mathbf{X}^t$ to compute the linear term $\langle [\nabla f(\mathbf{X}^t)(\mathbf{X}^t)^\mathsf{T}]_{\mathtt{BB}}, \mathbf{V} \rangle = \langle [\nabla f(\mathbf{X}^t)]_{\mathtt{B},:}^\mathsf{T} [\mathbf{X}^t]_{\mathtt{B},:}, \mathbf{V} \rangle$, 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* $\mathbf{Z} = \mathbf{U}_{\mathtt{B}}^\mathsf{T} \mathbf{X}^t$ *and* $\mathbf{P} \triangleq [\nabla f(\mathbf{X}^t)(\mathbf{X}^t)^\mathsf{T}]_{\mathtt{BB}} - \mathrm{mat}(\mathbf{Q}\mathrm{vec}(\mathbf{I}_k)) - \alpha \mathbf{I}_k$. *We have:*

- ***(a)*** *The subproblem in Equation (11) is equivalent to Problem (3) with* $\tilde{\mathbf{Q}} = \mathbf{Q} + \alpha \mathbf{I}$.
- ***(b)*** *Assume that Formula (9) is used to choose* $\mathbf{Q}$. *Problem (3) further reduces to the following problem:* $\bar{\mathbf{V}}^t \in \arg\min_{\mathbf{V} \in \mathrm{St}(k,k)} \mathcal{P}(\mathbf{V}) \triangleq \langle \mathbf{V}, \mathbf{P} \rangle + h(\mathbf{V}\mathbf{Z})$. *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 Lemma 2.3(b), when* $k > 2$, $h(\mathbf{X}) = 0$, *and* $\mathbf{Q}$ *is chosen to be a diagonal matrix as in Equation (9), the subproblem* $\bar{\mathbf{V}}^t \in \arg\min_{\mathbf{V} \in \mathrm{St}(k,k)} \mathcal{K}(\mathbf{V}; \mathbf{X}^t, \mathtt{B})$ *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* $(\bar{\mathbf{V}}^t; \mathbf{X}^t, \mathtt{B}) \leq \mathcal{K}(\mathbf{I}_k; \mathbf{X}^t, \mathtt{B})$ *can be found, then the sufficient descent condition remains valid, and convergence to a weaker optimality condition for the final solution* $\mathbf{X}^\infty$ *is still achievable (see Inequalities (42), (44)).*

► **Smallest Possible Subproblems When** $k = 2$. We now discuss how to solve the subproblems exactly when $k = 2$. 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* $\mathbf{V} \in \mathrm{St}(2, 2)$ *can be expressed as* $\mathbf{V} = \mathbf{V}_\theta^{\mathrm{rot}}$ *or* $\mathbf{V} = \mathbf{V}_\theta^{\mathrm{ref}}$ *for some* $\theta \in \mathbb{R}$, *where* $\mathbf{V}_\theta^{\mathrm{rot}} \triangleq \begin{pmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{pmatrix}$, $\mathbf{V}_\theta^{\mathrm{ref}} \triangleq \begin{pmatrix} -\cos(\theta) & \sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix}$. *We have* $\det(\mathbf{V}_\theta^{\mathrm{rot}}) = 1$ *and* $\det(\mathbf{V}_\theta^{\mathrm{ref}}) = -1$ *for any* θ.

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

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

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: $\min_{\mathbf{V}\in\mathrm{St}(2,2)} F(\mathbf{V}) \triangleq \|\mathbf{V} - \mathbf{A}\|_{\mathsf{F}}^2$, and $\min_{\mathbf{V}\in\mathrm{St}(2,2)} F(\mathbf{V}) \triangleq \|\mathbf{V} - \mathbf{B}\|_{\mathsf{F}}^2 + 5\|\mathbf{V}\|_1$, where $\mathbf{A} = \left(\begin{smallmatrix} 1 & 0 \\ -1 & -1 \end{smallmatrix}\right)$ and $\mathbf{B} = \left(\begin{smallmatrix} 1 & 0 \\ 1 & 2 \end{smallmatrix}\right)$. 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 shows that any orthogonal matrix $\mathbf{D} \in \mathrm{St}(n, n)$ and any point $\mathbf{X} \in \mathrm{St}(n, r)$ can be generated by composing simple 2-dimensional updates.

Theorem 3.1 (Basis Representation of Orthogonal Matrices)**.** *(Proof in Appendix E.1) Assume $k = 2$. For all $i \in [\mathrm{C}_n^k]$, 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 $\mathcal{V}_i \in \mathrm{St}(k, k)$. Then:*

- ***(a)*** *Any matrix $\mathbf{D} \in \mathrm{St}(n, n)$ can be expressed as $\mathbf{D} = \mathcal{W}_{\mathrm{C}_n^k} \ldots \mathcal{W}_2\mathcal{W}_1$ for suitable choice of $\mathcal{W}_i$ (equivalently, of $\mathcal{V}_i$). Furthermore, if $\forall i$, $\mathcal{V}_i = \mathbf{I}_2$, then $\mathbf{D} = \mathbf{I}_n$.*
- ***(b)*** *For any fixed reference point $\mathbf{X}^0 \in \mathrm{St}(n, r)$, every $\mathbf{X} \in \mathrm{St}(n, r)$ can be expressed as $\mathbf{X} = \mathcal{W}_{\mathrm{C}_n^k} \cdots \mathcal{W}_2\mathcal{W}_1\mathbf{X}^0$ for suitable $\mathcal{W}_i$.*

The above representation for $k = 2$ can in fact be extended to any block size $k \geq 2$, as stated next.

Corollary 3.2. *(Proof in Appendix E.2) The conclusion of Theorem 3.1 extends to all $k \geq 2$.*

Remark 3.3. ***(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 of Corollary 3.2 indicates that the proposed update scheme $\mathbf{X}^+ \Leftarrow \mathbf{X} + \mathrm{U}_{\mathrm{B}}(\mathbf{V} - \mathbf{I}_k)\mathrm{U}_{\mathrm{B}}^{\mathsf{T}}\mathbf{X}$ with $\mathbf{V} \in \mathrm{St}(k, k)$ 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 $\mathbf{\Lambda} \in \mathbb{R}^{r\times r}$ for the orthogonality constraint, we define the following Lagrangian function of Problem (1): $\mathcal{L}(\mathbf{X}, \mathbf{\Lambda}) = F(\mathbf{X}) + \frac{1}{2}\langle \mathbf{I}_r - \mathbf{X}^{\mathsf{T}}\mathbf{X}, \mathbf{\Lambda}\rangle$. Notably, the matrix $\mathbf{\Lambda}$ is symmetric, as $\mathbf{X}^{\mathsf{T}}\mathbf{X}$ is symmetric. We state the following definition of first-order optimality condition.

Definition 3.4. *Critical Point (Wen & Yin, 2013; Chen et al., 2020). A solution $\check{\mathbf{X}} \in \mathrm{St}(n, r)$ 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 $(\partial F(\check{\mathbf{X}}) \ominus \check{\mathbf{X}}[\partial F(\check{\mathbf{X}})]^{\mathsf{T}}\check{\mathbf{X}}) \triangleq \{\mathbf{G} - \check{\mathbf{X}}\mathbf{G}^{\mathsf{T}}\check{\mathbf{X}} \,|\, \mathbf{G} \in \partial F(\check{\mathbf{X}})\}$. Moreover, the corresponding multiplier satisfies $\mathbf{\Lambda} \in [\partial F(\check{\mathbf{X}})]^{\mathsf{T}}\check{\mathbf{X}}$.*

Remark 3.5. *The critical point condition in Lemma 3.4 can be equivalently expressed as (Absil et al., 2008; Jiang & Dai, 2015; Liu et al., 2016): $\mathbf{0} \in \mathbb{P}_{\mathrm{T}_{\mathbf{X}}\mathcal{M}}(\partial F(\mathbf{X}))$. Here, $\mathrm{T}_{\mathbf{X}}\mathcal{M}$ is the tangent space to $\mathcal{M}$ at $\mathbf{X} \in \mathcal{M}$ with $\mathrm{T}_{\mathbf{X}}\mathcal{M} = \{\mathbf{Y} \in \mathbb{R}^{n\times r} \,|\, \mathbf{X}^{\mathsf{T}}\mathbf{Y} + \mathbf{Y}^{\mathsf{T}}\mathbf{X} = \mathbf{0}\}$.*

► **Optimality Conditions for the Subproblems**. The Euclidean subdifferential of $\mathcal{K}(\mathbf{V};\mathbf{X}^t,\mathtt{B}^t)$ *w.r.t.* $\mathbf{V}$ is given by $\ddot{\mathbf{G}}(\mathbf{V}) \triangleq \ddot{\mathbf{\Delta}}(\mathbf{V}) + \mathrm{U}_{\mathtt{B}}^{\mathsf{T}}[\nabla f(\mathbf{X}^t) + \partial h(\mathbf{X}^{t+1})](\mathbf{X}^t)^{\mathsf{T}}\mathrm{U}_{\mathtt{B}}$, where $\ddot{\mathbf{\Delta}}(\mathbf{V}) = \mathrm{mat}((\mathbf{Q}+\alpha\mathbf{I}_k)\mathrm{vec}(\mathbf{V}-\mathbf{I}_k))$ and $\mathbf{X}^{t+1} = \mathbf{X}^t + \mathrm{U}_{\mathtt{B}}(\mathbf{V}-\mathbf{I}_k)\mathrm{U}_{\mathtt{B}}^{\mathsf{T}}\mathbf{X}^t$. Using Lemma 3.4, we set the Riemannian subdifferential of $\mathcal{K}(\mathbf{V};\mathbf{X}^t,\mathtt{B}^t)$ *w.r.t.* $\mathbf{V}$ to zero and obtain the following first-order optimality condition for $\bar{\mathbf{V}}^t$: $\mathbf{0} \in \partial_{\mathcal{M}}\mathcal{K}(\bar{\mathbf{V}}^t;\mathbf{X}^t,\mathtt{B}^t) \triangleq \ddot{\mathbf{G}}(\bar{\mathbf{V}}^t) \ominus \bar{\mathbf{V}}^t\ddot{\mathbf{G}}(\bar{\mathbf{V}}^t)^{\mathsf{T}}\bar{\mathbf{V}}^t$. This inclusion is a key ingredient in establishing the optimality hierarchy in Theorem 3.7(a) and the Riemannian subgradient lower bound in Lemma 4.4(a).

► **Optimality Conditions and Their Hierarchy**. We introduce the following new optimality condition of block-k stationary points.

Definition 3.6. *(Global) Block-k Stationary Point, abbreviated as* BS_k-point. Let $\alpha > 0$ and $k \geq 2$. A solution $\ddot{\mathbf{X}} \in \mathrm{St}(n,r)$ is called a block-k stationary point if: $\forall \mathtt{B} \in \{\mathcal{B}_i\}_{i=1}^{\mathrm{C}_n^k}$, $\mathbf{I}_k \in \arg\min_{\mathbf{V}\in\mathrm{St}(k,k)} \mathcal{K}(\mathbf{V};\ddot{\mathbf{X}},\mathtt{B})$, where $\mathcal{K}(\cdot;\cdot,\cdot)$ is defined in Equation (10).

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

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

Theorem 3.7. *(Proof in Appendix E.3) We establish the following relationships:*

(a) $\{\text{critical points } \ddot{\mathbf{X}}\} \supseteq \{\mathrm{BS}_2\text{-points } \ddot{\mathbf{X}}\}$.
(b) $\{\mathrm{BS_k}\text{-points } \ddot{\mathbf{X}}\} \supseteq \{\text{global optimal points } \bar{\mathbf{X}}\}$, *where* $k \in \{2,3,\ldots,n\}$.
(c) $\{\mathrm{BS_k}\textit{-points } \ddot{\mathbf{X}}\} \supseteq \{\mathrm{BS_{k+1}}\textit{-points } \ddot{\mathbf{X}}\}$, *where* $k \in \{2,3,\ldots,n-1\}$.
(d) *The reverse of the above three inclusions may not always hold true.*

Remark 3.8. ***(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* $\mathrm{BS_k}$*-points deterministically requires solving all* C_n^k *subproblems. However, by randomly selecting the working set* $\mathtt{B}$ *from the* C_n^k *possible combinations* $\{\mathcal{B}_i\}_{i=1}^{\mathrm{C}_n^k}$*, one can test whether* $\mathbf{X}$ *is a* $\mathrm{BS_k}$*-point in expectation.*

4 Convergence Analysis

This section establishes the iteration complexity and non-ergodic (last-iterate) 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 $\bar{\mathbf{V}}^t \in \arg\min_{\mathbf{V}\in\mathrm{St}(k,k)} \mathcal{K}(\mathbf{V};\mathbf{X}^t,\mathtt{B}^t)$ 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 $\xi^t \triangleq (\mathtt{B}^1,\mathtt{B}^2,\ldots,\mathtt{B}^t)$. We denote $\mathbf{X}^\infty$ as an arbitrary limit point of **OBCD**.

4.1 Iteration Complexity

Initially, we introduce the notation of ϵ-BS_k*-point* as follows.

Definition 4.1. *(ϵ-BS_k-point)* Given any constant $\epsilon > 0$, a point $\ddot{\mathbf{X}}$ is called an ϵ-BS_k*-point* if: $\frac{1}{\mathrm{C}_n^k}\sum_{i=1}^{\mathrm{C}_n^k} \mathrm{dist}(\mathbf{I}_k, \arg\min_{\mathbf{V}} \mathcal{K}(\mathbf{V};\ddot{\mathbf{X}},\mathcal{B}_i))^2 \leq \epsilon$, where $\mathcal{K}(\cdot;\cdot,\cdot)$ is defined in Equation (10). Here, the set $\{\mathcal{B}_1,\mathcal{B}_2,...,\mathcal{B}_{\mathrm{C}_n^k}\}$ denotes all possible combinations of the index vectors choosing k items from n without repetition, and $\mathrm{dist}(\Xi,\Xi')$ 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* $t \geq 0$*:*

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

(b) *If the* $\mathtt{B}^t$ *is selected from* $\{\mathcal{B}_i\}_{i=1}^{\mathtt{C}_n^k}$ *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. At the point $\mathbf{V} = \mathbf{I}_k$, the Riemannian subdifferential of $\mathcal{K}(\mathbf{V}; \mathbf{X}^t, \mathtt{B}^t)$ is $\partial_{\mathcal{M}}\mathcal{K}(\mathbf{I}_k; \mathbf{X}^t, \mathtt{B}^t) = \mathrm{U}_{\mathtt{B}^t}^{\mathsf{T}}(\mathbb{D} \ominus \mathbb{D}^{\mathsf{T}})\mathrm{U}_{\mathtt{B}^t}$, where $\mathbb{D} = [\nabla f(\mathbf{X}^t) + \partial h(\mathbf{X}^t)][\mathbf{X}^t]^{\mathsf{T}}$. We next derive a Riemannian subgradient lower bound in terms of the iterate gap.

Lemma 4.4. *(Proof in Appendix F.2,* **Riemannian Subgradient Lower Bound for the Iterates Gap**) Assume that $F(\cdot)$ is C_F-Lipschitz continuous on $\mathrm{St}(n, r)$, i.e., $\|\mathbf{G}\|_{\mathsf{F}} \leq C_F$ for all $\mathbf{X} \in \mathrm{St}(n, r)$ and all $\mathbf{G} \in \partial F(\mathbf{X})$. We have:

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

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

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* $\tilde{c}$ *as in Theorem 4.2 and* $\{\phi, \gamma\}$ *as in Lemma 4.4.* **OBCD** finds an ϵ*-critical point* of Problem (1), i.e., $\mathbb{E}_{\xi^{\bar{t}}}[\mathrm{dist}^2(\mathbf{0}, \partial_{\mathcal{M}}F(\mathbf{X}^{\bar{t}+1}))] \leq \epsilon$, in at most $T+1$ iterations in expectation, where $\bar{t} \in [T]$ and $T \geq \lceil \frac{\gamma^2\phi^2\tilde{c}}{\epsilon} \rceil$.

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 Kurdyka-Łojasiewicz (KL) function.*

Remark 4.8. *Semi-algebraic functions constitute a broad class of KL functions, including real polynomials, norm functions* $\|\mathbf{x}\|_p$ *with* $p \geq 0$*, rank functions, and indicator functions of sets such as the Stiefel manifold and the positive semidefinite cone (Attouch et al., 2010).*

We present the following useful proposition regrading to the KL function.

Proposition 4.9. *(***Kurdyka-Łojasiewicz Property**, see, e.g.,(Attouch et al., 2010; Bolte et al., 2014)). Let $F_\iota : \mathbb{R}^{m\times n} \to (-\infty, +\infty]$ be a KL function and $\mathbf{X}^\infty \in \mathrm{dom}\, F_\iota$. Then there exist $\sigma \in [0, 1)$, $\eta \in (0, +\infty]$, a neighborhood Υ of $\mathbf{X}^\infty$, and a concave continuous function $\varphi(t) = ct^{1-\sigma}$ with $c > 0$ and $t \in [0, \eta)$ such that for all $\mathbf{X}' \in \Upsilon$ satisfying $F_\iota(\mathbf{X}') \in (F_\iota(\mathbf{X}^\infty), F_\iota(\mathbf{X}^\infty) + \eta)$, it holds that $\mathrm{dist}(\mathbf{0}, \partial F_\iota(\mathbf{X}'))\, \varphi'\big(F_\iota(\mathbf{X}') - F_\iota(\mathbf{X}^\infty)\big) \geq 1$.

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 4.10. *(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 $D_i = \sum_{j=i}^{\infty} E_{j+1}$. Under the continuity assumption in Lemma 4.4, there exists a sufficiently large $t_\star$ such that, for all $t \geq t_\star$, 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, $\gamma \triangleq (\mathrm{C}_n^k/\mathrm{C}_{n-2}^{k-2})^{1/2}$, ϕ is defined in Lemma 4.4, and $\varphi(\cdot)$ is the desingularization function defined in Proposition 4.9.

(b) It holds that $\sum_{j=t}^{\infty} E_{j+1} \leq E_t + 2\kappa\varphi_t$. The sequence $\{E_t\}_{t=1}^{\infty}$ has the finite length property that $D_t \triangleq \sum_{j=t}^{\infty} E_{j+1}$ is always upper-bounded by a certain constant for all $t \geq t_\star$.

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

Theorem 4.11. *(Proof in Appendix F.5). Based on the continuity assumption made in Lemma 4.4, for all* $t \geq t_\star$*, we have:*

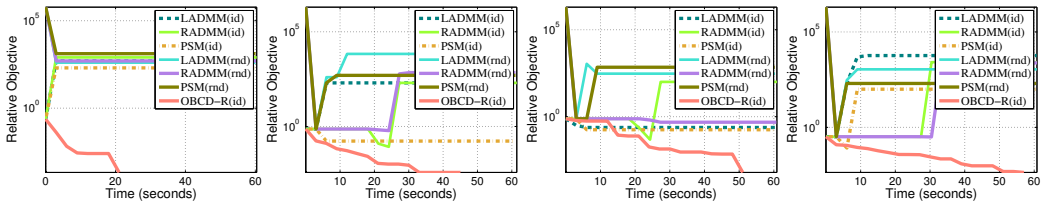
data-m-n	LADMM (id)	RADMM (id)	SPM (id)	LADMM (rnd)	RADMM (rnd)	SPM (rnd)	OBCD-R (id)
$r = 20$, $\lambda = 10$, time limit=40							
w1a-2477-300	199.897	219.698	199.897	259.825	239.717	259.672	199.667
TDT2-500-1000	199.997	359.382	199.997	389.376	269.292	389.260	199.258
20News-8000-1000	199.995	219.673	199.995	239.301	219.243	349.228	199.222
sector-6412-1000	199.980	349.793	199.980	749.996	249.813	369.651	199.649
E2006-2000-1000	199.999	239.115	199.999	269.128	219.084	709.095	199.077
MNIST-60000-784	199.985	379.893	199.985	289.917	339.910	1339.774	199.896
Gisette-3000-1000	199.980	339.979	199.980	539.979	369.981	1639.952	199.979
CnnCal-3000-1000	199.981	429.979	199.981	689.970	379.979	909.931	199.946
Cifar-1000-1000	199.979	479.979	199.979	1449.982	429.975	2169.934	199.974
randn-500-1000	199.980	469.980	199.980	409.980	389.980	1349.975	199.977

data-m-n	LADMM (id)	RADMM (id)	SPM (id)	LADMM (rnd)	RADMM (rnd)	SPM (rnd)	OBCD-R (id)
$r = 20$, $\lambda = 50$, time limit=40							
w1a-2477-300	999.891	1099.730	1099.889	1249.723	1049.707	1649.675	999.667
TDT2-500-1000	1049.997	1099.288	999.460	1049.282	1249.280	2149.271	999.257
20News-8000-1000	1149.995	1149.501	999.549	3649.247	1049.326	1799.228	999.222
sector-6412-1000	2449.886	1799.904	999.816	1549.998	1749.952	1399.651	999.649
E2006-2000-1000	1099.283	1249.109	999.284	1849.115	1349.085	2549.136	999.077
MNIST-60000-784	999.985	1699.913	2849.852	1399.921	1649.905	4349.781	999.896
Gisette-3000-1000	999.980	1649.980	999.980	10399.983	2249.976	6899.967	999.979
CnnCal-3000-1000	999.981	2499.981	1049.969	4599.973	2649.981	3499.938	999.946
Cifar-1000-1000	1099.979	1449.978	999.979	2149.979	3149.974	4349.972	999.974
randn-500-1000	1349.980	2449.980	3949.977	1299.981	1749.980	4249.976	999.977

data-m-n	LADMM (id)	RADMM (id)	SPM (id)	LADMM (rnd)	RADMM (rnd)	SPM (rnd)	OBCD-R (id)
$r = 20$, $\lambda = 100$, time limit=40							
w1a-2477-300	2499.912	2799.713	2199.819	2399.723	2499.708	3299.662	1999.667
TDT2-500-1000	2199.515	2199.302	1999.432	8799.310	2699.278	2499.257	1999.258
20News-8000-1000	2699.480	2199.262	1999.440	2099.242	1999.230	3999.224	1999.222
sector-6412-1000	7799.995	4599.977	2099.716	3099.999	4399.973	2199.651	1999.649
E2006-2000-1000	2099.207	3199.083	1999.284	2599.106	2299.085	4399.081	1999.077
MNIST-60000-784	1999.984	3199.904	11799.715	3199.922	3599.907	8299.829	1999.896
Gisette-3000-1000	2199.980	4299.979	1999.980	2499.982	2799.981	11499.971	1999.979
CnnCal-3000-1000	2499.981	4399.982	11499.907	4399.975	3899.983	6799.938	1999.946
Cifar-1000-1000	1999.979	4999.979	1999.979	5199.979	4399.978	8799.969	1999.974
randn-500-1000	6699.980	4099.980	7899.977	2599.980	3299.980	9099.976	1999.977

data-m-n	LADMM (id)	RADMM (id)	SPM (id)	LADMM (rnd)	RADMM (rnd)	SPM (rnd)	OBCD-R (id)
$r = 20$, $\lambda = 500$, time limit=40							
w1a-2477-300	11999.706	10999.702	16499.714	10499.702	9999.711	14499.667	9999.667
TDT2-500-1000	10499.273	15999.294	10999.395	10499.368	15499.281	12499.256	9999.258
20News-8000-1000	9999.347	11499.281	11499.328	10999.454	10499.258	14499.232	9999.222
sector-6412-1000	13999.997	16999.992	12999.660	22999.999	18999.986	13499.649	9999.649
E2006-2000-1000	9999.918	14499.080	9999.284	26499.095	10499.082	21499.081	9999.077
MNIST-60000-784	19499.965	20499.886	39499.844	11999.911	16999.905	47999.705	9999.896
Gisette-3000-1000	14999.980	16499.979	9999.980	15499.980	16999.978	36499.977	9999.979
CnnCal-3000-1000	12499.980	33999.979	28999.936	15499.974	52999.977	26999.936	9999.946
Cifar-1000-1000	19999.979	31499.980	9999.979	37999.979	21499.977	42999.953	9999.974
randn-500-1000	19499.981	33499.981	19999.979	19999.980	44999.981	17999.978	9999.977

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



(a) w1a-2477-300 (b) TDT2-500-1000 (c) 20News-8000-1000 (d) sector-6412-100

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

(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 $\mathbb{E}_{\xi^{t-1}}[\|\mathbf{X}^t - \mathbf{X}^\infty\|_\mathsf{F}] \leq \dot{c}\dot{\tau}^t$.*
(c) *If $\sigma \in (\frac{1}{2}, 1)$, then there exist $\dot{c} > 0$ such that $\mathbb{E}_{\xi^{t-1}}[\|\mathbf{X}^t - \mathbf{X}^\infty\|_\mathsf{F}] \leq \frac{\dot{c}}{t^{\dot{\tau}}}$, where $\dot{\tau} \triangleq \frac{1-\sigma}{2\sigma-1} > 0$.*

Remark 4.12. *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 4.11 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. We describe the application of L_0-regularized SPCA in the sequel, while additional applications for L_1-regularized SPCA and nonnegative PCA can be found in Appendix Section G.2.

► **Compared Methods on L_0-Regularized SPCA**. 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 Penalty-based Splitting Method (PSM) (Yuan, 2024; 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 PSM(rnd). For **OBCD**, we adopt a random working set strategy with identity initialization, denoted as **OBCD-R**(id).

► **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. The code for all three applications used to reproduce the experiments can be found in the **supplemental material**.

[2] Although 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.

► **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-regularized PCA, 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.

LLM USAGE

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

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Appendix

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, $\mathcal{M} \triangleq \mathrm{St}(n, r)$ 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 $\{\mathcal{B}_1, \mathcal{B}_2, ..., \mathcal{B}_{\mathrm{C}_n^k}\}$ 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 $\mathcal{B}_i \in \mathbb{N}^k,\ \forall i \in [\mathrm{C}_n^k]$. 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: $\|\mathbf{x}\| = \|\mathbf{x}\|_2 = \sqrt{\langle \mathbf{x}, \mathbf{x}\rangle}$
- $\mathbf{x}_i$: the i-th element of vector $\mathbf{x}$
- $\mathbf{X}_{i,j}$ or $\mathbf{X}_{ij}$: the (i^{th}, j^{th}) element of matrix $\mathbf{X}$
- $\mathrm{vec}(\mathbf{X})$: $\mathrm{vec}(\mathbf{X}) \in \mathbb{R}^{nr\times 1}$, the vector formed by stacking the column vectors of $\mathbf{X}$
- $\mathrm{mat}(\mathbf{x})$: $\mathrm{mat}(\mathbf{x}) \in \mathbb{R}^{n\times r}$, Convert $\mathbf{x} \in \mathbb{R}^{nr\times 1}$ into a matrix with $\mathrm{mat}(\mathrm{vec}(\mathbf{X})) = \mathbf{X}$
- $\mathbf{X}^\mathsf{T}$: the transpose of the matrix $\mathbf{X}$
- $\mathrm{sign}(t)$: the signum function, $\mathrm{sign}(t) = 1$ if $t \geq 0$ and $\mathrm{sign}(t) = -1$ 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
- $\mathbf{X} \succeq \mathbf{0}$(or $\succ \mathbf{0}$) : the Matrix $\mathbf{X}$ is symmetric positive semidefinite (or definite)
- $\mathrm{tr}(\mathbf{A})$: Sum of the elements on the main diagonal $\mathbf{X}$: $\mathrm{tr}(\mathbf{A}) = \sum_i \mathbf{A}_{i,i}$
- $\langle \mathbf{X}, \mathbf{Y}\rangle$: 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: $(\sum_{ij} \mathbf{X}_{ij}^2)^{1/2}$
- $\|\mathbf{X}\|_{\mathsf{sp}}$: 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 $\|\mathbf{X}\|_1 = \sum_{i,j} |\mathbf{X}_{i,j}|$
- $\|\max(|\mathbf{X}|, \tau)\|_1$: the capped-$\ell_1$ norm of $\mathbf{X}$ with $\|\max(|\mathbf{X}|, \tau)\|_1 = \sum_{i,j} \max(|\mathbf{X}_{i,j}|, \tau)$
- $\nabla f(\mathbf{X})$: 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 $\iota_{\geq 0}(\mathbf{X}) = \left\{ \begin{smallmatrix} 0, & \mathbf{X} \geq \mathbf{0}; \\ \infty, & \text{else.} \end{smallmatrix} \right\}$
- $\mathbb{P}_{\Xi}(\mathbf{Z})$: 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 $\mathbb{P}_{\mathcal{M}}(\mathbf{Y}) = \arg\min_{\mathbf{X}^\mathsf{T}\mathbf{X} = \mathbf{I}_r} \|\mathbf{X} - \mathbf{Y}\|_{\mathsf{F}}^2$
- $\text{dist}(\Xi, \Xi')$: the distance between two sets with $\text{dist}(\Xi, \Xi') \triangleq \inf_{\mathbf{X} \in \Xi, \mathbf{X}' \in \Xi'} \|\mathbf{X} - \mathbf{X}'\|_{\mathsf{F}}$
- $\mathbb{A} + \mathbb{B}$, $\mathbb{A} - \mathbb{B}$: 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 $\partial F(\mathbf{X})$ with $\|\partial F(\mathbf{X})\|_{\mathsf{F}} = \inf_{\mathbf{Y} \in \partial F(\mathbf{X})} \|\mathbf{Y}\|_{\mathsf{F}}$

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 $\text{dom}(F) \triangleq \{\mathbf{X} \in \mathbb{R}^{n \times r} : |F(\mathbf{X})| < +\infty\}$. The Fréchet subdifferential of F at $\mathbf{X} \in \text{dom}(F)$ is defined as

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

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

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

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.,

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

(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 $\mathbf{Y} = \hat{\mathbf{U}} \text{Diag}(\mathbf{s}) \hat{\mathbf{V}}^\mathsf{T}$ 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

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

The tangent and norm space to $\mathcal{M}$ at $\mathbf{X} \in \mathcal{M}$ are denoted as $\mathrm{T}_{\mathbf{X}}\mathcal{M}$ and $\mathrm{N}_{\mathbf{X}}\mathcal{M}$, 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 $\mathrm{T}_{\mathbf{X}}\mathcal{M} = \{\mathbf{Y} \in \mathbb{R}^{n \times r} | \mathcal{A}_X(\mathbf{Y}) = \mathbf{0}\}$ and $\mathrm{N}_{\mathbf{X}}\mathcal{M} = \{2\mathbf{X}\boldsymbol{\Lambda} \,|\, \boldsymbol{\Lambda} = \boldsymbol{\Lambda}^\mathsf{T}, \boldsymbol{\Lambda} \in \mathbb{R}^{r \times r}\}$. 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 $\partial_{\mathcal{M}} F(\mathbf{X}) = \mathbb{P}_{\mathrm{T}_{\mathbf{X}}\mathcal{M}}(\partial F(\mathbf{X}))$. 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 $\mathbf{0}_{k,k} = \mathrm{U}_{\mathtt{B}}^\mathsf{T} \mathbf{W} \mathrm{U}_{\mathtt{B}}$ for all $\mathtt{B} \in \{\mathcal{B}_i\}_{i=1}^{\mathrm{C}_n^k}$, 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 $|\mathtt{B}| = k = 1$. 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:*

$$\|\mathbf{A} - \mathbf{A}^\mathsf{T}\|_\mathsf{F} \le 2\|\mathbf{A} - \mathbf{C}\|_\mathsf{F} + \|\mathbf{C} - \mathbf{C}^\mathsf{T}\|_\mathsf{F}.$$

Proof. We derive: $\|\mathbf{A} - \mathbf{A}^\mathsf{T}\|_\mathsf{F} = \|(\mathbf{A} - \mathbf{C}) + (\mathbf{C} - \mathbf{C}^\mathsf{T}) + (\mathbf{C}^\mathsf{T} - \mathbf{A}^\mathsf{T})\|_\mathsf{F} \overset{①}{\le} \|\mathbf{A} - \mathbf{C}\|_\mathsf{F} + \|\mathbf{C} - \mathbf{C}^\mathsf{T}\|_\mathsf{F} + \|\mathbf{C}^\mathsf{T} - \mathbf{A}^\mathsf{T}\|_\mathsf{F} = 2\|\mathbf{A} - \mathbf{C}\|_\mathsf{F} + \|\mathbf{C} - \mathbf{C}^\mathsf{T}\|_\mathsf{F}$, where step ① 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 $\mathbf{A}^\mathsf{T} = -\mathbf{A}$. We have:*

$$\det\left((\mathbf{I}_2 + \tfrac{\tau}{2}\mathbf{A})^{-1}(\mathbf{I}_k - \tfrac{\tau}{2}\mathbf{A})\right) = 1.$$

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

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

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

□

Lemma A.4. *For any $\mathbf{W} \in \mathbb{R}^{n\times n}$, we have*

$$\sum_{i=1}^{\mathrm{C}_n^k} \|\mathbf{W}(\mathcal{B}_i, \mathcal{B}_i)\|_\mathsf{F}^2 = \mathrm{C}_{n-2}^{k-2}\sum_i\sum_{j,j\neq i}\mathbf{W}_{ij}^2 + \tfrac{k}{n}\mathrm{C}_n^k\sum_i \mathbf{W}_{ii}^2.$$

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

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

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

We first focus on the term Γ_1. We have:

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

where step ① uses the fact that $\|\mathtt{B}^\mathsf{T}\mathrm{Diag}(\mathbf{w})\mathtt{B}\|_\mathsf{F}^2 = \|[\mathrm{Diag}(\mathbf{w})]_{\mathtt{B}\mathtt{B}}\|_\mathsf{F}^2 = \|\mathbf{w}_\mathtt{B}\|_2^2$ for any $\mathtt{B} \in \{\mathcal{B}_i\}_{i=1}^{\mathrm{C}_n^k}$; step ② uses the observation that $\mathbf{w}_i$ appears in the term $\sum_{i=1}^{\mathrm{C}_n^k}\|\mathbf{w}_{\mathcal{B}_i}\|_2^2$ a total of $(\mathrm{C}_n^k\cdot\frac{k}{n})$ 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:

$$\Gamma_2 = \textstyle\sum_{i=1}^{\mathrm{C}_n^k}\|\mathbf{U}_{\mathcal{B}_i}^\mathsf{T}\mathbf{W}'\mathbf{U}_{\mathcal{B}_i}\|_\mathsf{F}^2 \overset{①}{=} \sum_i\sum_{j\neq i}[\mathrm{C}_{n-2}^{k-2}(\mathbf{W}'_{ij})^2] \overset{②}{=} \mathrm{C}_{n-2}^{k-2}\textstyle\sum_i\sum_{j,j\neq i}(\mathbf{W}_{ij})^2, \quad (14)$$

where step ① uses the fact that the term $\sum_{i=1}^{\mathrm{C}_n^k}\|\mathbf{U}_{\mathcal{B}_i}^\mathsf{T}\mathbf{W}'\mathbf{U}_{\mathcal{B}_i}\|_\mathsf{F}^2$ 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. □

Lemma A.5. *Assume* $\mathbf{QR} = \mathbf{X} \in \mathbb{R}^{n\times n}$*, 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: $\mathbf{R}\mathbf{R}^\mathsf{T} \overset{①}{=} (\mathbf{Q}\mathbf{X})(\mathbf{Q}\mathbf{X})^\mathsf{T} = \mathbf{Q}\mathbf{X}\mathbf{X}^\mathsf{T}\mathbf{Q}^\mathsf{T} \overset{②}{=} \mathbf{I}$, where step ① uses $\mathbf{R} = \mathbf{Q}^\mathsf{T}\mathbf{X}$; step ② 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* $\mathrm{T}_\mathbf{X}\mathcal{M} \triangleq \{\mathbf{Y} \in \mathbb{R}^{n\times r} \,|\, \mathcal{A}_X(\mathbf{Y}) = \mathbf{0}\}$ *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:*

$$(\mathbf{G} - \tfrac{1}{2}\mathbf{X}\mathcal{A}_\mathbf{X}(\mathbf{G})) = \arg\min_{\mathbf{Y}\in\mathrm{T}_\mathbf{X}\mathcal{M}} \|\mathbf{Y} - \mathbf{G}\|_\mathsf{F}^2.$$

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* $\mathbf{X} \in \mathrm{St}(n,r)$*, it holds that*

$$\mathrm{dist}(\mathbf{0}, \partial F_\iota(\mathbf{X})) \le \mathrm{dist}(\mathbf{0}, \partial_\mathcal{M} F(\mathbf{X})).$$

Proof. We let $\mathbf{G} \in \partial F(\mathbf{X})$ and define $\mathcal{A}_\mathbf{X}(\mathbf{G}) \triangleq \mathbf{X}^\mathsf{T}\mathbf{G} + \mathbf{G}^\mathsf{T}\mathbf{X}$.

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

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

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:*

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* $\sin(\theta) = \frac{-\tan(\theta)}{\sqrt{1+\tan^2(\theta)}}$.

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. *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 $i \geq 1$, we have:

$$\sum_{t=i}^{T} w_t = \sum_{t=i}^{T}(p_t - p_{t+1}) = p_i - p_{T+1} \overset{①}{\leq} p_i, \tag{15}$$

where step ① uses $p_i \geq 0$ for all i.

Second, we obtain:

$$\begin{aligned} E_{t+1} &\overset{①}{\leq} \sqrt{E_t w_t} \\ &\overset{②}{\leq} \sqrt{\tfrac{\alpha}{2}(E_t)^2 + (w_t)^2/(2\alpha)},\ \forall \alpha > 0 \\ &\overset{③}{\leq} \sqrt{\tfrac{\alpha}{2}} \cdot E_t + w_t\sqrt{1/(2\alpha)},\ \forall \alpha > 0. \end{aligned} \tag{16}$$

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 (16) over t from i to T, we have:

$$\begin{aligned} &\textstyle\sum_{t=i}^{T} w_t\sqrt{1/(2\alpha)} \\ &\geq \{\textstyle\sum_{t=i}^{T} E_{t+1}\} - \sqrt{\tfrac{\alpha}{2}}\{\textstyle\sum_{t=i}^{T} E_t\} \\ &= \{E_{T+1} + \textstyle\sum_{t=i}^{T-1} E_{t+1}\} - \sqrt{\tfrac{\alpha}{2}}\{E_i + \textstyle\sum_{t=i}^{T-1} E_{t+1}\} \\ &= E_{T+1} - \sqrt{\tfrac{\alpha}{2}}E_i + (1 - \sqrt{\tfrac{\alpha}{2}})\textstyle\sum_{t=i}^{T-1} E_{t+1} \\ &\overset{①}{\geq} -\sqrt{\tfrac{\alpha}{2}}E_i + (1 - \sqrt{\tfrac{\alpha}{2}})\textstyle\sum_{t=i}^{T-1} E_{t+1}, \end{aligned}$$

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

$$\begin{aligned} \textstyle\sum_{t=i}^{T-1} E_{t+1} &\leq (1 - \sqrt{\tfrac{\alpha}{2}})^{-1} \cdot \{\sqrt{\tfrac{\alpha}{2}}E_i + \sqrt{\tfrac{1}{2\alpha}}\textstyle\sum_{t=i}^{T} w_t\} \\ &\overset{①}{=} E_i + 2\textstyle\sum_{t=i}^{T} w_t \\ &\overset{②}{\leq} E_i + 2p_i, \end{aligned}$$

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 (15). Letting $T \to \infty$, we conclude this lemma.

□

Lemma A.10. *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 $\breve{h}(s) \triangleq -\frac{1}{\tau} \cdot s^{-\tau}$. We derive:

$$\begin{aligned} 1 &\overset{①}{\leq} a(D_{t-1} - D_t) \cdot h(D_t) \\ &\overset{②}{\leq} a(D_{t-1} - D_t) \cdot \kappa h(D_{t-1}) \\ &\overset{③}{\leq} a\kappa \textstyle\int_{D_t}^{D_{t-1}} h(s) ds \\ &\overset{④}{=} a\kappa \cdot (\breve{h}(D_{t-1}) - \breve{h}(D_t)) \\ &\overset{⑤}{=} a\kappa \cdot \tfrac{1}{\tau} \cdot ([D_t]^{-\tau} - [D_{t-1}]^{-\tau}), \end{aligned}$$

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 $\nabla\breve{h}(s) = h(s)$; step ⑤ uses the definition of $\breve{h}(\cdot)$. This leads to:

$$[D_t]^{-\tau} - [D_{t-1}]^{-\tau} \geq \tfrac{\tau}{\kappa\alpha}. \tag{17}$$

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

$$\begin{aligned} h(D_t) > \kappa h(D_{t-1}) &\overset{①}{\Rightarrow} [D_t]^{-(\tau+1)} > \kappa \cdot [D_{t-1}]^{-(\tau+1)} \\ &\overset{②}{\Rightarrow} ([D_t]^{-(\tau+1)})^{\frac{\tau}{\tau+1}} > \kappa^{\frac{\tau}{\tau+1}} \cdot ([D_{t-1}]^{-(\tau+1)})^{\frac{\tau}{\tau+1}} \\ &\Rightarrow [D_t]^{-\tau} > \kappa^{\frac{\tau}{\tau+1}} \cdot [D_{t-1}]^{-\tau}, \end{aligned} \tag{18}$$

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:

$$\begin{aligned} [D_t]^{-\tau} - [D_{t-1}]^{-\tau} &\overset{①}{\geq} (\kappa^{\frac{\tau}{\tau+1}} - 1) \cdot [D_{t-1}]^{-\tau} \\ &\overset{②}{\geq} (\kappa^{\frac{\tau}{\tau+1}} - 1) \cdot [D_0]^{-\tau}, \end{aligned} \tag{19}$$

where step ① uses Inequality (18); step ② uses $\tau > 0$ and $D_{t-1} \leq D_0$ for all $t \geq 1$.

In view of Inequalities (17) and (19), we have:

$$[D_t]^{-\tau} - [D_{t-1}]^{-\tau} \geq \underbrace{\min(\tfrac{\tau}{\kappa\alpha}, (\kappa^{\frac{\tau}{\tau+1}} - 1) \cdot [D_0]^{-\tau})}_{\triangleq \ddot{c}}. \tag{20}$$

Telescoping Inequality (20) over t from 1 to T, we have:

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

This leads to:

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

□

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:

$$\min_{\theta} \ \tfrac{1}{2}\|\mathbf{V}\|_{\mathbf{Q}}^2 + \langle \mathbf{V}, \mathbf{P} \rangle + h(\mathbf{VZ}), \ s.t. \ \mathbf{V} \in \{\mathbf{V}_\theta^{\mathrm{rot}}, \mathbf{V}_\theta^{\mathrm{ref}}\},$$

which can be further rewritten as:

$$\bar{\theta} \in \arg\min_{\theta} \ \tfrac{1}{2}\mathrm{vec}(\mathbf{V})^{\mathsf{T}}\mathbf{Q}\mathrm{vec}(\mathbf{V}) + \langle \mathbf{V}, \mathbf{P}\rangle + h(\mathbf{V}\mathbf{Z}), \ s.t. \ \mathbf{V} \triangleq \left(\begin{smallmatrix} \pm\cos(\theta) & \sin(\theta) \\ \mp\sin(\theta) & \cos(\theta) \end{smallmatrix}\right),$$

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:

$$\begin{aligned} \min_{\theta} \quad & h\left(\cos(\theta)\mathbf{x} + \sin(\theta)\mathbf{y}\right) + a\cos(\theta) + b\sin(\theta) \\ & + c\cos^2(\theta) + d\cos(\theta)\sin(\theta) + e\sin^2(\theta), \end{aligned} \tag{21}$$

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 (21) 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 (21).

Lemma B.1. *We define $\breve{F}(\tilde{c},\tilde{s}) \triangleq a\tilde{c} + b\tilde{s} + c\tilde{c}^2 + d\tilde{c}\tilde{s} + e\tilde{s}^2 + h\left(\tilde{c}\mathbf{x} + \tilde{s}\mathbf{y}\right)$, and $w \triangleq c - e$. The optimal solution $\bar{\theta}$ to (21) can be computed as:*

$$[\cos(\bar{\theta}), \sin(\bar{\theta})] \in \arg\min_{[c,s]} \ \breve{F}(c,s), \ s.t. \ [c,s] \in \left\{[c_1,s_1],[c_2,s_2],[0,1],[0,-1]\right\},$$

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:

$$\bar{t}_+ \in \arg\min_t \ p(t) \triangleq \tfrac{a+bt}{\sqrt{1+t^2}} + \tfrac{w+dt}{1+t^2} + h(\tfrac{\mathbf{x}+t\mathbf{y}}{\sqrt{1+t^2}}), \tag{22}$$

$$\bar{t}_- \in \arg\min_t \ \tilde{p}(t) \triangleq \tfrac{-a-bt}{\sqrt{1+t^2}} + \tfrac{w+dt}{1+t^2} + h(\tfrac{-\mathbf{x}-t\mathbf{y}}{\sqrt{1+t^2}}). \tag{23}$$

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

With the identity $\sin^2(\theta) = 1 - \cos^2(\theta)$, Problem (21) can be equivalently written as:

$$\begin{aligned} \bar{\theta} \in \arg\min_{\theta} \quad & h(\cos(\theta)\mathbf{x} + \sin(\theta)\mathbf{y}) + a\cos(\theta) + b\sin(\theta) \\ & + w\cos^2(\theta) + d\cos(\theta)\sin(\theta) + e. \end{aligned} \tag{24}$$

We first consider the case $\cos(\theta) \neq 0$. By Lemma A.8, there are two possible parameterizations for $(\cos(\theta), \sin(\theta))$ in Problem (24).

Case a). $\cos(\theta) = \frac{1}{\sqrt{1+\tan^2(\theta)}}$ and $\sin(\theta) = \frac{\tan(\theta)}{\sqrt{1+\tan^2(\theta)}}$. Then Problem (21) becomes:

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

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

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

Hence the corresponding optimal trigonometric pair is

$$\cos(\bar{\theta}_+) = \tfrac{1}{\sqrt{1+(\bar{t}_+)^2}}, \ \sin(\bar{\theta}_+) = \tfrac{\bar{t}_+}{\sqrt{1+(\bar{t}_+)^2}}. \tag{25}$$

Case b). $\cos(\theta) = \frac{-1}{\sqrt{1+\tan(\theta)^2}}$ and $\sin(\theta) = \frac{-\tan(\theta)}{\sqrt{1+\tan(\theta)^2}}$. In this case, Problem (21) reduces to

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

Again letting $t = \tan\theta$, we obtain

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

Thus, the corresponding optimal trigonometric pair is

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

Combining (25) and (26), when $\cos(\theta) \neq 0$ the optimal solution $\bar{\theta}$ to (24) satisfies $[\cos(\bar{\theta}), \sin(\bar{\theta})] \in \arg\min_{c,s}\ \breve{F}(c,s),\ s.t.\ [c,s] \in \{[\cos(\bar{\theta}_+), \sin(\bar{\theta}_+)], [\cos(\bar{\theta}_-), \sin(\bar{\theta}_-)]\}$. Including the case $\cos(\theta) = 0$, that is, $[c,s] \in \{[0,1],[0,-1]\}$, the final selection rule for the optimal pair is

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

Note that $\{\cos(\bar{\theta}), \sin(\bar{\theta})\}$ uniquely determines $\bar{\theta}$, and the objective in Problem (21) depends only on $\{\cos(\theta), \sin(\theta)\}$ for some θ. Thus, it is not necessary to explicitly recover the angles $\bar{\theta}_+$ and $\bar{\theta}_-$; it suffices to work with their cosine–sine representations.

□

We describe our **BSM** to solve Problem (22); our approach can be naturally extended to tackle Problem (23). **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 $\mathbf{y}_i \neq 0$. If this is not true and there exists $\mathbf{y}_i = 0$ for some i, then $\{\mathbf{x}_i, \mathbf{y}_i\}$ 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 (22) reduces to the following problem:

$$\min_t p(t) \triangleq \tfrac{a+bt}{\sqrt{1+t^2}} + \tfrac{w+dt}{1+t^2} + \lambda\|\mathbf{x}+t\mathbf{y}\|_0. \tag{27}$$

Given the limiting subdifferential of the ℓ_0 norm function can be computed as $\partial\|t\|_0 \in \begin{cases} \mathbb{R}, & t=0; \\ \{0\}, & \text{else.} \end{cases}$ (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: $0 = \nabla p(t) = [b(1+t^2) - (a+bt)t] \cdot \sqrt{1+t^2} \cdot t^\circ + [d(1+t^2) - (w+dt)(2t)] \cdot t^\circ$, where $t^\circ = (1+t^2)^{-2}$. Since $t^\circ > 0$, 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 analytically 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 (27) 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 (22) reduces to the following problem:

$$\bar{t} \in \arg\min_t p(t) \triangleq \tfrac{a+bt}{\sqrt{1+t^2}} + \tfrac{w+dt}{1+t^2} + \tfrac{\lambda\|\mathbf{x}+t\mathbf{y}\|_1}{\sqrt{1+t^2}}. \tag{28}$$

Setting the subgradient of $p(\cdot)$ to zero yields: $0 \in \partial p(t) = t^\circ[d(1+t^2) - (w+dt)2t + (b-at) \cdot \sqrt{1+t^2}] + t^\circ\lambda \cdot \sqrt{1+t^2} \cdot [\langle \text{sign}(\mathbf{x}+t\mathbf{y}), \mathbf{y}\rangle(1+t^2) - \|\mathbf{x}+t\mathbf{y}\|_1 t]$, 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, $\text{sign}(\mathbf{x}+t\mathbf{y}) \triangleq \mathbf{o}$ 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 (28) contains at most $2r + (4r+1)\times 4$ breakpoints.

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

Since the function $h(\mathbf{x}) \triangleq \iota_{\geq 0}(\mathbf{x})$ is scale-invariant with $h(t\mathbf{x}) = h(\mathbf{x})$ forall $t \geq 0$, Problem (22) reduces to the following problem:

$$\bar{t} \in \arg\min_t p(t) \triangleq \tfrac{a+bt}{\sqrt{1+t^2}} + \tfrac{w+dt}{1+t^2},\ s.t.\ \mathbf{x}+t\mathbf{y} \geq \mathbf{0}. \tag{29}$$

We define $I \triangleq \{i|\mathbf{y}_i > 0\}$ and $J \triangleq \{i|\mathbf{y}_i < 0\}$. It is not difficult to verity that $\{x+t\mathbf{y} \geq 0\} \Leftrightarrow \{-\frac{\mathbf{x}_I}{\mathbf{y}_I} \leq t, t \leq -\frac{\mathbf{x}_J}{\mathbf{y}_J}\} \Leftrightarrow \{lb \triangleq \max(-\frac{\mathbf{x}_I}{\mathbf{y}_I}) \leq t \leq \min(-\frac{\mathbf{x}_J}{\mathbf{y}_J}) \triangleq ub\}$. 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 (29) 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 $\mathbf{Q}$, (***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:

$$\min_{\mathbf{V}\in\text{St}(2,2)} F(\mathbf{V}) \triangleq \|\mathbf{V}-\mathbf{A}\|_\text{F}^2, \text{ with } \mathbf{A} = \left(\begin{smallmatrix} 1 & 0 \\ -1 & -1 \end{smallmatrix}\right). \tag{30}$$

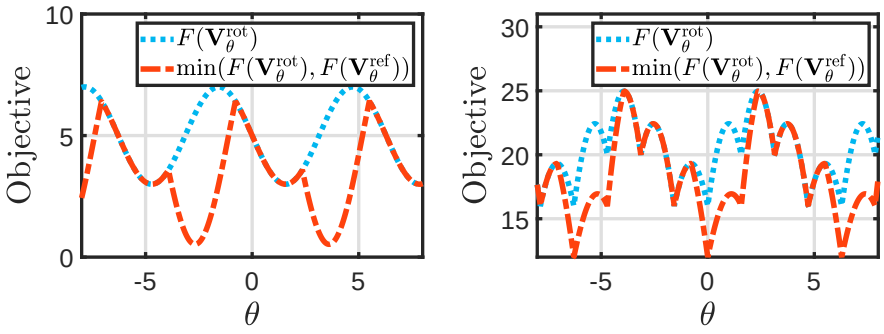
$$\min_{\mathbf{V}\in\text{St}(2,2)} F(\mathbf{V}) \triangleq \|\mathbf{V}-\mathbf{B}\|_\text{F}^2 + 5\|\mathbf{V}\|_1, \text{ with } \mathbf{B} = \left(\begin{smallmatrix} 1 & 0 \\ 1 & 2 \end{smallmatrix}\right). \tag{31}$$

Figure 2 shows the geometric visualizations of Problems (30) and (31) 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 BS_2-*point*, while the two respective examples contain 4 and 8 critical points. Therefore, the optimality condition of BS_2-points might be much stronger than that of critical points.

BS_2-points vs. Critical Point: Algorithm Instance Study. We briefly review methods that seek critical points of Problem (30) and demonstrate that they may lead to suboptimal solutions for Problem (30). As a representative example, we consider the well-known feasible method based on the Cayley transform (Wen & Yin, 2013). According to Equation (7) in (Wen & Yin, 2013), the update rule is:

$$\mathbf{X}^{t+1} \Leftarrow \mathbf{Q}\mathbf{X}^t,\ \mathbf{Q} \triangleq [(\mathbf{I}_2 + \tfrac{\tau}{2}\tilde{\mathbf{A}})^{-1}(\mathbf{I}_2 - \tfrac{\tau}{2}\tilde{\mathbf{A}})], \tag{32}$$

where $\tau \in \mathbb{R}$, and $\tilde{\mathbf{A}} \in \mathbb{R}^{2\times 2}$ is a suitable skew-symmetric matrix. Lemma A.3 shows that the matrix $\mathbf{Q}$ is always a rotation matrix. Consequently, if $\mathbf{X}^0$ is initialized as a rotation matrix with $\det(\mathbf{Q}) = 1$, all iterates $\mathbf{X}^{t+1}$ remain rotation matrices, which in general do not coincide with the optimal solution.



(a) $\min_{\mathbf{V}\in\mathrm{St}(2,2)} F(\mathbf{V}) \triangleq \|\mathbf{V}-\mathbf{A}\|_{\mathsf{F}}^2$ (b) $\min_{\mathbf{V}\in\mathrm{St}(2,2)} F(\mathbf{V}) \triangleq \|\mathbf{V}-\mathbf{B}\|_{\mathsf{F}}^2 + 5\|\mathbf{V}\|_1$

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

C.2 Computing the Matrix $\mathbf{Q}$

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* $\mathbf{Q}_2 = \mathrm{U}_{\mathrm{B}}^{\mathsf{T}}\mathbf{H}_2\mathrm{U}_{\mathrm{B}} \in \mathbb{R}^{k\times k}$. ***(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: $\mathbf{Q} \triangleq (\mathbf{Z}^{\mathsf{T}} \otimes \mathrm{U}_{\mathrm{B}})^{\mathsf{T}}\mathbf{H}(\mathbf{Z}^{\mathsf{T}} \otimes \mathrm{U}_{\mathrm{B}}) = (\mathbf{Z}^{\mathsf{T}} \otimes \mathrm{U}_{\mathrm{B}})^{\mathsf{T}}(\mathbf{H}_1 \otimes \mathbf{H}_2)(\mathbf{Z}^{\mathsf{T}} \otimes \mathrm{U}_{\mathrm{B}}) = (\mathbf{Z}^{\mathsf{T}} \otimes \mathrm{U}_{\mathrm{B}})^{\mathsf{T}}[(\mathbf{H}_1\mathbf{Z}^{\mathsf{T}}) \otimes (\mathbf{H}_2\mathrm{U}_{\mathrm{B}})] = (\mathbf{Z}\mathbf{H}_1\mathbf{Z}^{\mathsf{T}}) \otimes (\mathrm{U}_{\mathrm{B}}^{\mathsf{T}}\mathbf{H}_2\mathrm{U}_{\mathrm{B}}) = \mathbf{Q}_1 \otimes \mathbf{Q}_2$.

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

□

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* $\mathbf{Q} = L\|\mathbf{Z}\|_{\mathsf{sp}}^2 \cdot \mathbf{I}$.

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

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

□

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 $N_1 \times \mathcal{O}(n^2 r)$, 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 $\mathbf{X}^{t+1} = \mathbf{X}^t + \mathrm{U}_{\mathtt{B}}(\mathbf{V} - \mathbf{I})\mathrm{U}_{\mathtt{B}}^{\mathsf{T}}\mathbf{X}^t$, we efficiently reconstruct $\mathbf{C}\mathbf{X}^{t+1}$ by updating $\mathbf{Y}^{t+1} = \mathbf{Y}^t + \mathbf{C}\mathrm{U}_{\mathtt{B}}(\mathbf{V} - \mathbf{I})\mathrm{U}_{\mathtt{B}}^{\mathsf{T}}\mathbf{X}^t$ in $\mathcal{O}(nr)$ time. (***ii***) Computing the matrix $\mathbf{P}$ as shown in (3) involves matrix multiplication between matrices $[\nabla f(\mathbf{X}^t)]_{\mathtt{B}:} \in \mathbb{R}^{k\times r}$ and $[[\mathbf{X}^t]_{\mathtt{B}:}]^{\mathsf{T}} \in \mathbb{R}^{r\times k}$, 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 $\bar{\mathbf{V}}^t \in \arg\min_{\mathbf{V}\in\mathrm{St}(k,k)} \mathcal{K}(\mathbf{V}; \mathbf{X}^t, \mathtt{B})$ in Algorithm 1 reduces to:

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

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

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

$\min_{\mathbf{V}\in\mathrm{St}(2,2)} \langle \mathbf{V}, (\nabla f(\mathbf{X}^t)[\mathbf{X}^t]^{\mathsf{T}})_{\mathtt{BB}} \rangle + h(\mathbf{V}\mathrm{U}_{\mathtt{B}}\mathbf{X}^t)$ with $\mathtt{B} = [3, 4]$.

$\ldots$

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

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 $k \triangleq |\mathtt{B}| > 2$ 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 $|x|_0 = \begin{cases} 0, & x = 0; \\ 1, & \text{else.} \end{cases}$.

The Fréchet subdifferential of the function $h(x) = |x|_0$ at $x \in \mathrm{dom}(h)$ 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 $x \in \mathrm{dom}(h)$ 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: $\hat{\partial}h(x) = \{\xi \in \mathbb{R} : \lim_{z\to x} \inf_{z\neq x} \frac{-\langle \xi, z-x\rangle}{|z-x|} \geq 0\} = \{0\}$. (***ii***) $x = 0$. We have: $\hat{\partial}h(x) = \{\xi \in \mathbb{R} : \lim_{z\to x} \inf_{z\neq x} \frac{|z|_0 - \langle \xi, z-x\rangle}{|z-x|} \geq 0\} = \{\xi \in \mathbb{R} : \lim_{z\to x} \inf_{z\neq x} \frac{1-\langle \xi, z\rangle}{|z|} \geq 0\} = \mathbb{R}$.

We therefore conclude that $[\partial\|\mathbf{X}\|_0]_{i,j} \in \begin{cases} \mathbb{R}, & \mathbf{X}_{i,j} = 0; \\ \{0\}, & \text{else.} \end{cases}$ 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 $\mathtt{B} \in \{\mathcal{B}_i\}_{i=1}^{\mathrm{C}_n^k}$, we have:

$$
\begin{aligned}
& [\mathbf{X}^+]^\mathsf{T}\mathbf{X}^+ - \mathbf{X}^\mathsf{T}\mathbf{X} \\
\overset{①}{=}\ & [\mathbf{X} + \mathrm{U}_\mathtt{B}(\mathbf{V}-\mathbf{I}_k)\mathrm{U}_\mathtt{B}^\mathsf{T}\mathbf{X}]^\mathsf{T}[\mathbf{X} + \mathrm{U}_\mathtt{B}(\mathbf{V}-\mathbf{I}_k)\mathrm{U}_\mathtt{B}^\mathsf{T}\mathbf{X}] - \mathbf{X}^\mathsf{T}\mathbf{X} \\
=\ & \mathbf{X}^\mathsf{T}\mathrm{U}_\mathtt{B}(\mathbf{V}-\mathbf{I}_k)\mathrm{U}_\mathtt{B}^\mathsf{T}\mathbf{X} + [\mathrm{U}_\mathtt{B}(\mathbf{V}-\mathbf{I}_k)\mathrm{U}_\mathtt{B}^\mathsf{T}\mathbf{X}]^\mathsf{T}\mathbf{X} + [\mathrm{U}_\mathtt{B}(\mathbf{V}-\mathbf{I}_k)\mathrm{U}_\mathtt{B}^\mathsf{T}\mathbf{X}]^\mathsf{T}[\mathrm{U}_\mathtt{B}(\mathbf{V}-\mathbf{I}_k)\mathrm{U}_\mathtt{B}^\mathsf{T}\mathbf{X}] \\
=\ & \mathbf{X}^\mathsf{T}\mathrm{U}_\mathtt{B}\left[(\mathbf{V}-\mathbf{I}_k+\mathbf{V}^\mathsf{T}-\mathbf{I}_k) + (\mathbf{V}-\mathbf{I}_k)^\mathsf{T}\mathrm{U}_\mathtt{B}^\mathsf{T}\mathrm{U}_\mathtt{B}(\mathbf{V}-\mathbf{I}_k)\right]\mathrm{U}_\mathtt{B}^\mathsf{T}\mathbf{X} \\
\overset{②}{=}\ & \mathbf{X}^\mathsf{T}\mathrm{U}_\mathtt{B}\left[(\mathbf{V}-\mathbf{I}_k+\mathbf{V}^\mathsf{T}-\mathbf{I}_k) + (\mathbf{V}-\mathbf{I}_k)^\mathsf{T}(\mathbf{V}-\mathbf{I}_k)\right]\mathrm{U}_\mathtt{B}^\mathsf{T}\mathbf{X} \\
=\ & \mathbf{X}^\mathsf{T}\mathrm{U}_\mathtt{B}(\mathbf{V}-\mathbf{I}_k+\mathbf{V}^\mathsf{T}-\mathbf{I}_k+\mathbf{V}^\mathsf{T}\mathbf{V}-\mathbf{V}^\mathsf{T}-\mathbf{V}+\mathbf{I}_k)\mathrm{U}_\mathtt{B}^\mathsf{T}\mathbf{X} \\
=\ & \mathbf{X}^\mathsf{T}\mathrm{U}_\mathtt{B}(-\mathbf{I}_k+\mathbf{V}^\mathsf{T}\mathbf{V})\mathrm{U}_\mathtt{B}^\mathsf{T}\mathbf{X} \\
\overset{③}{=}\ & \mathbf{X}^\mathsf{T}\mathrm{U}_\mathtt{B}\cdot\mathbf{0}\cdot\mathrm{U}_\mathtt{B}^\mathsf{T}\mathbf{X} \\
=\ & \mathbf{0},
\end{aligned}
$$

where step ① uses $\mathbf{X}^+ = \mathbf{X} + \mathrm{U}_\mathtt{B}(\mathbf{V}-\mathbf{I}_k)\mathrm{U}_\mathtt{B}^\mathsf{T}\mathbf{X}$; step ② uses $\mathrm{U}_\mathtt{B}^\mathsf{T}\mathrm{U}_\mathtt{B} = \mathbf{I}_k$; 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 $\mathbf{X}^+ \triangleq \mathbf{X} + \mathrm{U}_\mathtt{B}(\mathbf{V}-\mathbf{I}_k)\mathrm{U}_\mathtt{B}^\mathsf{T}\mathbf{X}$, $\underline{\mathbf{Q}} \triangleq (\mathbf{Z}^\mathsf{T}\otimes\mathrm{U}_\mathtt{B})^\mathsf{T}\mathbf{H}(\mathbf{Z}^\mathsf{T}\otimes\mathrm{U}_\mathtt{B})$, and $\mathbf{Z} \triangleq \mathrm{U}_\mathtt{B}^\mathsf{T}\mathbf{X}$.

Part (a). We derive the following results:

$$
\begin{aligned}
\|\mathbf{X}^+ - \mathbf{X}\|_\mathbf{H}^2 &\overset{①}{=} \|\mathrm{U}_\mathtt{B}(\mathbf{V}-\mathbf{I}_k)\mathbf{Z}\|_\mathbf{H}^2 \\
&\overset{②}{=} \mathrm{vec}(\mathrm{U}_\mathtt{B}(\mathbf{V}-\mathbf{I}_k)\mathbf{Z})^\mathsf{T}\mathbf{H}\mathrm{vec}(\mathrm{U}_\mathtt{B}(\mathbf{V}-\mathbf{I}_k)\mathbf{Z}) \\
&\overset{③}{=} \mathrm{vec}(\mathbf{V}-\mathbf{I}_k)^\mathsf{T}(\mathbf{Z}^\mathsf{T}\otimes\mathrm{U}_\mathtt{B})^\mathsf{T}\mathbf{H}(\mathbf{Z}^\mathsf{T}\otimes\mathrm{U}_\mathtt{B})\mathrm{vec}(\mathbf{V}-\mathbf{I}_k) \\
&\overset{④}{=} \|\mathbf{V}-\mathbf{I}_k\|^2_{(\mathbf{Z}^\mathsf{T}\otimes\mathrm{U}_\mathtt{B})^\mathsf{T}\mathbf{H}(\mathbf{Z}^\mathsf{T}\otimes\mathrm{U}_\mathtt{B})} \\
&\overset{⑤}{=} \|\mathbf{V}-\mathbf{I}_k\|^2_{\underline{\mathbf{Q}}},
\end{aligned}
$$

where step ① uses $\mathbf{X}^+ \triangleq \mathbf{X} + \mathrm{U}_\mathtt{B}(\mathbf{V}-\mathbf{I}_k)\mathbf{Z}$; step ② uses $\|\mathbf{X}\|_\mathbf{H}^2 = \mathrm{vec}(\mathbf{X})^\mathsf{T}\mathbf{H}\mathrm{vec}(\mathbf{X})$; step ③ uses $(\mathbf{Z}^\mathsf{T}\otimes\mathbf{R})\mathrm{vec}(\mathbf{U}) = \mathrm{vec}(\mathbf{RUZ})$ 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 $\underline{\mathbf{Q}}$.

Part (b). We derive the following equalities:

$$
\begin{aligned}
\|\mathbf{X}^+ - \mathbf{X}\|_\mathsf{F}^2 &\overset{①}{=} \|\mathrm{U}_\mathtt{B}(\mathbf{V}-\mathbf{I}_k)\mathbf{Z}\|_\mathsf{F}^2 \\
&\overset{②}{=} \|(\mathbf{V}-\mathbf{I}_k)\mathbf{Z}\|_\mathsf{F}^2 \\
&= \langle(\mathbf{V}-\mathbf{I}_k)^\mathsf{T}(\mathbf{V}-\mathbf{I}_k), \mathbf{Z}\mathbf{Z}^\mathsf{T}\rangle \\
&\overset{③}{=} 2\langle\mathbf{I}_k-\mathbf{V}, \mathbf{Z}\mathbf{Z}^\mathsf{T}\rangle + \langle\mathbf{V}-\mathbf{V}^\mathsf{T}, \mathbf{Z}\mathbf{Z}^\mathsf{T}\rangle. \\
&\overset{④}{=} 2\langle\mathbf{I}_k-\mathbf{V}, \mathbf{Z}\mathbf{Z}^\mathsf{T}\rangle + 0.
\end{aligned}
$$

where step ① uses $\mathbf{X}^+ \triangleq \mathbf{X} + \mathrm{U}_\mathtt{B}(\mathbf{V}-\mathbf{I}_k)\mathbf{Z}$; step ② uses the fact that $\|\mathrm{U}_\mathtt{B}\mathbf{V}\|_\mathsf{F}^2 = \|\mathbf{V}\|_\mathsf{F}^2$ 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:

$$\begin{aligned}\|\mathbf{X}^+ - \mathbf{X}\|_{\mathsf{F}}^2 &= \|\mathrm{U}_{\mathrm{B}}(\mathbf{V}-\mathbf{I}_k)\mathrm{U}_{\mathrm{B}}^{\mathsf{T}}\mathbf{X}\|_{\mathsf{F}}^2 \\ &\overset{①}{\leq} \|\mathrm{U}_{\mathrm{B}}\|_{\mathsf{sp}}^2 \cdot \|(\mathbf{V}-\mathbf{I}_k)\mathrm{U}_{\mathrm{B}}^{\mathsf{T}}\mathbf{X}\|_{\mathsf{F}}^2 \\ &\overset{②}{\leq} \|\mathrm{U}_{\mathrm{B}}\|_{\mathsf{sp}}^2 \cdot \|\mathbf{V}-\mathbf{I}_k\|_{\mathsf{F}}^2 \cdot \|\mathrm{U}_{\mathrm{B}}^{\mathsf{T}}\|_{\mathsf{sp}}^2 \cdot \|\mathbf{X}\|_{\mathsf{sp}}^2 \\ &\overset{③}{=} \|\mathbf{V}-\mathbf{I}_k\|_{\mathsf{F}}^2 \\ &\overset{④}{=} 2\langle \mathbf{I}_k - \mathbf{V}, \mathbf{I}_k\rangle,\end{aligned}$$

where step ① and step ② uses the norm inequality that $\|\mathbf{AX}\|_{\mathsf{F}} \leq \|\mathbf{A}\|_{\mathsf{F}} \cdot \|\mathbf{X}\|_{\mathsf{sp}}$ for any $\mathbf{A}$ and $\mathbf{X}$; step ③ uses $\|\mathrm{U}_{\mathrm{B}}\|_{\mathsf{sp}} = \|\mathrm{U}_{\mathrm{B}}^{\mathsf{T}}\|_{\mathsf{sp}} = \|\mathbf{X}\|_{\mathsf{sp}} = 1$ 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 $\mathcal{K}(\mathbf{V}; \mathbf{X}^t, \mathtt{B}) \triangleq \frac{1}{2}\|\mathbf{V}-\mathbf{I}_k\|_{\mathbf{Q}+\alpha\mathbf{I}}^2 + h(\mathbf{VZ}) + \langle \mathbf{V}, [\nabla f(\mathbf{X}^t)(\mathbf{X}^t)^{\mathsf{T}}]_{\mathtt{BB}}\rangle + \ddot{c}$, where $\mathbf{Z} \triangleq \mathrm{U}_{\mathrm{B}}^{\mathsf{T}}\mathbf{X}^t$, and $\ddot{c} = h(\mathrm{U}_{\mathrm{B}^c}^{\mathsf{T}}\mathbf{X}^t) + f(\mathbf{X}^t) - \langle \mathbf{I}_k, [\nabla f(\mathbf{X}^t)(\mathbf{X}^t)^{\mathsf{T}}]_{\mathtt{BB}}\rangle$ is a constant.

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

$$\begin{aligned}&\mathcal{K}(\mathbf{V}; \mathbf{X}^t, \mathtt{B}) \\ \triangleq\ & \ddot{c} + \tfrac{1}{2}\|\mathbf{V}-\mathbf{I}_k\|_{\mathbf{Q}+\alpha\mathbf{I}_k}^2 + \langle \mathbf{V}, [\nabla f(\mathbf{X}^t)(\mathbf{X}^t)^{\mathsf{T}}]_{\mathtt{BB}}\rangle + h(\mathbf{VZ}) \\ =\ & \ddot{c} + \tfrac{1}{2}\|\mathbf{V}-\mathbf{I}_k\|_{\mathbf{Q}}^2 + \tfrac{\alpha}{2}\|\mathbf{V}-\mathbf{I}_k\|_{\mathsf{F}}^2 + \langle \mathbf{V}, [\nabla f(\mathbf{X}^t)(\mathbf{X}^t)^{\mathsf{T}}]_{\mathtt{BB}}\rangle + h(\mathbf{VZ}) \\ \overset{①}{=}\ & \ddot{c} + \tfrac{1}{2}\|\mathbf{V}\|_{\mathbf{Q}}^2 - \langle \mathbf{V}, \mathrm{mat}(\mathbf{Q}\mathrm{vec}(\mathbf{I}_k))\rangle + \tfrac{1}{2}\|\mathbf{I}_k\|_{\mathbf{Q}}^2 + \alpha\langle \mathbf{I}_k, \mathbf{I}_k - \mathbf{V}\rangle + \langle \mathbf{V}, [\nabla f(\mathbf{X}^t)(\mathbf{X}^t)^{\mathsf{T}}]_{\mathtt{BB}}\rangle + h(\mathbf{VZ}) \\ \overset{②}{=}\ & \ddot{c} + \tfrac{1}{2}\|\mathbf{V}\|_{\mathbf{Q}}^2 + \langle \mathbf{V}, \underbrace{[\nabla f(\mathbf{X}^t)(\mathbf{X}^t)^{\mathsf{T}}]_{\mathtt{BB}} - \mathrm{mat}(\mathbf{Q}\mathrm{vec}(\mathbf{I}_k)) - \alpha\mathbf{I}_k}_{\triangleq \mathbf{P}}\rangle + h(\mathbf{VZ}) + \tfrac{1}{2}\|\mathbf{I}_k\|_{\mathbf{Q}}^2,\end{aligned}$$

where step ① uses Lemma 2.2(c) that: $\frac{1}{2}\|\mathbf{V}-\mathbf{I}_k\|_{\mathsf{F}}^2 = \langle \mathbf{I}_k, \mathbf{I}_k - \mathbf{V}\rangle$; 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 $\mathbf{V} \in \mathrm{St}(k,k)$, the term $\frac{1}{2}\|\mathbf{V}\|_{\mathbf{Q}}^2$ simplifies to a constant with $\frac{1}{2}\|\mathbf{V}\|_{\mathbf{Q}}^2 = \frac{1}{2}\varsigma k$. We can deduce from (3):

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

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:

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

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: $\mathbf{\Lambda} = -\mathbf{P}^{\mathsf{T}}\bar{\mathbf{V}}^t \overset{①}{=} -[\tilde{\mathbf{U}}\mathrm{Diag}(\mathbf{s})\tilde{\mathbf{V}}^{\mathsf{T}}]^{\mathsf{T}} \cdot [-\tilde{\mathbf{U}}\tilde{\mathbf{V}}^{\mathsf{T}}] = \tilde{\mathbf{V}}\mathrm{Diag}(\mathbf{s})\tilde{\mathbf{U}}^{\mathsf{T}}\tilde{\mathbf{U}}\tilde{\mathbf{V}}^{\mathsf{T}} \overset{②}{=} \tilde{\mathbf{V}}\mathrm{Diag}(\mathbf{s})\tilde{\mathbf{V}}^{\mathsf{T}} \overset{③}{\succeq} \mathbf{0}$, where step ① 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 ② uses $\tilde{\mathbf{U}}^{\mathsf{T}}\tilde{\mathbf{U}} = \mathbf{I}_k$; step ③ 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 $\mathbf{V} \in \mathrm{St}(2,2)$ 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 $\mathbf{V}_\theta^{\mathrm{rot}}$ and Jacobi reflection matrix $\mathbf{V}_\theta^{\mathrm{ref}}$:

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

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

□

E PROOF FOR SECTION 3

```
function [Q,R] = JacobiGivensQR(X)
n = size(X,1); Q = eye(n); R = X;
for j=1:n
   for i=n:-1:(j+1)
      B = [i-1;i]; V = Givens(R(i-1,j),R(i,j));
      R(B,:) = V'*R(B,:); Q(:,B) = Q(:,B)*V;
      if (i==j+1 && R(j,j)<0)
         V = [-1 0; 0 -1]; % or V = [-1 0; 0 1];
         R(B,:) = V'*R(B,:); Q(:,B) = Q(:,B)*V;
      end
   end
end
if(R(n,n)<0)
    V = [1 0;0 -1]; R(B,:) = V'*R(B,:); Q(:,B) = Q(:,B)*V;
end

function V = Givens(a,b)
% Find a Givens rotation that V'*[a;b] = [r;0]
if (b==0)
    c = 1; s = 0;
else
    if (abs(b) > abs(a))
        tau = -a/b; s = 1/sqrt(1+tau^2); c = s*tau;
    else
        tau = -b/a; c = 1/sqrt(1+tau^2); s = c*tau;
    end
end
V = [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 $\mathbf{X} = \mathbf{QR}$, 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 $\mathbf{X} \in \mathrm{St}(n, n)$ into the form $\mathbf{X} = \mathbf{QR}$, where $\mathbf{Q} = \mathbf{X}$ and $\mathbf{R} = \mathbf{I}_n$, using a sequence of 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 $\mathbf{V} = \left[\begin{smallmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{smallmatrix}\right]$ 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 $\mathbf{V} \triangleq \left(\begin{smallmatrix} -1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$ to the two rows $\mathtt{B} = [i-1, i]$ to ensure that[3] $\mathbf{R}_{i-1,i-1} = 1$.
- **d)** Line 13-15 is executed only once when $\det(\mathbf{X}) = -1$. In such cases, we have $\mathbf{R}_{\mathtt{BB}} = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$ and $\det(\mathbf{R}_{\mathtt{BB}}) = -1$, where $\mathtt{B} = [n-1, n]$ is the two indices for the final rotation or reflection step. To ensure that the resulting $\mathbf{R}_{\mathtt{BB}}$ is an identify matrix, **Jacobi-Givens-QR** employs a reflection matrix $\mathbf{V} = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$, leading to $\mathbf{V}^\mathsf{T}\mathbf{R}_{\mathtt{BB}} = \mathbf{I}_2$.

Therefore, we establish the conclusion that any orthogonal matrix $\mathbf{X} \in \mathrm{St}(n,n)$ can be expressed as $\mathbf{D} = \mathcal{W}_{\mathrm{C}_n^k} ... \mathcal{W}_2 \mathcal{W}_1$, where $\mathcal{W}_i = \mathbf{U}_{\mathcal{B}_i} \mathcal{V}_i \mathbf{U}_{\mathcal{B}_i}^\mathsf{T} + \mathbf{U}_{\mathcal{B}_i^c} \mathbf{U}_{\mathcal{B}_i^c}^\mathsf{T}$, 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 $\mathbf{X} \in \mathrm{St}(n,r)$ and $\mathbf{X}^0 \in \mathrm{St}(n,r)$, 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 $\mathbf{X}[\mathbf{X}^0]^\mathsf{T}$ has the following singular value decomposition:

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

Therefore, we have the following equalities:

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

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

Furthermore, we derive the following results:

$$\begin{aligned}
& \mathbf{z} \in \{0,1\}^n \\
\Rightarrow\ & \mathrm{Diag}(\mathbf{z})^\mathsf{T} = \mathrm{Diag}(\mathbf{z})\mathrm{Diag}(\mathbf{z})^\mathsf{T} \\
\Rightarrow\ & \mathbf{U}[\mathrm{Diag}(\mathbf{z})^\mathsf{T} - \mathrm{Diag}(\mathbf{z})\mathrm{Diag}(\mathbf{z})^\mathsf{T}]\mathbf{U}^\mathsf{T}\mathbf{X} = \mathbf{0} \\
\overset{①}{\Rightarrow}\ & \mathbf{U}[\mathbf{V}^\mathsf{T}\mathbf{X}^0\mathbf{X}^\mathsf{T}\mathbf{U} - \mathbf{U}^\mathsf{T}\mathbf{X}(\mathbf{X}^0)^\mathsf{T}\mathbf{V}\mathbf{V}^\mathsf{T}\mathbf{X}^0\mathbf{X}^\mathsf{T}\mathbf{U}]\mathbf{U}^\mathsf{T}\mathbf{X} = \mathbf{0} \\
\Rightarrow\ & \mathbf{U}\mathbf{V}^\mathsf{T}\mathbf{X}^0\mathbf{X}^\mathsf{T}\mathbf{U}\mathbf{U}^\mathsf{T}\mathbf{X} - \mathbf{U}\mathbf{U}^\mathsf{T}\mathbf{X}(\mathbf{X}^0)^\mathsf{T}\mathbf{V}\mathbf{V}^\mathsf{T}\mathbf{X}^0\mathbf{X}^\mathsf{T}\mathbf{U}\mathbf{U}^\mathsf{T}\mathbf{X} = \mathbf{0} \\
\overset{②}{\Rightarrow}\ & \mathbf{U}\mathbf{V}^\mathsf{T}\mathbf{X}^0 - \mathbf{X} = \mathbf{0} \\
\overset{③}{\Rightarrow}\ & \bar{\mathbf{D}} \cdot \mathbf{X}^0 - \mathbf{X} = \mathbf{0},
\end{aligned}$$

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 $\bar{\mathbf{D}} \in \mathrm{St}(n,n)$ can be represented as $\bar{\mathbf{D}} = \mathcal{W}_{\mathrm{C}_n^k} ... \mathcal{W}_2 \mathcal{W}_1$, 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 $\mathcal{V}_i \in \mathrm{St}(2,2)$ (as established in the first part of this theorem), we can conclude that any matrix $\mathbf{X} \in \mathrm{St}(n,r)$ can be expressed as $\mathbf{X} = \bar{\mathbf{D}}\mathbf{X}^0 = \mathcal{W}_{\mathrm{C}_n^k} ... \mathcal{W}_2 \mathcal{W}_1 \mathbf{X}^0$.

□

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

E.2 Proof of Corollary 3.2

Proof. We denote e_i as the i-th canonical basis vector in $\mathbb{R}^n$.

We denote the set $\{\mathcal{B}_1, \mathcal{B}_2, ..., \mathcal{B}_{C_n^k}\}$ as all possible combinations of the index vectors choosing k items from n without repetition.

Part (a). Fix any $k \geq 2$. By Theorem 3.1(a) for the case $k = 2$, for every $\mathbf{D} \in \mathrm{St}(n, n)$ there exist index pairs (p_i, q_i) and matrices $\mathcal{V}_i^{(2)} \in \mathrm{St}(2, 2)$ such that

$$\mathbf{D} = \mathcal{W}_{C_n^2}^{(2)} \cdots \mathcal{W}_2^{(2)} \mathcal{W}_1^{(2)},$$

where

$$\mathcal{W}_i^{(2)} = \mathbf{I}_n + \mathbf{U}_{\mathcal{B}_i}^{(2)} \big(\mathcal{V}_j^{(2)} - \mathbf{I}_2\big) [\mathbf{U}_{\mathcal{B}_i}^{(2)}]^\top, \quad \mathbf{U}_{\mathcal{B}_i}^{(2)} = [e_{p_i}, e_{q_i}] \in \mathbb{R}^{n \times 2}.$$

We let

$$\mathcal{V}_i \triangleq \begin{pmatrix} \mathcal{V}_i^{(2)} & \mathbf{0} \\ \mathbf{0} & \mathbf{I}_{k-2} \end{pmatrix} \in \mathrm{St}(k, k), \qquad \mathcal{W}_i \triangleq \mathbf{I}_n + \mathbf{U}_{\mathcal{B}_i} \big(\mathcal{V}_i - \mathbf{I}_k\big) \mathbf{U}_{\mathcal{B}_i}^\top.$$

By construction, $\mathcal{W}_j$ acts as $\mathcal{V}_j^{(2)}$ on the two coordinates p_j, q_j and as the identity on all other coordinates, hence $\mathcal{W}_j = \mathcal{W}_j^{(2)}$ as linear operators on $\mathbb{R}^n$. Therefore

$$\mathbf{D} = \mathcal{W}_{C_n^2}^{(2)} \cdots \mathcal{W}_1^{(2)} = \mathcal{W}_{C_n^2} \cdots \mathcal{W}_1,$$

which proves the first part of this corollary for any $k \geq 2$.

Part (b). A similar argument to that used in the proof of Theorem 3.1(b) yields the second part of this corollary.

□

E.3 Proof for Theorem 3.7

Proof. We use $\bar{\mathbf{X}}$, $\ddot{\mathbf{X}}$, and $\check{\mathbf{X}}$ to denote a *global optimal point*, a BS$_k$*-point*, and a *critical point* of Problem (1), respectively.

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

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

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

$$\begin{aligned}
\mathbf{0}_{n,n} = \mathbf{G}\ddot{\mathbf{X}}^\mathsf{T} - \ddot{\mathbf{X}}\mathbf{G}^\mathsf{T} \quad &\Rightarrow \quad (\mathbf{0}_{n,n} \cdot \ddot{\mathbf{X}}) = (\mathbf{G}\ddot{\mathbf{X}}^\mathsf{T} - \ddot{\mathbf{X}}\mathbf{G}^\mathsf{T})\ddot{\mathbf{X}} \\
&\overset{①}{\Rightarrow} \quad \mathbf{0}_{n,r} = \mathbf{G} - \ddot{\mathbf{X}}\mathbf{G}^\mathsf{T}\ddot{\mathbf{X}}, \\
&\Rightarrow \quad \ddot{\mathbf{X}}^\mathsf{T} \cdot \mathbf{0}_{n,r} = \ddot{\mathbf{X}}^\mathsf{T}(\mathbf{G} - \ddot{\mathbf{X}}\mathbf{G}^\mathsf{T}\ddot{\mathbf{X}}) \\
&\overset{②}{\Rightarrow} \quad \mathbf{0}_{r,r} = \ddot{\mathbf{X}}^\mathsf{T}\mathbf{G} - \mathbf{G}^\mathsf{T}\ddot{\mathbf{X}} \\
&\Rightarrow \quad \mathbf{0}_{n,n} = \ddot{\mathbf{X}}(\ddot{\mathbf{X}}^\mathsf{T}\mathbf{G} - \mathbf{G}^\mathsf{T}\ddot{\mathbf{X}})\ddot{\mathbf{X}}^\mathsf{T} \\
&\overset{③}{\Rightarrow} \quad \mathbf{0}_{n,n} = \ddot{\mathbf{X}}\underbrace{\ddot{\mathbf{X}}^\mathsf{T}\mathbf{G}\ddot{\mathbf{X}}^\mathsf{T}}_{\triangleq \mathbf{G}^\mathsf{T}} - \underbrace{\ddot{\mathbf{X}}\mathbf{G}^\mathsf{T}\ddot{\mathbf{X}}}_{\triangleq \mathbf{G}}\ddot{\mathbf{X}}^\mathsf{T},
\end{aligned} \tag{39}$$

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 $\{\mathrm{BS_k\text{-}points}\,\ddot{\mathbf{X}}\} \supseteq \{\mathrm{global\,optimal\,points}\,\bar{\mathbf{X}}\}$ for all $k \in \{2,3,\ldots,n\}$. We define $\mathcal{X}^{\star}_{\mathtt{B}}(\mathbf{V}) \triangleq \bar{\mathbf{X}} + \mathrm{U}_{\mathtt{B}}(\mathbf{V}-\mathbf{I}_k)\mathrm{U}_{\mathtt{B}}^{\mathsf{T}}\bar{\mathbf{X}}$, and $\mathcal{K}(\mathbf{V};\mathbf{X},\mathtt{B}) \triangleq f(\mathbf{X}) + \langle \mathbf{V}-\mathbf{I}_k, [\nabla f(\mathbf{X})(\mathbf{X})^{\mathsf{T}}]_{\mathtt{BB}}\rangle + \frac{1}{2}\|\mathbf{V}-\mathbf{I}_k\|^2_{\mathbf{Q}+\alpha\mathbf{I}_k} + h(\mathrm{U}_{\mathtt{B}^c}^{\mathsf{T}}\mathbf{X}) + h(\mathbf{V}\mathrm{U}_{\mathtt{B}}^{\mathsf{T}}\mathbf{X})$. We let $\mathbf{V}_{(i)} \in \mathrm{St}(k,k)$ and $\mathcal{B}_i \in \{\mathcal{B}_i\}_{i=1}^{\mathrm{C}_n^k}$. We derive:

$$
\begin{aligned}
& \mathcal{K}(\mathbf{I}_2;\bar{\mathbf{X}},\mathcal{B}_i),\ \forall \mathcal{B}_i \\
\overset{①}{=}\ & F(\bar{\mathbf{X}}) = h(\bar{\mathbf{X}}) + f(\bar{\mathbf{X}}) \\
\overset{②}{\leq}\ & h(\mathbf{X}) + f(\mathbf{X}), \forall \mathbf{X} \in \mathrm{St}(n,r) \\
\overset{③}{\leq}\ & h(\bar{\mathbf{X}} + \mathbf{U}_{\mathcal{B}_i}(\mathbf{V}_{(i)}-\mathbf{I}_k)\mathbf{U}_{\mathcal{B}_i}^{\mathsf{T}}\bar{\mathbf{X}}) + f(\bar{\mathbf{X}} + \mathrm{U}_{\mathcal{B}_i}(\mathbf{V}_{(i)}-\mathbf{I}_k)\mathbf{U}_{\mathcal{B}_i}^{\mathsf{T}}\bar{\mathbf{X}}),\ \forall \mathbf{V}_{(i)},\ \forall \mathcal{B}_i \\
\overset{④}{=}\ & h(\mathcal{X}^{\star}_{\mathcal{B}_i}(\mathbf{V}_{(i)})) + f(\mathcal{X}^{\star}_{\mathcal{B}_i}(\mathbf{V}_{(i)})),\ \forall \mathbf{V}_{(i)},\ \forall \mathcal{B}_i \\
\overset{⑤}{=}\ & \mathcal{K}(\mathbf{V}_{(i)};\bar{\mathbf{X}},\mathcal{B}_i),\ \forall \mathbf{V}_{(i)},\ \forall \mathcal{B}_i \\
\leq\ & \min_{\mathbf{V}\in\mathrm{St}(k,k)} \mathcal{K}(\mathbf{V};\bar{\mathbf{X}},\mathcal{B}_i),\ \forall \mathcal{B}_i,
\end{aligned}
\tag{40}
$$

where step ① uses the definition of $\mathcal{K}(\mathbf{V};\mathbf{X},\mathtt{B}) \triangleq f(\mathbf{X}) + \langle \mathbf{V}-\mathbf{I}_k, [\nabla f(\mathbf{X})(\mathbf{X})^{\mathsf{T}}]_{\mathtt{BB}}\rangle + \frac{1}{2}\|\mathbf{V}-\mathbf{I}_k\|^2_{\mathbf{Q}+\alpha\mathbf{I}_k} + h(\mathrm{U}_{\mathtt{B}^c}^{\mathsf{T}}\mathbf{X}) + h(\mathbf{V}\mathrm{U}_{\mathtt{B}}^{\mathsf{T}}\mathbf{X})$; step ② uses the definition of $\bar{\mathbf{X}}$; step ③ uses the basis representation of orthogonal matrices for all $k \geq 2$, as shown in Corollary 3.2; step ④ uses the definition of $\mathcal{X}^{\star}_{\mathtt{B}}(\mathbf{V})$; step ⑤ uses the same strategy as in deriving Inequality (10). This leads to:

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

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

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

Part (d). The inclusion $\{\mathrm{critical\,points}\,\check{\mathbf{X}}\} \subseteq \{\mathrm{BS_k\text{-}points}\,\ddot{\mathbf{X}}\}$ 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 $\{\mathrm{BS_2\text{-}points}\,\ddot{\mathbf{X}}\} \subseteq \{\mathrm{global\,optimal\,points}\,\bar{\mathbf{X}}\}$ and $\{\mathrm{BS_k}\textit{-points}\,\ddot{\mathbf{X}}\} \subseteq \{\mathrm{BS_{k+1}}\textit{-points}\,\ddot{\mathbf{X}}\}$ may not always hold true.

□

F Proof for Section 4

F.1 Proof for Theorem 4.2

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

$$
\begin{aligned}
h(\mathbf{X}^{t+1}) - h(\mathbf{X}^t) &\overset{①}{=} h(\mathrm{U}_{\mathtt{B}}\bar{\mathbf{V}}^t\mathrm{U}_{\mathtt{B}}^{\mathsf{T}}\mathbf{X}^t + \mathrm{U}_{\mathtt{B}^c}\mathrm{U}_{\mathtt{B}^c}^{\mathsf{T}}\mathbf{X}^t) - h(\mathrm{U}_{\mathtt{B}}\mathrm{U}_{\mathtt{B}}^{\mathsf{T}}\mathbf{X}^t + \mathrm{U}_{\mathtt{B}^c}\mathrm{U}_{\mathtt{B}^c}^{\mathsf{T}}\mathbf{X}^t) \\
&\overset{②}{=} h(\mathrm{U}_{\mathtt{B}}\bar{\mathbf{V}}^t\mathrm{U}_{\mathtt{B}}^{\mathsf{T}}\mathbf{X}^t) + h(\mathrm{U}_{\mathtt{B}^c}\mathrm{U}_{\mathtt{B}^c}^{\mathsf{T}}\mathbf{X}^t) - h(\mathrm{U}_{\mathtt{B}}\mathrm{U}_{\mathtt{B}}^{\mathsf{T}}\mathbf{X}^t) - h(\mathrm{U}_{\mathtt{B}^c}\mathrm{U}_{\mathtt{B}^c}^{\mathsf{T}}\mathbf{X}^t) \\
&\overset{③}{=} h(\bar{\mathbf{V}}^t\mathrm{U}_{\mathtt{B}}^{\mathsf{T}}\mathbf{X}^t) - h(\mathrm{U}_{\mathtt{B}}^{\mathsf{T}}\mathbf{X}^t),
\end{aligned}
\tag{41}
$$

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

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

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

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

$$\begin{aligned} f(\mathbf{X}^{t+1}) - f(\mathbf{X}^t) &\overset{①}{\leq} \langle \mathcal{X}_{\mathtt{B}}^t(\bar{\mathbf{V}}^t) - \mathbf{X}^t, \nabla f(\mathbf{X}^t)\rangle + \tfrac{1}{2}\|\mathcal{X}_{\mathtt{B}}^t(\bar{\mathbf{V}}^t) - \mathbf{X}^t\|_{\mathbf{H}}^2 \\ &\overset{②}{=} \langle \mathrm{U}_{\mathtt{B}}(\bar{\mathbf{V}}^t - \mathbf{I}_k)\mathrm{U}_{\mathtt{B}}^{\mathsf{T}}\mathbf{X}^t, \nabla f(\mathbf{X}^t)\rangle + \tfrac{1}{2}\|\bar{\mathbf{V}}^t - \mathbf{I}_k\|_{\underline{\mathbf{Q}}}^2 \\ &\overset{③}{\leq} \langle \bar{\mathbf{V}}^t - \mathbf{I}_k, [\nabla f(\mathbf{X}^t)(\mathbf{X}^t)^{\mathsf{T}}]_{\mathtt{BB}}\rangle + \tfrac{1}{2}\|\bar{\mathbf{V}}^t - \mathbf{I}_k\|_{\mathbf{Q}}^2, \end{aligned} \tag{43}$$

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

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

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

where step ① uses Lemma 2.2(c).

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

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

$$\mathbb{E}_{\xi^t}[F(\mathbf{X}^{t+1})] - F(\mathbf{X}^t) \leq -\mathbb{E}_{\xi^t}[\tfrac{\alpha}{2}\|\bar{\mathbf{V}}^t - \mathbf{I}_k\|_{\mathsf{F}}^2].$$

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

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

where $\mathbf{X}^\infty$ 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

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

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

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

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 $\frac{\tilde{c}}{T+1} \leq \epsilon$.

□

F.2 Proof of Lemma 4.4

Proof. 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:

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

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

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

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

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

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

$$\begin{aligned} & \mathbf{0}_{k,k} = (\Upsilon_1 + \Upsilon_2) - \bar{\mathbf{V}}^t(\Upsilon_1 + \Upsilon_2)^{\mathsf{T}}\bar{\mathbf{V}}^t \\ \overset{①}{\Rightarrow} \quad & \mathbf{0}_{k,k} = \Upsilon_1 + \Omega_1 + \Omega_2 - \bar{\mathbf{V}}^t(\Upsilon_1 + \Omega_1 + \Omega_2)^{\mathsf{T}}\bar{\mathbf{V}}^t \\ \Rightarrow \quad & \Omega_1 = \bar{\mathbf{V}}^t(\Upsilon_1 + \Omega_1 + \Omega_2)^{\mathsf{T}}\bar{\mathbf{V}}^t - \Upsilon_1 - \Omega_2, \end{aligned} \tag{50}$$

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

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

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

Using the definition $\xi^t \triangleq (\mathtt{B}^1, \mathtt{B}^2, \ldots, \mathtt{B}^t)$, we have:

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

Third, we derive the following results:

$$\begin{aligned}
& \mathbb{E}_{\xi^{t+1}}[\mathrm{dist}(\mathbf{0}, \partial_{\mathcal{M}}\mathcal{K}(\mathbf{I}_k; \mathbf{X}^{t+1}, \mathtt{B}^{t+1}))] = \mathbb{E}_{\xi^{t+1}}[\|\partial_{\mathcal{M}}\mathcal{K}(\mathbf{I}_k; \mathbf{X}^{t+1}, \mathtt{B}^{t+1})\|_{\mathsf{F}}] \\
\overset{①}{=}\ & \mathbb{E}_{\xi^{t+1}}[\|\mathrm{U}_{\mathtt{B}^{t+1}}^{\mathsf{T}}\{\partial F(\mathbf{X}^{t+1})[\mathbf{X}^{t+1}]^{\mathsf{T}} \ominus \mathbf{X}^{t+1}[\partial F(\mathbf{X}^{t+1})]^{\mathsf{T}}\}\mathrm{U}_{\mathtt{B}^{t+1}}\|_{\mathsf{F}}] \\
\overset{②}{=}\ & \mathbb{E}_{\xi^t}[\|\mathrm{U}_{\mathtt{B}^t}^{\mathsf{T}}\{\partial F(\mathbf{X}^{t+1})[\mathbf{X}^{t+1}]^{\mathsf{T}} \ominus \mathbf{X}^{t+1}[\partial F(\mathbf{X}^{t+1})]^{\mathsf{T}}\}\mathrm{U}_{\mathtt{B}^t}\|_{\mathsf{F}}] \\
\overset{③}{\leq}\ & \mathbb{E}_{\xi^t}[\|\Omega_0 - \Omega_0^{\mathsf{T}}\|_{\mathsf{F}}] \\
\overset{④}{\leq}\ & 2\mathbb{E}_{\xi^t}[\|\Omega_0 - \Omega_1\|_{\mathsf{F}}] + \mathbb{E}_{\xi^t}[\|\Omega_1 - \Omega_1^{\mathsf{T}}\|_{\mathsf{F}}] \\
\overset{⑤}{=}\ & 2\mathbb{E}_{\xi^t}[\|\Omega_0 - \Omega_1\|_{\mathsf{F}}] + \mathbb{E}_{\xi^t}[\|\bar{\mathbf{V}}^t(\Upsilon_1 + \Omega_1 + \Omega_2)^{\mathsf{T}}\bar{\mathbf{V}}^t - \Upsilon_1 - \Omega_2 - \Omega_1^{\mathsf{T}}\|_{\mathsf{F}}] \\
\overset{⑥}{=}\ & 2\mathbb{E}_{\xi^t}[\|\Omega_0 - \Omega_1\|_{\mathsf{F}}] + \mathbb{E}_{\xi^t}[\|\bar{\mathbf{V}}^t\Upsilon_1^{\mathsf{T}}\bar{\mathbf{V}}^t - \Upsilon_1\|_{\mathsf{F}}] + \mathbb{E}_{\xi^t}[\|\bar{\mathbf{V}}^t\Omega_1^{\mathsf{T}}\bar{\mathbf{V}}^t - \Omega_1^{\mathsf{T}}\|_{\mathsf{F}}] \\
& + \mathbb{E}_{\xi^t}[\|\bar{\mathbf{V}}^t\Omega_2^{\mathsf{T}}\bar{\mathbf{V}}^t - \Omega_2\|_{\mathsf{F}}]
\end{aligned} \tag{52}$$

where step ① uses the definition of $\partial_{\mathcal{M}}\mathcal{K}(\mathbf{V}; \mathbf{X}^{t+1}, \mathtt{B}^{t+1})$ 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:

$$\begin{aligned}
& 2\mathbb{E}_{\xi^t}[\|\Omega_0 - \Omega_1\|_{\mathsf{F}}] \\
\leq\ & 2\mathbb{E}_{\xi^t}[\|\mathrm{U}_{\mathtt{B}^t}^{\mathsf{T}}[\nabla f(\mathbf{X}^{t+1}) + \mathbb{H}^{t+1}][\mathbf{X}^{t+1} - \mathbf{X}^t]^{\mathsf{T}}\mathrm{U}_{\mathtt{B}^t}\|_{\mathsf{F}}] \\
\overset{①}{=}\ & 2\mathbb{E}_{\xi^t}[\|\mathrm{U}_{\mathtt{B}^t}^{\mathsf{T}}[\nabla f(\mathbf{X}^{t+1}) + \mathbb{H}^{t+1}][\mathrm{U}_{\mathtt{B}}(\bar{\mathbf{V}}^t - \mathbf{I}_k)\mathrm{U}_{\mathtt{B}^t}\mathbf{X}^t]^{\mathsf{T}}\mathrm{U}_{\mathtt{B}^t}\|_{\mathsf{F}}] \\
\overset{②}{\leq}\ & 2C_F\mathbb{E}_{\xi^t}[\|\bar{\mathbf{V}}^t - \mathbf{I}_k\|_{\mathsf{F}}],
\end{aligned} \tag{53}$$

where step ① uses $\mathbf{X}^{t+1} = \mathbf{X}^t + \mathrm{U}_{\mathtt{B}}(\bar{\mathbf{V}}^t - \mathbf{I}_k)\mathrm{U}_{\mathtt{B}}^{\mathsf{T}}\mathbf{X}^t$; step ② uses the inequality $\|\mathbf{XY}\|_{\mathsf{F}} \leq \|\mathbf{X}\|_{\mathsf{F}}\|\mathbf{Y}\|_{\mathsf{sp}}$ for all $\mathbf{X}$ and $\mathbf{Y}$ repeatedly, and the fact that $\|\mathbf{G}\|_{\mathsf{F}} \leq C_F$ for all $\mathbf{X} \in \mathrm{St}(n, r)$ and all $\mathbf{G} \in \partial F(\mathbf{X})$.

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

$$\begin{aligned}
& \mathbb{E}_{\xi^t}[\|\bar{\mathbf{V}}^t\Upsilon_1^{\mathsf{T}}\bar{\mathbf{V}}^t - \Upsilon_1\|_{\mathsf{F}}] \\
\overset{①}{\leq}\ & \mathbb{E}_{\xi^t}[\|\bar{\mathbf{V}}^t\Upsilon_1^{\mathsf{T}}\bar{\mathbf{V}}^t\|_{\mathsf{F}}] + \mathbb{E}_{\xi^t}[\|\Upsilon_1\|_{\mathsf{F}}] \\
\overset{②}{\leq}\ & 2\mathbb{E}_{\xi^t}[\|\Upsilon_1\|_{\mathsf{F}}] \\
\overset{③}{=}\ & 2\mathbb{E}_{\xi^t}[\|\mathrm{mat}((\mathbf{Q} + \alpha\mathbf{I}_k)\mathrm{vec}(\bar{\mathbf{V}}^t - \mathbf{I}_k))\|_{\mathsf{F}}] \\
\leq\ & 2\|\mathbf{Q} + \alpha\mathbf{I}_k\|_{\mathsf{sp}} \cdot \mathbb{E}_{\xi^t}[\|\bar{\mathbf{V}}^t - \mathbf{I}_k)\|_{\mathsf{F}}] \\
\overset{④}{\leq}\ & 2(L_f + \alpha) \cdot \mathbb{E}_{\xi^t}[\|\bar{\mathbf{V}}^t - \mathbf{I}_k)\|_{\mathsf{F}}]
\end{aligned} \tag{54}$$

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

$$\begin{aligned}
& \mathbb{E}_{\xi^t}[\|\bar{\mathbf{V}}^t\Omega_1^{\mathsf{T}}\bar{\mathbf{V}}^t - \Omega_1^{\mathsf{T}}\|_{\mathsf{F}}] \\
\overset{①}{=} \; & \mathbb{E}_{\xi^t}[\|\bar{\mathbf{V}}^t\Omega_1^{\mathsf{T}}(\bar{\mathbf{V}}^t - \mathbf{I}_k) + (\bar{\mathbf{V}}^t - \mathbf{I}_k)\Omega_1^{\mathsf{T}}\|_{\mathsf{F}}] \\
\overset{②}{\leq} \; & 2\mathbb{E}_{\xi^t}[\|\Omega_1\|_{\mathsf{sp}} \cdot \|(\bar{\mathbf{V}}^t - \mathbf{I}_k)\|_{\mathsf{F}}] \\
\overset{③}{\leq} \; & 2\mathbb{E}_{\xi^t}[\|\nabla f(\mathbf{X}^{t+1}) + \mathbb{H}^{t+1}\|_{\mathsf{sp}} \cdot \|(\bar{\mathbf{V}}^t - \mathbf{I}_k)\|_{\mathsf{F}}] \\
\leq \; & 2C_F\mathbb{E}_{\xi^t}[\|(\bar{\mathbf{V}}^t - \mathbf{I}_k)\|_{\mathsf{F}}] \qquad (55)
\end{aligned}$$

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 $\|\Omega_1\|_{\mathsf{sp}} = \|\mathrm{U}_{\mathrm{B}^t}^{\mathsf{T}}[\nabla f(\mathbf{X}^{t+1}) + \mathbb{H}^{t+1}][\mathbf{X}^t]^{\mathsf{T}}\mathrm{U}_{\mathrm{B}^t}\|_{\mathsf{sp}} \leq \|\nabla f(\mathbf{X}^{t+1}) + \mathbb{H}^{t+1}\|_{\mathsf{sp}} \leq \|\nabla f(\mathbf{X}^{t+1}) + \mathbb{H}^{t+1}\|_{\mathsf{F}}$ which can be derived using the norm inequality.

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:

$$\begin{aligned}
& \mathbb{E}_{\xi^t}[\|\bar{\mathbf{V}}^t\Omega_2^{\mathsf{T}}\bar{\mathbf{V}}^t - \Omega_2\|_{\mathsf{F}}] \\
\overset{①}{\leq} \; & \mathbb{E}_{\xi^t}[\|\bar{\mathbf{V}}^t\Omega_2^{\mathsf{T}}\bar{\mathbf{V}}^t\|_{\mathsf{F}}] + \mathbb{E}[\|\Omega_2\|_{\mathsf{F}}] \\
\overset{②}{\leq} \; & 2\mathbb{E}_{\xi^t}[\|\Omega_2\|_{\mathsf{F}}] \\
\overset{③}{=} \; & 2\mathbb{E}_{\xi^t}[\|\mathrm{U}_{\mathrm{B}^t}^{\mathsf{T}}[\nabla f(\mathbf{X}^t) - \nabla f(\mathbf{X}^{t+1})][\mathbf{X}^t]^{\mathsf{T}}\mathrm{U}_{\mathrm{B}^t}\|_{\mathsf{F}}] \\
\overset{④}{\leq} \; & 2\mathbb{E}_{\xi^t}[\|\nabla f(\mathbf{X}^t) - \nabla f(\mathbf{X}^{t+1})\|_{\mathsf{F}}] \\
\overset{⑤}{\leq} \; & 2L_f\mathbb{E}_{\xi^t}[\|\mathbf{X}^t - \mathbf{X}^{t+1}\|_{\mathsf{F}}] \\
\overset{⑥}{\leq} \; & 2L_f\mathbb{E}_{\xi^t}[\|\bar{\mathbf{V}}^t - \mathbf{I}_k\|_{\mathsf{F}}], \qquad (56)
\end{aligned}$$

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 Lemma 2.2(c).

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

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

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

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

$$\begin{aligned}
\|\mathbf{D}^t\|_{\mathsf{F}}^2 &= \textstyle\sum_i \sum_{j\neq i}(\mathbf{D}_{ij}^t)^2 + \sum_i \sum_{j=i}(\mathbf{D}_{ij}^t)^2 \\
&\overset{①}{=} \textstyle\sum_i \sum_{j\neq i}(\mathbf{D}_{ij}^t)^2 \\
&\overset{②}{=} \textstyle\frac{1}{\mathrm{C}_{n-2}^{k-2}} \sum_{i=1}^{\mathrm{C}_n^k} \|\mathbf{U}_{\mathcal{B}_i}^{\mathsf{T}}\mathbf{D}^t\mathbf{U}_{\mathcal{B}_i}\|_{\mathsf{F}}^2 \\
&\overset{③}{=} \textstyle\frac{1}{\mathrm{C}_{n-2}^{k-2}} \cdot \mathrm{C}_n^k\mathbb{E}_{\mathrm{B}^t}[\|\mathrm{U}_{\mathrm{B}^t}^{\mathsf{T}}\mathbf{D}^t\mathrm{U}_{\mathrm{B}^t}\|_{\mathsf{F}}^2] \\
&\overset{④}{=} \gamma^2\mathbb{E}_{\mathrm{B}^t}[\|\mathrm{U}_{\mathrm{B}^t}^{\mathsf{T}}\mathbf{D}^t\mathrm{U}_{\mathrm{B}^t}\|_{\mathsf{F}}^2], \qquad (57)
\end{aligned}$$

where step ① uses the fact that $\mathbf{D}_{ii}^t = 0$ for all $i \in [n]$; step ② uses Claim (***a***) of this lemma with $\mathbf{D}_{ii}^t = 0$ for all $i \in [n]$; step ③ uses $\mathbb{E}_{\mathrm{B}^t}[\|\mathrm{U}_{\mathrm{B}^t}^{\mathsf{T}}\mathbf{W}\mathrm{U}_{\mathrm{B}^t}\|_{\mathsf{F}}^2] = \frac{1}{\mathrm{C}_n^k}\sum_{i=1}^{\mathrm{C}_n^k}\|\mathbf{U}_{\mathcal{B}_i}^{\mathsf{T}}\mathbf{W}\mathbf{U}_{\mathcal{B}_i}\|_{\mathsf{F}}^2$ as B^t are

chosen from $\{\mathcal{B}_i\}_{i=1}^{\mathrm{C}_n^k}$ randomly and uniformly; ④ uses the definition of γ. We further derive:

$$\begin{aligned}
\mathbb{E}_{\xi^t}\|\partial_{\mathcal{M}}F(\mathbf{X}^t)\|_{\mathsf{F}} &\overset{①}{=} \|\partial F(\mathbf{X}^t)\ominus \mathbf{X}^t[\partial F(\mathbf{X}^t)]^{\mathsf{T}}\mathbf{X}^t\|_{\mathsf{F}}\\
&\overset{②}{=} \|\partial F(\mathbf{X}^t)[\mathbf{X}^t]^{\mathsf{T}}\mathbf{X}^t\ominus \mathbf{X}^t[\partial F(\mathbf{X}^t)]^{\mathsf{T}}\mathbf{X}^t\|_{\mathsf{F}}\\
&\overset{③}{\leq} \|\partial F(\mathbf{X}^t)[\mathbf{X}^t]^{\mathsf{T}}\ominus \mathbf{X}^t[\partial F(\mathbf{X}^t)]^{\mathsf{T}}\|_{\mathsf{F}}\\
&\overset{④}{=} \gamma\mathbb{E}_{\mathtt{B}^t}[\|\mathrm{U}_{\mathtt{B}^t}^{\mathsf{T}}\{\partial F(\mathbf{X}^t)[\mathbf{X}^t]^{\mathsf{T}}\ominus \mathbf{X}^t[\partial F(\mathbf{X}^t)]^{\mathsf{T}}\}\mathrm{U}_{\mathtt{B}^t}\|_{\mathsf{F}}]\\
&\overset{⑤}{=} \gamma\|\partial_{\mathcal{M}}\mathcal{K}(\mathbf{I}_k;\mathbf{X}^t,\mathtt{B}^t)\|_{\mathsf{F}}
\end{aligned}\tag{58}$$

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 $\|\mathbf{A}\mathbf{X}\|_{\mathsf{F}}^2\leq\|\mathbf{A}\|_{\mathsf{F}}^2$ for all $\mathbf{X}\in\mathrm{St}(n,r)$; step ④ uses Equality (57); step ⑤ uses the definition of $\partial_{\mathcal{M}}\mathcal{K}(\mathbf{I}_k;\mathbf{X}^t,\mathtt{B}^t)$.

□

F.3 Proof of Theorem 4.6

Proof. We derive the following results:

$$\begin{aligned}
\mathbb{E}_{\xi^T}[\mathrm{dist}^2(\mathbf{0},\partial_{\mathcal{M}}F(\mathbf{X}^{T+1}))] &\overset{①}{=} \gamma^2\cdot\mathbb{E}_{\xi^{T+1}}[\mathrm{dist}^2(\mathbf{0},\partial_{\mathcal{M}}\mathcal{K}(\mathbf{I}_k;\mathbf{X}^{T+1},\mathtt{B}^{T+1}))]\\
&\overset{②}{\leq} \gamma^2\cdot\phi^2\cdot\mathbb{E}_{\xi^T}[\|\bar{\mathbf{V}}^T-\mathbf{I}_k\|_{\mathsf{F}}^2]\\
&\overset{③}{\leq} \gamma^2\cdot\phi^2\cdot\tfrac{\tilde{c}}{T+1},
\end{aligned}$$

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 4.10

Proof. By Theorem 4.2(a) and Theorem 4.6, the composite function $F_\iota(\mathbf{X})\triangleq F(\mathbf{X})+\iota_{\mathcal{M}}(\mathbf{X})$ is monotonically non-increasing, i.e., $F_\iota(\mathbf{X}^{t+1})\leq F_\iota(\mathbf{X}^t)$. Moreover, the sequence $\{\mathbf{X}^t\}_{t=1}^{\infty}$ has a limit point $\mathbf{X}^\infty$.

Since $F_\iota(\mathbf{X})\triangleq F(\mathbf{X})+\iota_{\mathcal{M}}(\mathbf{X})$ is a KL function by assumption, Proposition 4.9 implies that there exists an index $t_\star\in\mathbb{N}$ such that, for all $t\geq t_\star$,

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

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:

$$\begin{aligned}
&(F(\mathbf{X}^t)-F(\mathbf{X}^{t+1}))\varphi'(F(\mathbf{X}^t)-F(\mathbf{X}^\infty))\\
\leq\ &\underbrace{\varphi(F(\mathbf{X}^t)-F(\mathbf{X}^\infty))}_{\triangleq\varphi_t}-\varphi(F(\mathbf{X}^{t+1})-F(\mathbf{X}^\infty)).
\end{aligned}\tag{60}$$

Part (a). We derive the following inequalities:

$$
\begin{aligned}
(E_{t+1})^2 \triangleq \mathbb{E}_{\xi^t}[\|\bar{\mathbf{V}}^t - \mathbf{I}_k\|_{\mathsf{F}}^2] &\overset{①}{\leq} \tfrac{2}{\alpha} \cdot \mathbb{E}_{\xi^t}[F(\mathbf{X}^t) - F(\mathbf{X}^{t+1})] \\
&\overset{②}{\leq} \tfrac{2}{\alpha} \cdot \mathbb{E}_{\xi^t}[(\varphi_t - \varphi_{t+1}) \cdot \tfrac{1}{\varphi'(F(\mathbf{X}^t) - F(\mathbf{X}^\infty))}] \\
&\overset{③}{\leq} \tfrac{2}{\alpha} \cdot \mathbb{E}_{\xi^t}[(\varphi_t - \varphi_{t+1}) \cdot \operatorname{dist}(0, \partial F_\iota(\mathbf{X}^t))] \\
&\overset{④}{\leq} \tfrac{2}{\alpha} \cdot \mathbb{E}_{\xi^t}[(\varphi_t - \varphi_{t+1}) \cdot \|\partial_{\mathcal{M}} F(\mathbf{X}^t)\|_{\mathsf{F}}] \\
&\overset{⑤}{\leq} \tfrac{2}{\alpha} \cdot \mathbb{E}_{\xi^t}[(\varphi_t - \varphi_{t+1})\gamma \|\partial_{\mathcal{M}} \mathcal{K}(\mathbf{I}_k; \mathbf{X}^t, \mathtt{B}^t)\|_{\mathsf{F}}] \\
&\overset{⑥}{\leq} \tfrac{2}{\alpha} \cdot \mathbb{E}_{\xi^{t-1}}[(\varphi_t - \varphi_{t+1})\gamma\phi \|\bar{\mathbf{V}}^{t-1} - \mathbf{I}_k\|_{\mathsf{F}}] \\
&\overset{⑦}{=} \underbrace{\tfrac{2}{\alpha} \cdot \gamma\phi}_{\triangleq \kappa} \cdot (\varphi_t - \varphi_{t+1}) \cdot E_t,
\end{aligned}
$$

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.9 with $p_t = \kappa\varphi_t$ with $p_t \geq p_{t+1}$, for all $i \geq 1$, we have:

$$\textstyle\sum_{j=i}^{\infty} E_{j+1} \leq E_i + 2p_i.$$

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

$$D_t \leq E_t + 2p_t \overset{①}{=} E_t + 2\kappa\varphi_t \overset{②}{\leq} E_t + 2\kappa\varphi_1 \overset{③}{\leq} 2\sqrt{k} + 2\kappa\varphi_1,$$

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 4.11

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 $D_i = \sum_{j=i}^{\infty} E_{j+1}$.

We have: $D_{t-1} - D_t = E_t \leq 2\sqrt{k} \triangleq \overline{r}$.

First, we have:

$$
\begin{aligned}
\|\mathbf{X}^T - \mathbf{X}^\infty\|_{\mathsf{F}} &\overset{①}{\leq} \textstyle\sum_{j=T}^{\infty} \|\mathbf{X}^j - \mathbf{X}^{j+1}\|_{\mathsf{F}} \\
&\overset{②}{\leq} \textstyle\sum_{j=T}^{\infty} \|\bar{\mathbf{V}}^j - \mathbf{I}_k\|_{\mathsf{F}} \\
&\overset{③}{=} \textstyle\sum_{j=T}^{\infty} E_{j+1} \\
&\overset{④}{=} D_T,
\end{aligned}
$$

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:

$$\begin{aligned}\tfrac{1}{\varphi'(s^t)} &\overset{①}{\leq} \|\mathrm{dist}(\mathbf{0}, \partial F_\iota(\mathbf{X}^t))\|_{\mathsf{F}} \\ &\overset{②}{\leq} \|\partial_{\mathcal{M}} F(\mathbf{X}^t)\|_{\mathsf{F}} \\ &\overset{③}{\leq} \mathbb{E}_{\xi^t}[\gamma \|\partial_{\mathcal{M}} \mathcal{K}(\mathbf{I}_k; \mathbf{X}^t, \mathtt{B}^t)\|_{\mathsf{F}} \\ &\overset{④}{\leq} \mathbb{E}_{\xi^t}[\gamma\phi \|\bar{\mathbf{V}}^{t-1} - \mathbf{I}_k\|_{\mathsf{F}} \\ &\overset{⑤}{\leq} \gamma\phi E_t,\end{aligned}$$

where step ① uses uses Proposition 4.9 that $\mathrm{dist}(\mathbf{0}, \partial F_\iota(\mathbf{X}'))\varphi'(F_\iota(\mathbf{X}') - F_\iota(\mathbf{X}^\infty)) \geq 1$; 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 $E_t \triangleq \mathbb{E}_{\xi^{t-1}}[\|\bar{\mathbf{V}}^{t-1} - \mathbf{I}_k\|_{\mathsf{F}}^2]$.

Third, using the definition of D_t, we derive:

$$\begin{aligned}D_t &\triangleq \textstyle\sum_{i=t}^{\infty} E_{i+1} \\ &\overset{①}{\leq} E_t + 2\kappa\varphi_t \\ &\overset{②}{=} E_t + 2\kappa c \cdot \{[s^t]^\sigma\}^{\frac{1-\sigma}{\sigma}} \\ &\overset{③}{=} E_t + 2\kappa c \cdot \{c(1-\sigma) \cdot \tfrac{1}{\varphi'(s^t)}\}^{\frac{1-\sigma}{\sigma}} \\ &\overset{④}{=} E_t + 2\kappa c \cdot \{c(1-\sigma) \cdot \gamma\phi E_t\}^{\frac{1-\sigma}{\sigma}} \\ &\overset{⑤}{=} D_{t-1} - D_t + 2\kappa c \cdot \{c(1-\sigma) \cdot \gamma\phi (D_{t-1} - D_t)\}^{\frac{1-\sigma}{\sigma}} \\ &= D_{t-1} - D_t + \underbrace{2\kappa c \cdot [c(1-\sigma)\gamma\phi]^{\frac{1-\sigma}{\sigma}}}_{\triangleq \ddot{\kappa}} \cdot \{D_{t-1} - D_t\}^{\frac{1-\sigma}{\sigma}}, \end{aligned} \tag{61}$$

where step ① uses $\sum_{i=t}^{\infty} E_{i+1} \leq E_t + 2\kappa\varphi_t$, as shown in Theorem 4.10(***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):

$$\begin{aligned}0 &\leq -\tfrac{1}{\varphi'(s^t)} + \gamma\phi E_t \\ &\overset{①}{=} -\tfrac{1}{c(1-\sigma)\cdot[s^t]^{-\sigma}} + \gamma\phi E_t \\ &\overset{②}{=} -\tfrac{1}{c} + \gamma\phi E_t, \end{aligned} \tag{62}$$

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 $E_t \geq \frac{1}{c\gamma\phi} > 0$. 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 define $w \triangleq \frac{1-\sigma}{\sigma} \geq 1$. We have from Inequality (61):

$$\begin{aligned}D_t &\leq D_{t-1} - D_t + (D_{t-1} - D_t)^w \cdot \ddot{\kappa} \\ &\overset{①}{\leq} D_{t-1} - D_t + (D_{t-1} - D_t) \cdot \overline{r}^{w-1} \cdot \ddot{\kappa} \\ &\leq D_{t-1} \cdot \tfrac{\overline{r}^{w-1}\cdot\ddot{\kappa}+1}{\overline{r}^{w-1}\cdot\ddot{\kappa}+2}, \end{aligned} \tag{63}$$

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

$$D_T \leq D_1 \cdot \left(\tfrac{\overline{r}^{w-1}\cdot\ddot{\kappa}+1}{\overline{r}^{w-1}\cdot\ddot{\kappa}+2}\right)^{T-1}.$$

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 have from Inequality (61):

$$\begin{aligned} D_t &\leq D_{t-1} - D_t + \ddot{\kappa} \cdot (D_{t-1} - D_t)^{\frac{1-\sigma}{\sigma}} \\ &\overset{①}{=} \ddot{\kappa}(D_{t-1} - D_t)^w + (D_{t-1} - D_t)^w \cdot (E_t)^{1-w} \\ &\overset{②}{\leq} \ddot{\kappa}(D_{t-1} - D_t)^w + (D_{t-1} - D_t)^w \cdot \bar{r}^{1-w} \\ &= (D_{t-1} - D_t)^w \cdot \underbrace{(\ddot{\kappa} + \bar{r}^{1-w})}_{\triangleq \dot{\kappa}}, \end{aligned}$$

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 $\max_{x \in (0, \bar{r}]} x^{1-w} \leq \bar{r}^{1-w}$ if $w \in (0,1)$. We further obtain:

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

Applying Lemma A.10 with $a = \dot{\kappa}^{1/w}$, we have:

$$D_T \leq \mathcal{O}(T^{-1/\tau}) \overset{①}{=} \mathcal{O}(T^{-\frac{1}{1/w-1}}) \overset{②}{=} \mathcal{O}(T^{-\frac{1}{\frac{\sigma}{1-\sigma}-1}}) = \mathcal{O}(T^{-\frac{1-\sigma}{2\sigma-1}}),$$

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

□

G Additional Experiment Details and Results

This section provides additional experimental details and results for our proposed methods. We first introduce nonnegative PCA as an additional application, describe the datasets and experimental settings, and specify the compared baselines for ℓ_1-regularized SPCA and nonnegative PCA. We then report extended results on ℓ_0-regularized SPCA, ℓ_1-regularized SPCA, and nonnegative PCA, demonstrating the effectiveness and robustness of our algorithms across these settings.

G.1 Additional Application: Nonnegative PCA

Nonnegative PCA is an extension of PCA that imposes nonnegativity constraints on the principal vector (Zass & Shashua, 2006; Qian et al., 2021). This constraint leads to a nonnegative representation of loading vectors and it helps to capture data locality in feature selection. Nonnegative PCA can formulated as: $\min_{\mathbf{X} \in \mathrm{St}(n,r)} -\frac{1}{2}\langle \mathbf{CX}, \mathbf{X} \rangle, s.t. \mathbf{X} \geq \mathbf{0}$, where $\mathbf{C} \in \mathbb{R}^{n \times n}$ is the covariance matrix of the data.

G.2 Data Sets

To generate the data matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$, 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 $\mathbf{A} = \frac{\mathbf{A}}{\|\mathbf{A}\|_{\mathsf{F}}}$ and let $\mathbf{C} = \mathbf{A}^{\mathsf{T}}\mathbf{A} \in \mathbb{R}^{n \times n}$.

G.3 Additional Experiment Settings

► **Compared Methods on L_1-Regularized SPCA**. We benchmark **OBCD** against the following state-of-the-art algorithms: (i) Randomized Submanifold Subgradient Method (RSSM) (Cheung et al., 2024); (ii) Linearized Alternating Direction Method of Multiplier (LADMM) (He & Yuan, 2012); (iii) Riemannian Subgradient Method (RSubGrad) (Li et al., 2021); (iv) ADMM (Lai & Osher, 2014); (v) Manifold Proximal Gradient Method (ManPG) (Chen et al., 2020). For RSSM

and RSubGrad, the subgradient $\mathbf{G}^t \in \partial F(\mathbf{X}^t)$ at iterate $\mathbf{X}^t$ is taken as $\mathbf{G}^t = -\mathbf{C}\mathbf{X}^t + \lambda \mathrm{sign}(\mathbf{X}^t)$, since $\mathrm{sign}(\mathbf{X})$ is a valid subgradient of $\|\mathbf{X}\|_1$. All competing methods are initialized with a random matrix, producing five variants: RSSM(rnd), LADMM(rnd), RSubGrad(rnd), ADMM(rnd), and ManPG(rnd). For **OBCD**, we employ a random working-set rule with identity initialization, denoted by **OBCD-R**(id).

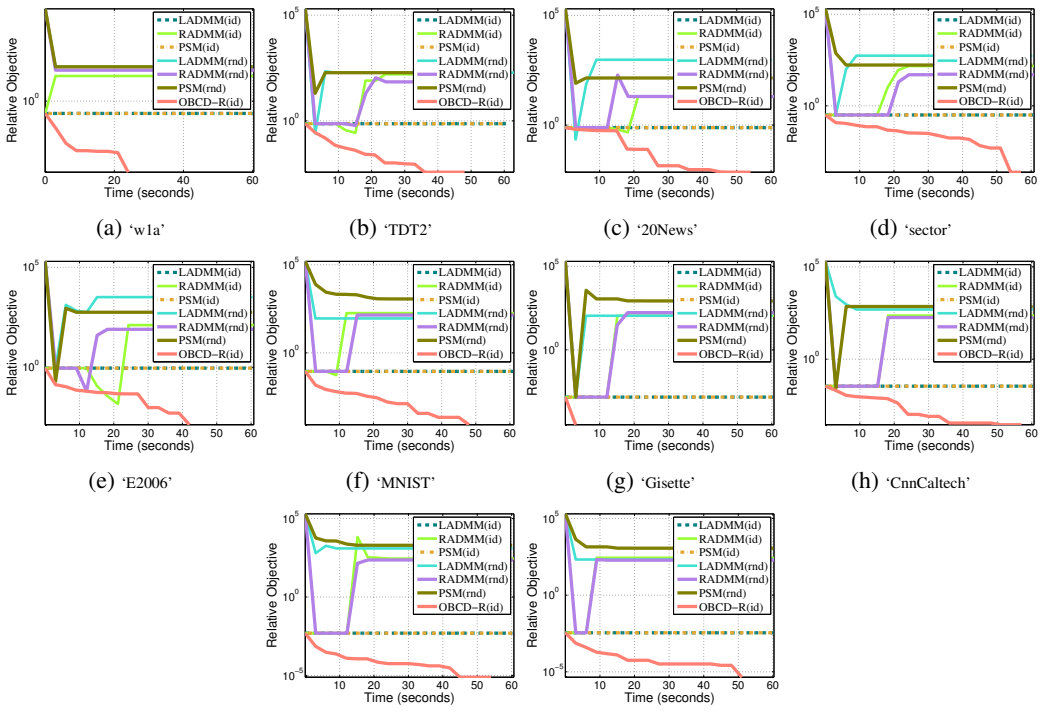
► **Compared Methods on Nonnegative PCA**. For Nonnegative PCA, we compare **OBCD** with two leading infeasible approaches: ***(i)*** Linearized ADMM (LADMM) (He & Yuan, 2012; Lai & Osher, 2014), ***(ii)*** Penalty-based Splitting Method (PSM) (Yuan, 2024; Chen, 2012), and ***(iii)*** Riemannian ADMM (RADMM) (Li et al., 2024a). Since LADMM, PSM, and RADMM are infeasible methods and may violate the nonnegativity constraints, we evaluate the quality of intermediate solutions using a surrogate objective, $f(\mathbf{X}) + 1000\|\min(\mathbf{0}, \mathbf{X})\|_{\mathsf{F}}$ with $\mathbf{X} \in \mathrm{St}(n, r)$, which penalizes any violation of feasibility.

G.4 Additional Experiment Results

► **Results on L_0-Regularized SPCA**. For $\lambda \in \{10, 50, 100, 500\}$, Figures 3-6 present the convergence curves of the compared methods on L_0-regularized SPCA. Across all setting, **OBCD-R** consistently achieves lower objective values than competing methods, further reinforcing the conclusions drawn in the main paper.

► **Results on L_1-Regularized SPCA**. For $\lambda \in \{10, 50, 100, 500\}$, Table 2 and Figures 7-10 report objective values obtained by all methods with $r = 20$. Two observations follow. ***(i)*** ManPG is generally faster than LADMM, ADMM and RSubGrad, which aligns with the findings reported in (Chen et al., 2020). ***(ii)*** **OBCD-R** consistently achieves lower objective values compared with {LADMM, ADMM, RSubGrad, ManPG}, demonstrating its superior solution quality.

► **Results on Nonnegative PCA**. For $r \in \{10, 20, 40, 80\}$, Table 3 reports objective values and feasibility violations measured by $\|\min(\mathbf{0}, \mathbf{X})\|_{\mathsf{F}}$, while Figures 11-14 show the surrogate objective $f(\mathbf{X}) + 1000\|\min(\mathbf{0}, \mathbf{X})\|_{\mathsf{F}}$. Two key conclusions can be drawn. ***(i)*** The proposed methods generally achieve the best overall performance, and **OBCD-R** often substantially outperforms LADMM, PSM, and RADMM by locating stronger stationary points.

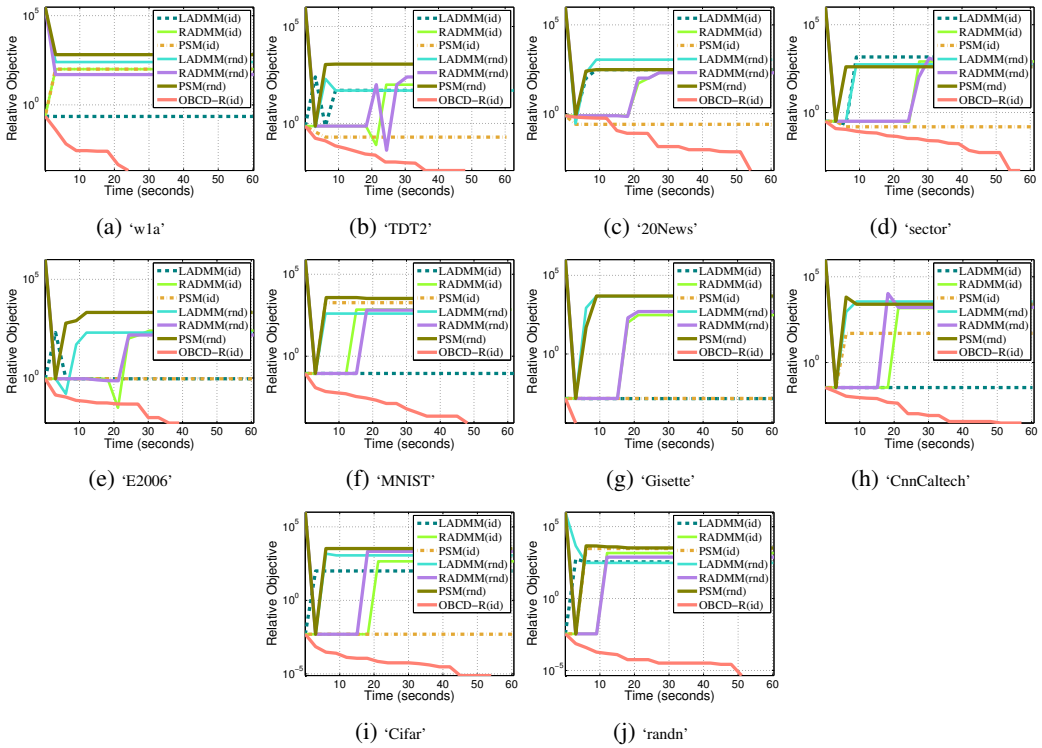


(a) 'w1a' (b) 'TDT2' (c) '20News' (d) 'sector'

(e) 'E2006' (f) 'MNIST' (g) 'Gisette' (h) 'CnnCaltech'

(i) 'Cifar' (j) 'randn'

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

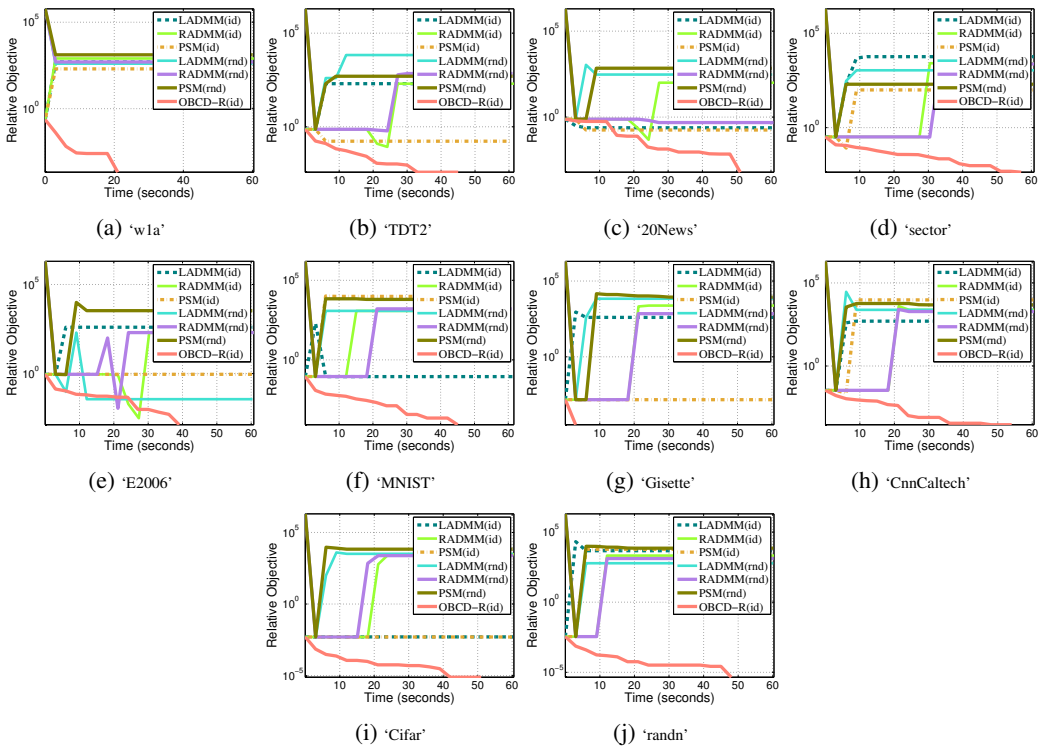


(a) 'w1a' (b) 'TDT2' (c) '20News' (d) 'sector'

(e) 'E2006' (f) 'MNIST' (g) 'Gisette' (h) 'CnnCaltech'

(i) 'Cifar' (j) 'randn'

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

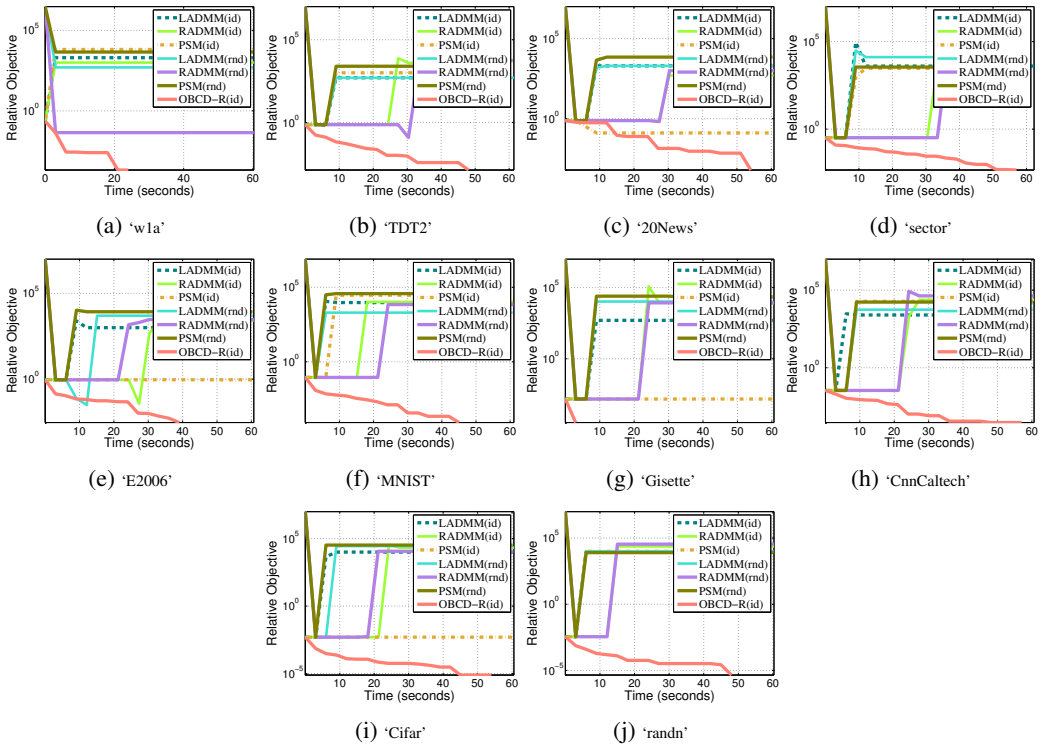


(a) 'w1a' (b) 'TDT2' (c) '20News' (d) 'sector'

(e) 'E2006' (f) 'MNIST' (g) 'Gisette' (h) 'CnnCaltech'

(i) 'Cifar' (j) 'randn'

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



(a) 'w1a' (b) 'TDT2' (c) '20News' (d) 'sector'

(e) 'E2006' (f) 'MNIST' (g) 'Gisette' (h) 'CnnCaltech'

(i) 'Cifar' (j) 'randn'

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

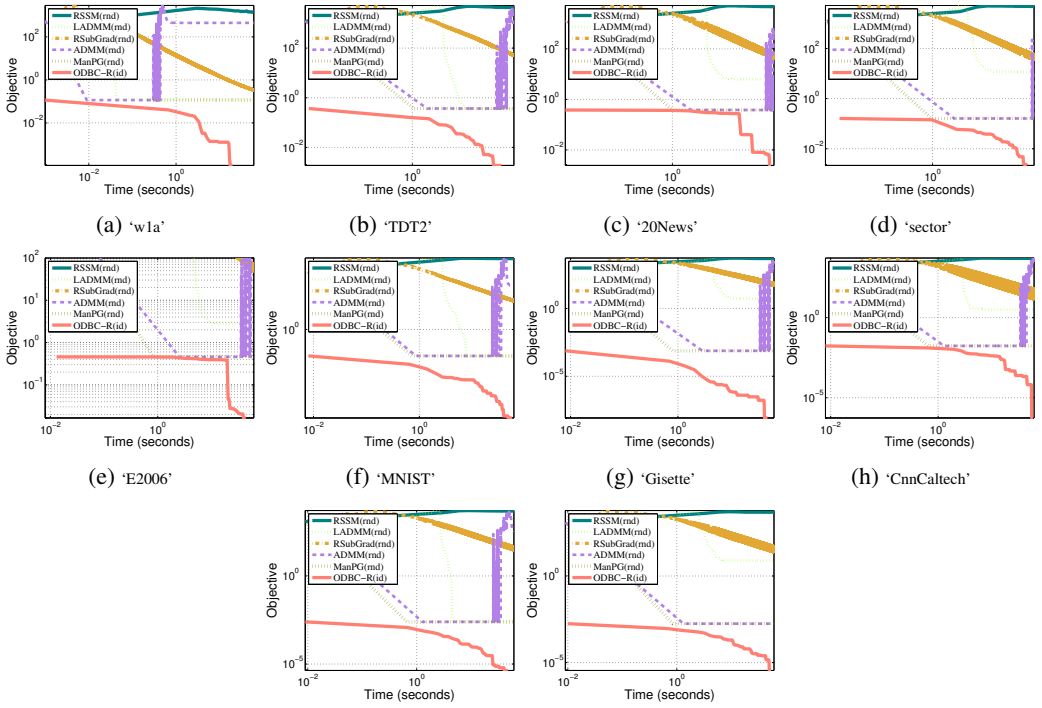
data-m-n	RSSM (rnd)	LADMM (rnd)	RSubGrad (rnd)	ADMM (rnd)	ManPG (rnd)	OBCD-R (id)
$r = 20$, $\lambda = 10$, time limit=60						
w1a-2477-300	1676.362	199.961	207.918	648.546	199.949	199.833
TDT2-500-1000	4798.905	199.997	376.695	2756.315	199.999	199.636
20News-8000-1000	5099.667	203.159	458.525	2976.634	199.997	199.673
sector-6412-1000	5088.999	211.558	257.937	2646.919	199.990	199.848
E2006-2000-1000	4791.094	201.933	240.895	2873.292	200.000	199.541
MNIST-60000-784	4491.492	199.990	304.146	3077.644	199.992	199.950
Gisette-3000-1000	5096.530	203.597	361.631	3054.472	199.990	199.989
CnnCaltech-3000-1000	5274.750	203.177	287.583	2952.906	199.990	199.977
Cifar-1000-1000	5326.610	199.990	452.860	3007.068	199.990	199.987
randn-500-1000	5299.246	207.757	267.307	2908.559	199.990	199.988

data-m-n	RSSM (rnd)	LADMM (rnd)	RSubGrad (rnd)	ADMM (rnd)	ManPG (rnd)	OBCD-R (id)
$r = 20$, $\lambda = 50$, time limit=60						
w1a-2477-300	11896.991	1017.039	1014.312	1948.020	999.949	999.833
TDT2-500-1000	24811.350	1142.577	5689.161	13596.188	999.999	999.643
20News-8000-1000	25660.045	1085.026	4852.847	15234.296	999.997	999.673
sector-6412-1000	25685.661	1076.243	5056.712	13985.491	999.990	999.834
E2006-2000-1000	23945.851	1085.356	4102.980	13800.413	1000.000	999.933
MNIST-60000-784	22829.255	1036.685	3035.519	15166.657	999.992	999.949
Gisette-3000-1000	25696.928	1125.509	4866.266	15083.925	999.990	999.989
CnnCaltech-3000-1000	26443.995	1075.923	5648.585	14435.979	999.990	999.977
Cifar-1000-1000	26174.415	1101.272	6080.349	14828.673	999.990	999.987
randn-500-1000	25917.437	1237.580	4616.156	14999.881	999.990	999.988

data-m-n	RSSM (rnd)	LADMM (rnd)	RSubGrad (rnd)	ADMM (rnd)	ManPG (rnd)	OBCD-R (id)
$r = 20$, $\lambda = 100$, time limit=60						
w1a-2477-300	25212.531	2024.330	2142.546	4172.640	1999.949	1999.833
TDT2-500-1000	49303.568	2210.215	13770.257	27221.640	1999.999	1999.636
20News-8000-1000	52028.247	2204.356	12741.678	30561.467	1999.997	1999.673
sector-6412-1000	51434.623	2222.103	17521.186	27816.620	1999.990	1999.834
E2006-2000-1000	48063.148	2140.058	11210.402	27411.269	2000.000	1999.933
MNIST-60000-784	46090.059	2057.976	11107.393	30906.421	1999.992	1999.949
Gisette-3000-1000	51396.503	2202.300	15971.871	30698.736	1999.990	1999.989
CnnCaltech-3000-1000	53046.484	2230.728	9917.898	29326.239	1999.990	1999.977
Cifar-1000-1000	52183.021	2282.490	16736.350	30070.764	1999.990	1999.987
randn-500-1000	52275.431	2309.568	14891.818	30522.549	1999.990	1999.988

data-m-n	RSSM (rnd)	LADMM (rnd)	RSubGrad (rnd)	ADMM (rnd)	ManPG (rnd)	OBCD-R (id)
$r = 20$, $\lambda = 500$, time limit=60						
w1a-2477-300	144765.556	9999.940	26452.425	14711.906	9999.949	9999.834
TDT2-500-1000	243550.365	11006.292	177896.188	137815.999	9999.999	9999.636
20News-8000-1000	257513.893	10188.884	193633.121	152343.022	9999.997	9999.675
sector-6412-1000	260801.229	9999.915	199887.443	138927.601	9999.990	9999.834
E2006-2000-1000	236514.992	10535.514	135563.372	143898.385	10000.000	9999.933
MNIST-60000-784	228035.432	10306.371	146677.728	145588.796	9999.992	9999.948
Gisette-3000-1000	261983.906	10313.107	202913.350	152724.051	9999.990	9999.989
CnnCaltech-3000-1000	259056.451	10418.351	166856.613	149325.559	9999.990	9999.977
Cifar-1000-1000	262258.151	10874.860	195776.730	150353.857	9999.990	9999.987
randn-500-1000	257825.619	10219.431	80831.264	137050.323	9999.990	9999.988

Table 2: Comparisons of objective values for L_1-regularized SPCA. The 1^{st}, 2^{nd}, and 3^{rd} best results are colored with red, green and blue, respectively.

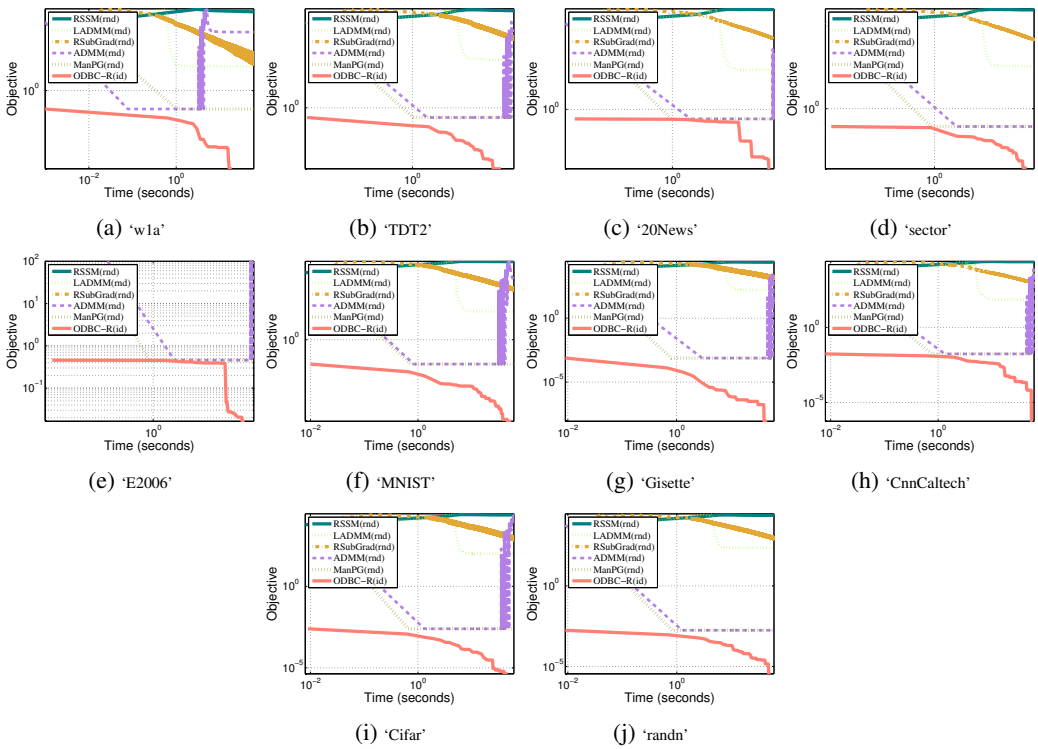


(a) 'w1a' (b) 'TDT2' (c) '20News' (d) 'sector'

(e) 'E2006' (f) 'MNIST' (g) 'Gisette' (h) 'CnnCaltech'

(i) 'Cifar' (j) 'randn'

Figure 7: The convergence curve for solving L_1-regularized SPCA with $\lambda = 10$.

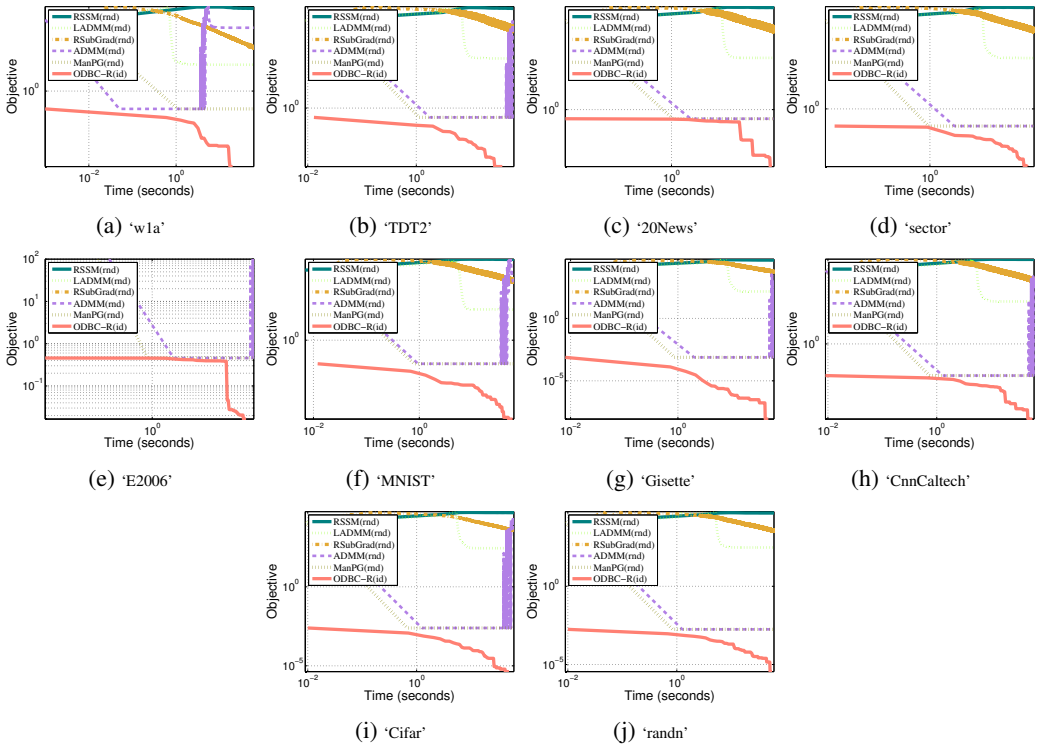


(a) 'w1a' (b) 'TDT2' (c) '20News' (d) 'sector'

(e) 'E2006' (f) 'MNIST' (g) 'Gisette' (h) 'CnnCaltech'

(i) 'Cifar' (j) 'randn'

Figure 8: The convergence curve for solving L_1-regularized SPCA with $\lambda = 50$.

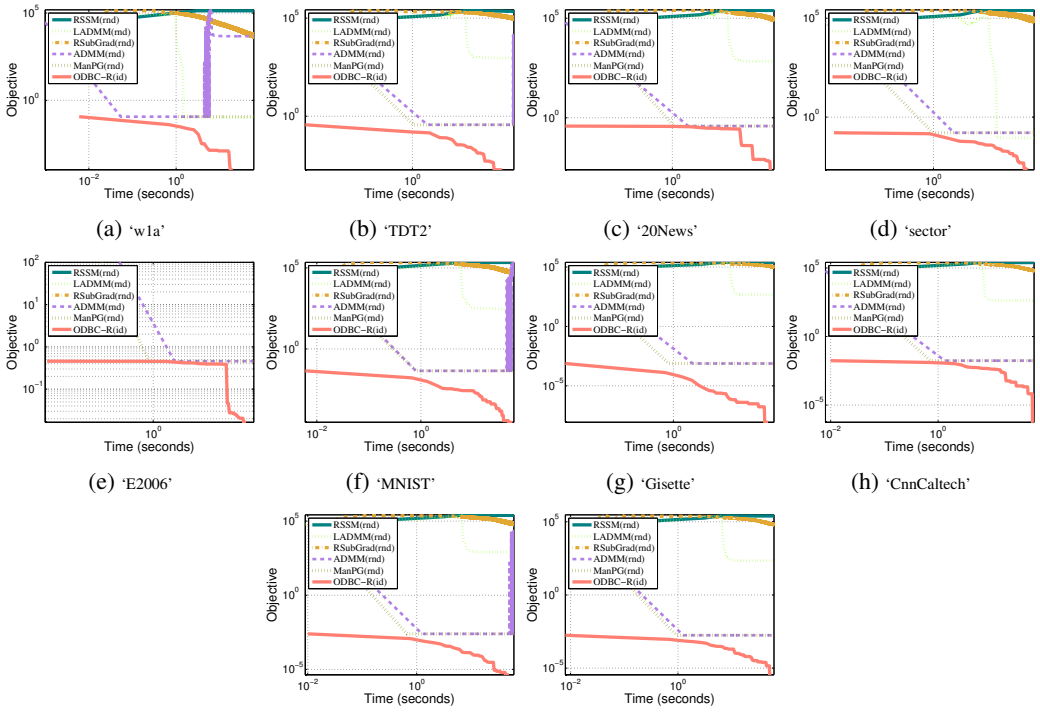


(a) 'w1a' (b) 'TDT2' (c) '20News' (d) 'sector'

(e) 'E2006' (f) 'MNIST' (g) 'Gisette' (h) 'CnnCaltech'

(i) 'Cifar' (j) 'randn'

Figure 9: The convergence curve for solving L_1-regularized SPCA with $\lambda = 100$.



(a) 'w1a' (b) 'TDT2' (c) '20News' (d) 'sector'

(e) 'E2006' (f) 'MNIST' (g) 'Gisette' (h) 'CnnCaltech'

(i) 'Cifar' (j) 'randn'

Figure 10: The convergence curve for solving L_1-regularized SPCA with $\lambda = 500$.

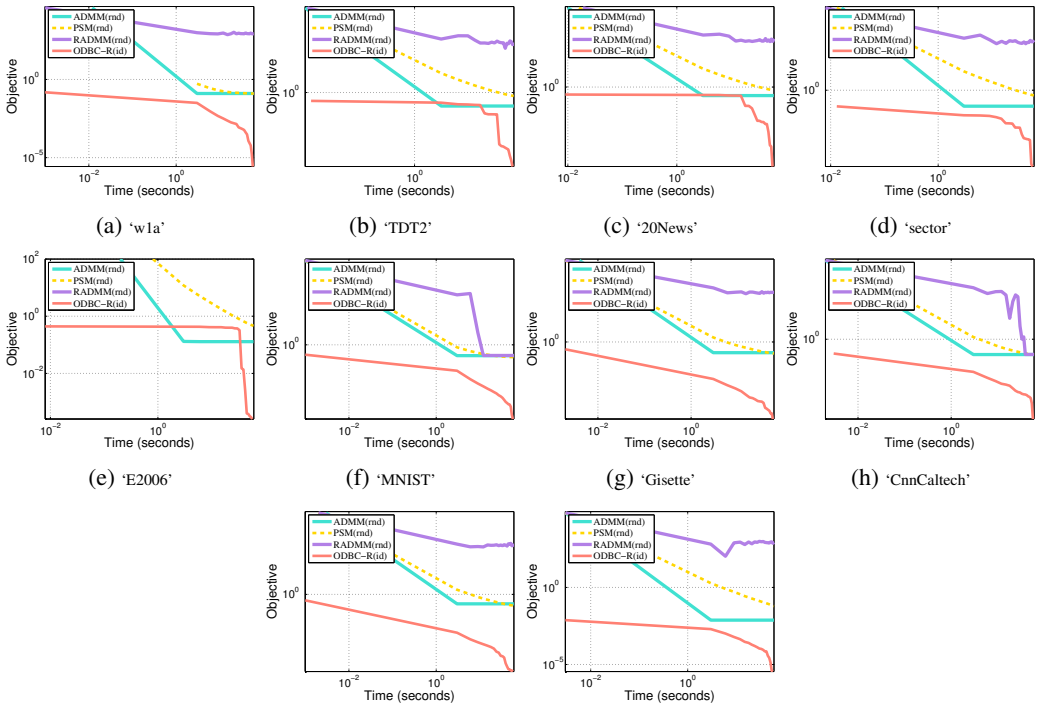
data-m-n	ADMM (rnd)	PSM (rnd)	RADMM (rnd)	OBCD-R(id) (id)
$r = 10$, time limit=60				
w1a-2477-300	-4.08e-02, 0e+00	-4.71e-02, 0e+00	-1.11e-02, 0e+00	-1.67e-01, 7e-15
TDT2-500-1000	-1.64e-01, 0e+00	-6.70e-02, 0e+00	-2.82e-03, 0e+00	-3.32e-01, 4e-15
20News-8000-1000	-4.82e-02, 0e+00	-9.14e-02, 0e+00	-8.43e-03, 0e+00	-3.49e-01, 2e-14
sector-6412-1000	-5.70e-03, 0e+00	-5.84e-03, 0e+00	-3.30e-03, 0e+00	-1.21e-01, 1e-15
E2006-2000-1000	-3.13e-01, 0e+00	-3.39e-01, 0e+00	-6.71e-03, 0e+00	-4.42e-01, 1e-14
MNIST-60000-784	-3.57e-02, 0e+00	-9.10e-02, 0e+00	-3.00e-02, 0e+00	-2.78e-01, 2e-14
Gisette-3000-1000	-1.41e-01, 0e+00	-2.34e-01, 0e+00	-6.84e-02, 0e+00	-3.72e-01, 2e-18
CnnCaltech-3000-1000	-2.28e-02, 0e+00	-6.58e-02, 0e+00	-2.10e-02, 0e+00	-1.38e-01, 0e+00
Cifar-1000-1000	-1.73e-01, 0e+00	-2.91e-01, 0e+00	-7.86e-02, 0e+00	-4.47e-01, 0e+00
randn-500-1000	-4.91e-03, 0e+00	-5.10e-03, 0e+00	-4.77e-03, 0e+00	-1.24e-02, 2e-14

data-m-n	ADMM (rnd)	PSM (rnd)	RADMM (rnd)	OBCD-R (id)
$r = 20$, time limit=60				
w1a-2477-300	-3.73e-02, 0e+00	-5.36e-02, 0e+00	-3.68e-02, 0e+00	-2.17e-01, 3e-15
TDT2-500-1000	-1.73e-03, 0e+00	-9.53e-02, 0e+00	-5.01e-03, 0e+00	-3.71e-01, 2e-15
20News-8000-1000	-1.31e-03, 0e+00	-3.14e-02, 0e+00	-7.71e-03, 0e+00	-3.78e-01, 4e-15
sector-6412-1000	-9.91e-03, 0e+00	-1.55e-02, 0e+00	-1.17e-02, 0e+00	-1.67e-01, 4e-15
E2006-2000-1000	-1.20e-03, 0e+00	-3.56e-01, 0e+00	-1.55e-03, 0e+00	-4.62e-01, 1e-14
MNIST-60000-784	-1.70e-02, 0e+00	-9.40e-02, 0e+00	-3.47e-02, 0e+00	-2.95e-01, 2e-14
Gisette-3000-1000	-2.23e-02, 0e+00	-2.31e-01, 0e+00	-6.05e-02, 0e+00	-3.80e-01, 7e-19
CnnCaltech-3000-1000	-1.05e-02, 0e+00	-6.87e-02, 0e+00	-3.34e-02, 0e+00	-1.52e-01, 2e-26
Cifar-1000-1000	-2.37e-02, 0e+00	-2.87e-01, 0e+00	-1.12e-01, 0e+00	-4.54e-01, 0e+00
randn-500-1000	-1.00e-02, 0e+00	-9.90e-03, 0e+00	-9.55e-03, 0e+00	-2.11e-02, 2e-14

data-m-n	ADMM (rnd)	PSM (rnd)	RADMM (rnd)	OBCD-R (id)
$r = 40$, time limit=60				
w1a-2477-300	-6.45e-02, 0e+00	-1.07e-01, 0e+00	-8.56e-02, 0e+00	-3.00e-01, 7e-15
TDT2-500-1000	-3.50e-02, 0e+00	-9.89e-02, 0e+00	-3.57e-02, 0e+00	-4.09e-01, 6e-15
20News-8000-1000	-1.92e-02, 0e+00	-3.43e-02, 0e+00	-1.11e-01, 0e+00	-4.14e-01, 2e-14
sector-6412-1000	-8.70e-02, 0e+00	-2.38e-02, 0e+00	-3.70e-02, 0e+00	-2.25e-01, 4e-15
E2006-2000-1000	-8.36e-03, 0e+00	-3.64e-01, 0e+00	-2.68e-02, 0e+00	-4.75e-01, 2e-14
MNIST-60000-784	-2.09e-02, 0e+00	-1.09e-01, 0e+00	-4.67e-02, 0e+00	-2.89e-01, 3e-14
Gisette-3000-1000	-2.59e-02, 0e+00	-2.63e-01, 0e+00	-1.47e-01, 0e+00	-3.69e-01, 6e-20
CnnCaltech-3000-1000	-2.03e-02, 0e+00	-8.75e-02, 0e+00	-4.74e-02, 0e+00	-1.49e-01, 0e+00
Cifar-1000-1000	-2.65e-02, 0e+00	-3.25e-01, 0e+00	-1.60e-01, 0e+00	-4.43e-01, 0e+00
randn-500-1000	-2.01e-02, 0e+00	-2.03e-02, 0e+00	-2.00e-02, 0e+00	-3.08e-02, 5e-16

data-m-n	ADMM (rnd)	PSM (rnd)	RADMM (rnd)	OBCD-R (id)
$r = 80$, time limit=60				
w1a-2477-300	-1.28e-01, 0e+00	-1.70e-01, 0e+00	-1.34e-01, 0e+00	-3.90e-01, 1e-16
TDT2-500-1000	-9.80e-02, 0e+00	-4.97e-02, 0e+00	-4.55e-02, 0e+00	-4.49e-01, 2e-14
20News-8000-1000	-2.93e-02, 0e+00	-3.04e-02, 0e+00	-2.23e-02, 0e+00	-4.47e-01, 3e-14
sector-6412-1000	-7.99e-02, 0e+00	-3.82e-02, 0e+00	-3.39e-02, 0e+00	-2.96e-01, 5e-15
E2006-2000-1000	-3.09e-03, 0e+00	-3.31e-01, 0e+00	-1.39e-01, 0e+00	-4.89e-01, 2e-14
MNIST-60000-784	-5.06e-02, 0e+00	-9.95e-02, 0e+00	-8.13e-02, 0e+00	-3.03e-01, 3e-14
Gisette-3000-1000	-6.51e-02, 0e+00	-2.64e-01, 0e+00	-2.35e-01, 0e+00	-3.56e-01, 0e+00
CnnCaltech-3000-1000	-4.77e-02, 0e+00	-1.02e-01, 0e+00	-8.91e-02, 0e+00	-1.61e-01, 0e+00
Cifar-1000-1000	-6.69e-02, 0e+00	-3.21e-01, 0e+00	-2.29e-01, 0e+00	-4.24e-01, 0e+00
randn-500-1000	-4.03e-02, 0e+00	-4.02e-02, 0e+00	-3.95e-02, 0e+00	-5.31e-02, 3e-14

Table 3: Comparisons of objective values and the violation of the nonnegative constraints ($\|\min(\mathbf{0}, \mathbf{X})\|_\mathsf{F}$) for nonnegative PCA for all the compared methods. The 1^{st}, 2^{nd}, and 3^{rd} best results are colored with red, green and blue, respectively.

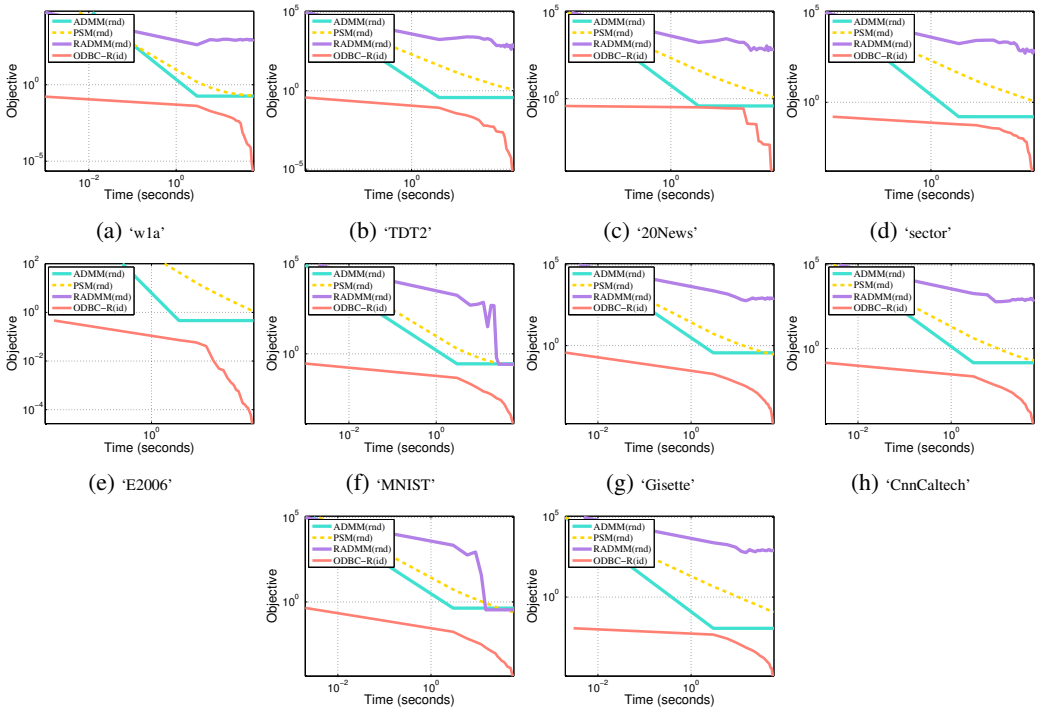


(a) 'w1a' (b) 'TDT2' (c) '20News' (d) 'sector'

(e) 'E2006' (f) 'MNIST' (g) 'Gisette' (h) 'CnnCaltech'

(i) 'Cifar' (j) 'randn'

Figure 11: The convergence curve of the surrogate objective $f(\mathbf{X}) + 1000\|\min(\mathbf{0}, \mathbf{X})\|_{\mathsf{F}}$ with $\mathbf{X} \in \mathrm{St}(n, r)$ for solving the nonnegative PCA problem with $r = 10$.

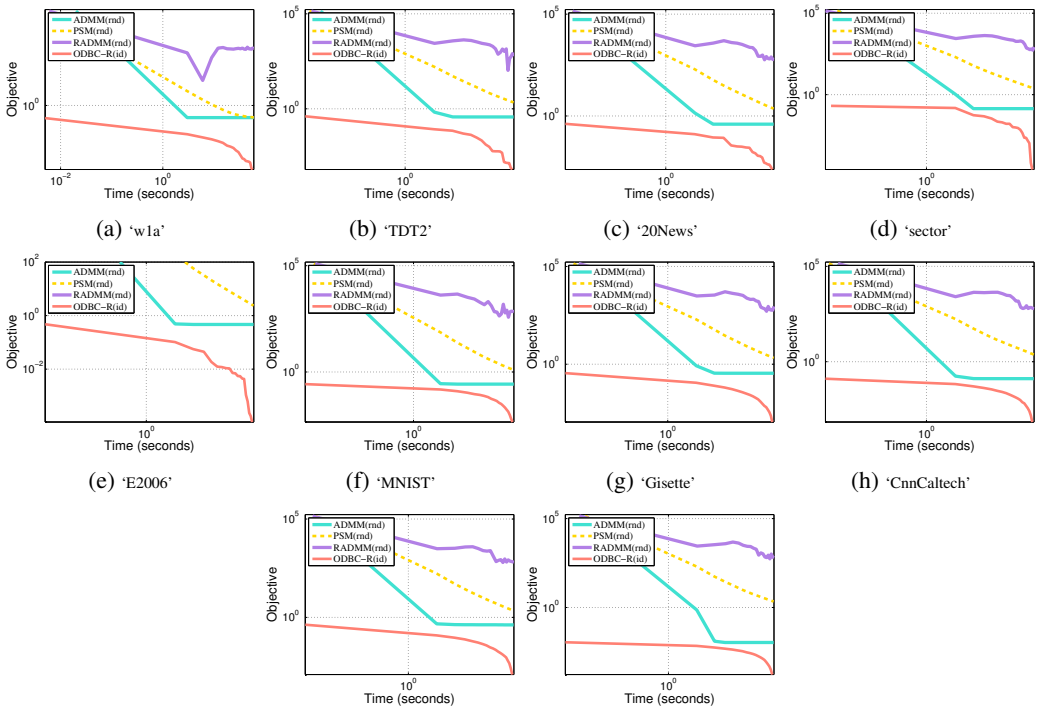


(a) 'w1a' (b) 'TDT2' (c) '20News' (d) 'sector'

(e) 'E2006' (f) 'MNIST' (g) 'Gisette' (h) 'CnnCaltech'

(i) 'Cifar' (j) 'randn'

Figure 12: The convergence curve of the surrogate objective $f(\mathbf{X}) + 1000\|\min(\mathbf{0}, \mathbf{X})\|_{\mathsf{F}}$ with $\mathbf{X} \in \mathrm{St}(n, r)$ for solving the nonnegative PCA problem with $r = 20$.

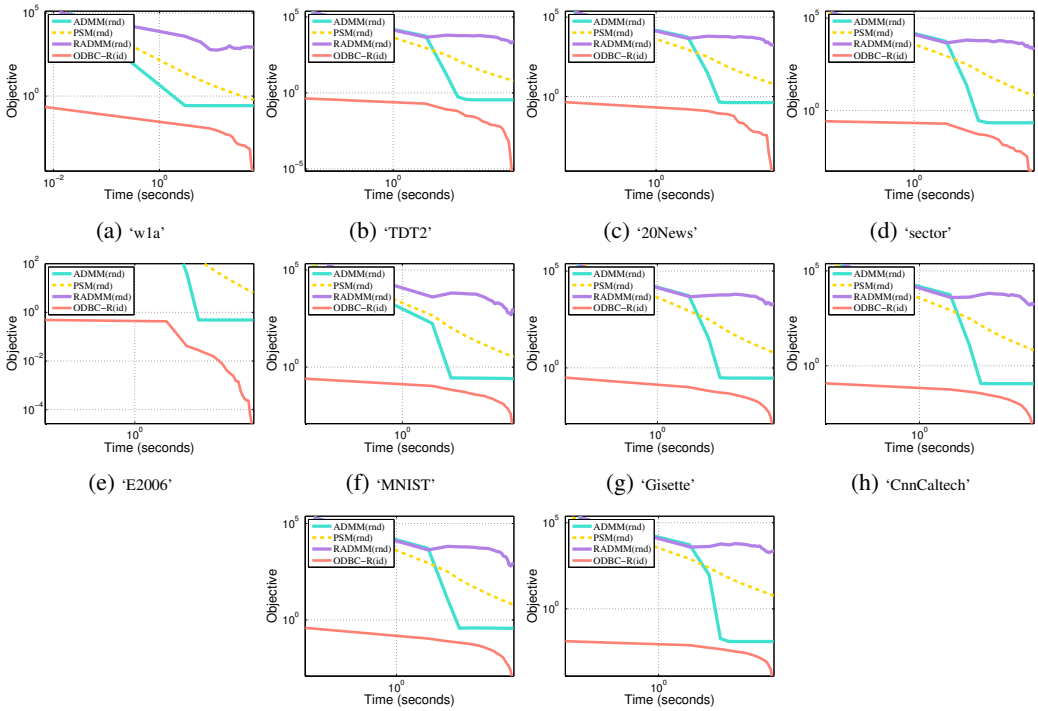


(a) 'w1a' (b) 'TDT2' (c) '20News' (d) 'sector'

(e) 'E2006' (f) 'MNIST' (g) 'Gisette' (h) 'CnnCaltech'

(i) 'Cifar' (j) 'randn'

Figure 13: The convergence curve of the surrogate objective $f(\mathbf{X}) + 1000\|\min(\mathbf{0}, \mathbf{X})\|_{\mathsf{F}}$ with $\mathbf{X} \in \mathrm{St}(n, r)$ for solving the nonnegative PCA problem with $r = 40$.



(a) 'w1a' (b) 'TDT2' (c) '20News' (d) 'sector'

(e) 'E2006' (f) 'MNIST' (g) 'Gisette' (h) 'CnnCaltech'

(i) 'Cifar' (j) 'randn'

Figure 14: The convergence curve of the surrogate objective $f(\mathbf{X}) + 1000\|\min(\mathbf{0}, \mathbf{X})\|_{\mathsf{F}}$ with $\mathbf{X} \in \mathrm{St}(n, r)$ for solving the nonnegative PCA problem with $r = 80$.