A Decomposition Algorithm for Sparse Generalized Eigenvalue Problem

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Abstract

Sparse generalized eigenvalue problem arises in a number of standard and modern statistical learning models, including sparse principal component analysis, sparse Fisher discriminant analysis and sparse canonical correlation analysis. However, this problem is difficult to solve since it is NP-hard. In this paper, we consider a new decomposition method to tackle this problem. Specifically, we use random or/and swapping strategies to find a working set and perform global combinatorial search over the small subset of variables. We consider a bisection search method and a coordinate descent method for solving the quadratic fractional programming subproblem. In addition, we provide theoretical analysis for the proposed decomposition algorithm. Extensive experiments on both real-world and synthetic data sets have shown that the proposed method achieves state-of-the-art performance in terms of accuracy.

1. Introduction

In this paper, we mainly focus on the following sparse generalized eigenvalue problem:

$$\begin{aligned}\min_{\mathbf{x}\neq\mathbf{0},\ \mathbf{x}\in\Omega}\ f(\mathbf{x}) \triangleq \frac{h(\mathbf{x})}{g(\mathbf{x})},\ s.t.\ \Omega \triangleq \{\mathbf{x} \mid \|\mathbf{x}\|_0 \leq s\} \\ h(\mathbf{x}) \triangleq \tfrac{1}{2}\mathbf{x}^T\mathbf{A}\mathbf{x},\ g(\mathbf{x}) \triangleq \tfrac{1}{2}\mathbf{x}^T\mathbf{C}\mathbf{x},\end{aligned} \tag{1}$$

where $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{A} \in \mathbb{R}^{n\times n}$ and $\mathbf{C} \in \mathbb{R}^{n\times n}$ are some symmetry matrices, and $s \in [1, n]$ is a positive integer. Here we assume that $\mathbf{C}$ is strictly positive definite.

We notice that the objective function and sparsity constraint in (1) is scale-invariant (multiplying $\mathbf{x}$ with a non-zero constant does not change the value of objective function and the satisfiability of sparsity constraint). Thus, it is equivalent to the following problem: $\min_{\mathbf{x}}\ \mathbf{x}^T\mathbf{A}\mathbf{x},\ s.t.\ \mathbf{x}^T\mathbf{C}\mathbf{x} = 1,\ \|\mathbf{x}\|_0 \leq s$. Moreover, without the sparsity constraint, Problem (1) reduces to the minimum generalized eigenvalue problem and it has several equivalent formulations [4]: $\min_{\mathbf{x}\neq\mathbf{0}}\ (\mathbf{x}^T\mathbf{A}\mathbf{x})/(\mathbf{x}^T\mathbf{C}\mathbf{x}) = \min\{\mathbf{x}^T\mathbf{A}\mathbf{x} : \mathbf{x}^T\mathbf{C}\mathbf{x} = 1\} = \min\{\lambda : \mathbf{A} - \lambda\mathbf{C} \succeq 0\} = \lambda_{\min}(\mathbf{C}^{-1/2}\mathbf{A}\mathbf{C}^{-1/2})$, where $\lambda_{\min}(\mathbf{X})$ denotes the smallest eigenvalue of a given matrix $\mathbf{X}$.

Problem (1) is closely related to the classical matrix computation in the literature [12, 11, 1]. Imposing an additional sparsity constraint on the solution reduces overfitting and improve the interpretability of the model for high-dimensional data analysis. This has motivated active research in developing methods that enforce sparsity on eigenvectors. For instance, the work of [17] proposes SCoTLASS by enforcing a sparsity constraint on the principal direction using a bounded ℓ_1 norm on the solution. The work of [33] reformulates the principle component analysis problem as a elastic-net regularized ridge regression problem, which can be solved efficiently using least angle regression. The work of [9] proposes a convex relaxation for the sparse PCA problem based on semidefinite programming.

One difficulty of solving (1) comes from the combinational nature of the cardinality constraint. To solve this problem, a conventional way is to simply replace ℓ_0 norm by its convex relaxation. Recently, non-convex approximation methods such as Schatten ℓ_p norm, re-weighted ℓ_1 norm, Capped ℓ_1 have been proposed to solve this problem for acquiring better accuracy than the convex methods [23]. However, all these approximation methods fails to directly control the sparsity of the solution. In contrast to the above relaxed approximation methods, iterative hard thresholding is a different approach by iteratively setting the small elements (in magnitude) to zero in a gradient descent manner. By using this strategy, it is able to control the sparsity of the solution directly and exactly. Due to its simplicity, it has been widely used and incorporated into the truncated power method [30] and truncated Rayleigh flow method [25].

Another difficulty of solving (1) is due to the non-convexity of the objective function. One popular way to overcome this difficulty is to remove the quadratic term using semi-definite programming lifting technique and reformulating (1) into the following low-rank sparse optimization problem: $\min_{\mathbf{X}\succeq 0}\ tr(\mathbf{A}\mathbf{X})/tr(\mathbf{C}\mathbf{X}),\ s.t.\ \|\mathbf{X}\|_0 \leq s^2,\ rank(\mathbf{X}) = 1$. We remark that the objective function

is both quasiconcave and quasiconvex (hence quasilinear), and one can constrain the denominator to be a positive constant using the scale-invariant property of the problem. Recently, convex semi-definite programming method drops the rank constraint and consider ℓ_1 relaxation for the sparsity constraint [9, 8, 19, 32]. It is shown to have strong guarantee under suitable assumptions. However, such a matrix lifting technique will incur expensive computation overhead.

In summary, existing methods for solving (1) suffer from the following limitations. (i) Semi-definite programming matrix methods are not scalable [9, 8, 19]. (ii) Convex/Non-convex approximation methods fail to directly control the low-rank and sparse property of the solution. (iii) Hard thresholding method [30, 18] only obtains weak optimality guarantee and suffers from poor accuracy in practice [3, 29].

Recently, the work of [3, 5] presents and analyzes a new optimality criterion which is based on coordinate-wise optimality for sparse optimization. They show that coordinate-wise optimality is strictly stronger than the optimality criterion based on hard thresholding. The work of [29] considers a new block-k optimal condition for general discrete optimization. It is shown to be stronger than the coordinate-wise condition since it includes coordinate-wise optimality as a special case with $k = 1$. Inspired by these works, we propose a new decomposition method for sparse generalized eigenvalue problem, along with using a greedy method based on the coordinate-wise optimality [5] for finding the working set.

Contributions: This paper makes the following contributions. **(i)** We propose a new decomposition algorithm for solving the generalized sparse eigenvalue problem (See Section 3). **(ii)** We discuss two methods to solve the sparse quadratic fractional programming subproblem (See Section 5). **(iii)** Convergence analysis for the proposed decomposition method is provided (See Section 5). **(iv)** Extensive experiments on real-world and synthetic data sets have shown that our method achieves state-of-the-art performance (See Section 7).

Notation: All vectors are column vectors and superscript T denotes transpose. $\mathbf{X}_{i,j}$ denotes the (i^{th}, j^{th}) element of matrix $\mathbf{X}$ and $\mathbf{x}_i$ denotes the i-th element of vector $\mathbf{x}$. $\mathbf{e}_i$ denotes a unit vector with a 1 in the i^{th} entry and 0 in all other entries. $\text{diag}(\mathbf{x})$ denotes a diagonal matrix formed with $\mathbf{x}$ as its principal diagonal. $\div$ denotes the element-wise division between two vectors. For any partition of the index vector $[1, 2, ..., n]$ into $[B, N]$ with $B \in \mathbb{N}^k$, $N \in \mathbb{N}^{n-k}$, we denote $\mathbf{U}_B \in \mathbb{R}^{n\times k}$, $\mathbf{U}_N \in \mathbb{R}^{n\times(n-k)}$ with $\mathbf{U}(B(i), i) = 1,\ \forall i = 1, ..., k$ and $\mathbf{U}(N(i), i) = 1,\ \forall i = 1, 2, ..., n-k$. Therefore, we have $\mathbf{x} = \mathbf{U}_B\mathbf{x}_B + \mathbf{U}_N\mathbf{x}_N$. Finally, we use C_k^i to denote the number of possible combinations choosing i items from k.

2. Generalized Eigenvalue Problems

A number of standard and modern statistical learning models can be formulated as the sparse generalized eigenvalue problem, which we present some instances below.

A1: Principle Component Analysis (PCA). Consider a data matrix $\mathbf{X} \in \mathbb{R}^{m\times d}$, where each row represents an independent sample. The covariance matrix $\mathbf{\Sigma}$ is computed by $\mathbf{\Sigma} = \frac{1}{m-1}\sum_{i=1}^m(\mathbf{z}_i - \boldsymbol{\mu})(\mathbf{z}_i - \boldsymbol{\mu})^T \in \mathbb{R}^{d\times d}$, where $\mathbf{z}_i$ denotes i^{th} column of $\mathbf{Z}$ and $\mu = \sum_{i=1}^m \mathbf{z}_i \in \mathbb{R}^d$. PCA can be cast into the following optimization problem: $\min_{\mathbf{x}\neq 0}\ (-\mathbf{x}^T\mathbf{\Sigma}\mathbf{x})/(\mathbf{x}^T\mathbf{x})$.

A2: Fisher Discriminant Analysis (FDA). Given observations with two distinct classes with $\boldsymbol{\mu}_i$ and $\mathbf{\Sigma}_i$ being the mean vector and covariance matrix of class i ($i = 1$ or 2), respectively. FDA seeks a projection vector such that the between-class variance is large relative to the within-class variance, leading to the following problem: $\min_{\mathbf{x}\neq 0}\ \frac{-\mathbf{x}^T((\boldsymbol{\mu}_1-\boldsymbol{\mu}_2)(\boldsymbol{\mu}_1-\boldsymbol{\mu}_2)^T)\mathbf{x}}{\mathbf{x}^T(\mathbf{\Sigma}_1+\mathbf{\Sigma}_2)\mathbf{x}}$.

A3: Canonical Correlation Analysis (CCA). Given two classes of data $\mathcal{X}$ and $\mathcal{Y}$, CCA exploits the relation of the samples by solving the following variational formulation: $\max_{\mathbf{u}\neq 0,\ \mathbf{v}\neq 0}\ \mathbf{u}^T\mathbf{\Sigma}_{xy}\mathbf{v},\ s.t.\ \mathbf{u}^T\mathbf{\Sigma}_{xx}\mathbf{u} = \mathbf{v}^T\mathbf{\Sigma}_{yy}\mathbf{v} = 1$, where $\mathbf{\Sigma} \triangleq \left(\begin{smallmatrix}\mathbf{\Sigma}_{xx} & \mathbf{\Sigma}_{xy}\\ \mathbf{\Sigma}_{yx} & \mathbf{\Sigma}_{yy}\end{smallmatrix}\right)$ is the covariance matrix between sample from $\mathcal{X}$ and $\mathcal{Y}$. Defining $\mathbf{A} \triangleq \left(\begin{smallmatrix}\mathbf{0} & \mathbf{\Sigma}_{xy}\\ \mathbf{\Sigma}_{yx} & \mathbf{0}\end{smallmatrix}\right)$ and $\mathbf{C} \triangleq \left(\begin{smallmatrix}\mathbf{\Sigma}_{xx} & \mathbf{0}\\ \mathbf{0} & \mathbf{\Sigma}_{yy}\end{smallmatrix}\right)$, and $\mathbf{x} \triangleq \left(\begin{smallmatrix}\mathbf{u}\\ \mathbf{v}\end{smallmatrix}\right)$, we can rewrite CCA as the following equivalent optimization problem: $\min_{\mathbf{x}}\ \frac{-\mathbf{x}^T\mathbf{A}\mathbf{x}}{\mathbf{x}^T\mathbf{C}\mathbf{x}}$.

Incorporated with the sparsity constraint, the applications listed above become special cases of the general optimization models in (1).

3. The Proposed Decomposition Algorithm

This section presents our decomposition algorithm for solving (1), which is based on the following notation of block-k optimality for general non-convex constrained optimization.

Definition 1. *(Block-k Optimal Solution) We let $\mathbf{x} = \mathbf{U}_B\mathbf{x}_B + \mathbf{U}_N\mathbf{x}_N$. A solution $\mathbf{x}$ is the block-k optimal solution if and only if it holds that:*

$$\forall |B| = k,\ \mathbf{x}_B = \arg\min_{\mathbf{x}_B}\ f\left(\mathbf{U}_B\mathbf{x}_B + \mathbf{U}_N\mathbf{x}_N\right),$$
$$s.t.\ \left(\mathbf{U}_B\mathbf{x}_B + \mathbf{U}_N\mathbf{x}_N\right) \in \Omega,\ N \triangleq \{1, 2, ..., n\} \setminus B.$$

In other words, a solution is the block-k optimal solution if and only if every block coordinate of size k achieves the global optimal solution.

The basic idea of the decomposition method is that in each iteration, the indices $\{1, ..., n\}$ of decision variable are separated to two sets B and N, where B is the working set and $N = \{1, ..., n\} \setminus B$. The vector $\mathbf{x}_N$ is fixed so the objective value becomes a subproblem with the variable $\mathbf{x}_B$

Algorithm 1 A Decomposition Algorithm for Sparse Generalized Eigenvalue Problem as in (1).

1: Specify the working set parameter k and the proximal term parameter θ.
2: Find an initial feasible solution $\mathbf{x}^0$ and set $t = 0$.
3: **while** not converge **do**
4: (**S1**) Use some strategy to find a working set B whose size is k. Define $N \triangleq \{1, 2, ..., n\} \setminus B$.
5: (**S2**) Solve the following subproblem with the variable $\mathbf{x}_B$ using combinatorial search:

$$\mathbf{x}_B^{t+1} \Leftarrow \arg\min_{\mathbf{x}_B} \frac{h(\mathbf{x}_B, \mathbf{x}_N^t) + \frac{\theta}{2}\|\mathbf{x}_B - \mathbf{x}_B^t\|_2^2}{g(\mathbf{x}_B, \mathbf{x}_N^t)} \quad s.t.\ \|\mathbf{x}_B\|_0 + \|\mathbf{x}_N^t\|_0 \leq s \tag{2}$$

6: (S3) Increment t by 1.
7: **end while**

is solved. Note that B is updated in each iteration t. To simplify the notation, we use B instead of B^t. Therefore, we can rewrite $h(\cdot)$ and $g(\cdot)$ in Problem (1) as:

$$h(\mathbf{x}_B, \mathbf{x}_N) = \tfrac{1}{2}\mathbf{x}_B^T\mathbf{A}_{BB}\mathbf{x}_B + \tfrac{1}{2}\mathbf{x}_N^T\mathbf{A}_{NN}\mathbf{x}_N + \langle \mathbf{x}_B, \mathbf{A}_{BN}\mathbf{x}_N\rangle$$
$$g(\mathbf{x}_B, \mathbf{x}_N) = \tfrac{1}{2}\mathbf{x}_B^T\mathbf{C}_{BB}\mathbf{x}_B + \tfrac{1}{2}\mathbf{x}_N^T\mathbf{C}_{NN}\mathbf{x}_N + \langle \mathbf{x}_B, \mathbf{C}_{BN}\mathbf{x}_N\rangle.$$

Our proposed algorithm iteratively solves the small-sized optimization problem in (2) until convergence. We summarize our algorithm in Algorithm 1.

Remarks. **(i)** The concept of block-k optimality has been introduced in [29]. This paper extends their method for minimizing convex quadratic functions to handle general non-convex objective functions. **(ii)** Algorithm 1 relies on solving a small-sized non-convex optimization problem. However, using the specific structure of the objective function and the sparsity constraint, we can develop an efficient and practical algorithm to solve it globally. **(iii)** We introduce a new proximal point strategy for the sub-problem in (2). This is to guarantee sufficient descent condition and global convergence of Algorithm 1 (refer to Lemma 2 and Theorem 2). **(iv)** When the dimension n is small [1] and the parameter setting $\theta = 0,\ k = n$ is used, the subproblem is equivalent to the original problem and Algorithm 1 finds the global optimal solution of the optimization problem.

4. Finding a Working Set

This subsection shows how to find the working set (refer to Step **S2** in Algorithm 1). This problem is challenging for two aspects. **(i)** Unlike convex methods that one can find the working set using the KKT primal-dual residual [16, 7], there is no general criteria to find the working set for non-convex problem. **(ii)** There are C_n^k possible combinations of choice for the working set of size k. One cannot expect to use the cyclic strategy and alternatingly minimize over all the possible combinations due to large computational complexity when k is large.

We propose to use the following two strategies to find the working set:

• Random Strategy. We uniformly select one combination (which contains k coordinates) from the whole working set of size C_n^k. In expectation, our algorithm is still guaranteed to find the block-k stationary point.

• Swapping Strategy. We denote $\mathcal{S}(\mathbf{x})$ and $\mathcal{Z}(\mathbf{x})$ as the index of non-zero elements and zero elements of $\mathbf{x}$, respectively. Based on the current solution $\mathbf{x}^t$, our method enumerates all the possible pairs (i, j) with $i \in \mathcal{S}(\mathbf{x}^t)$ and $j \in \mathcal{Z}(\mathbf{x}^t)$ that leads to the greatest descent $\mathbf{d}$ by changing the two coordinates from zero/non-zero to non-zero/zero, as follows:

$$\mathbf{D}_{i,j} = \min_\beta\ f(\mathbf{x}^t + \beta\mathbf{e}_i - \mathbf{x}_j^t\mathbf{e}_j) - f(\mathbf{x}^t). \tag{3}$$

We then pick the top pairs of coordinates that lead to the greatest descent by measuring $\mathbf{D} \in \mathbb{R}^{|\mathcal{S}(\mathbf{x})|\times|\mathcal{Z}(\mathbf{x})|}$. Specifically, we denote $P \in \mathbb{N}^n$ and $S \in \mathbb{N}^n$ as the index pairs of the sorted version of $\mathbf{D}$ with $\mathbf{D}_{P_1,S_1} \leq \mathbf{D}_{P_2,S_2} \leq \mathbf{D}_{P_3,S_3} \leq, ..., \mathbf{D}_{P_n,S_n}$. Assuming that k is an even number, we simply pick the top-$(k/2)$ nonoverlapping elements of the sequence P and S respectively as the working set.

We now discuss how to solve the one-dimensional non-convex subproblem in (3) to obtain $\mathbf{D}_{i,j}$. We start from the following lemma.

Lemma 1. *Assume* $\tau \triangleq \frac{1}{2}\bar{r}\beta^2 + \bar{s}\beta + \bar{t} > 0\ \forall\beta$. *The following one-dimensional non-convex optimization problem:*

$$\min_\beta \psi(\beta) \triangleq \frac{\frac{1}{2}\bar{a}\beta^2 + \bar{b}\beta + \bar{c}}{\frac{1}{2}\bar{r}\beta^2 + \bar{s}\beta + \bar{t}},\ s.t.\ \bar{L} \leq \beta \leq \bar{U} \tag{4}$$

admits a closed-form solution which can be expressed as: $\beta^* = \arg\min_\beta\ f(\beta),\ \beta \in \{\Pi(\beta_1), \Pi(\beta_2)\}$, *where* $\beta_1 = (-\vartheta - \sqrt{\vartheta^2 - 2\pi\iota})/\pi,\ \beta_2 = (-\vartheta + \sqrt{\vartheta^2 - 2\pi\iota})/\pi,\ \pi \triangleq \bar{a}\bar{s} - \bar{b}\bar{r},\ \vartheta \triangleq \bar{a}\bar{t} - \bar{c}\bar{r},\ \iota \triangleq \bar{t}\bar{b} + \bar{c}\bar{s}$, *and* $\Pi(\beta) \triangleq \min(\bar{U}, \max(\bar{L}, \beta))$.

Proof. Dropping the bound constraint and setting the gradient of $\psi(\beta)$ to zero, we have $0 = \psi'(\beta) = ((\bar{a}\beta+\bar{b})(\frac{1}{2}\bar{r}\beta^2 + \bar{s}\beta + \bar{t}) - (\frac{1}{2}\bar{a}\beta^2 + \bar{b}\beta + \bar{c})(\bar{r}\beta + \bar{s}))/\tau^2$. Noticing $\tau > 0$, we obtain the following first-order optimal condition for ψ: $0 = (\bar{a}\beta + \bar{b})(\frac{1}{2}\bar{r}\beta^2 + \bar{s}\beta + \bar{t}) - (\frac{1}{2}\bar{a}\beta^2 + \bar{b}\beta + \bar{c})(\bar{r}\beta + \bar{s})$. It can be simplified as: $0 = \frac{1}{2}\beta^2\pi + \beta\vartheta + \iota$. Solving this equation, we have two solutions β_1 and β_2. We select the one between $\Pi(\beta_1)$ and $\Pi(\beta_2)$ that leads to a lower objective value as the optimal solution. □

Denoting $\mathbf{v} \triangleq \mathbf{x}^t - \mathbf{x}_j^t\mathbf{e}_j$ and incorporating the specific form of $f(\cdot)$, we obtain: $\min_\beta\ f(\mathbf{v} + \beta\mathbf{e}_i) =$

[1] The popular pit props dataset [15, 22] only contains 13 dimensions.

$\min_\beta \frac{\frac{1}{2}(\mathbf{v}+\beta\mathbf{e}_i)^T\mathbf{A}(\mathbf{v}+\beta\mathbf{e}_i)}{\frac{1}{2}(\mathbf{v}+\alpha\mathbf{e}_i)^T\mathbf{C}(\mathbf{v}+\beta\mathbf{e}_i)}$. By applying Lemma 1 with $\bar{L} = -\infty$, $\bar{U} = \infty$, $\bar{a} = \mathbf{A}_{i,i}$, $\bar{b} = (\mathbf{Av})_i$, $\bar{c} = \frac{1}{2}\mathbf{v}^T\mathbf{Av}$, $\bar{r} = \mathbf{C}_{i,i}$, $\bar{s} = (\mathbf{Cv})_i$, $\bar{t} = \frac{1}{2}\mathbf{v}^T\mathbf{Cv}$, we obtain the global optimal solution for (3).

5. Solving the Subproblem

The subproblem (2) in Algorithm 1 reduces to the following quadratic fractional programming problem subject to sparsity constraint:

$$\min_{\mathbf{z}\in\mathbb{R}^k} p(\mathbf{z}) \triangleq \frac{\frac{1}{2}\mathbf{z}^T\bar{\mathbf{Q}}\mathbf{z} + \bar{\mathbf{p}}^T\mathbf{z} + \bar{w}}{\frac{1}{2}\mathbf{z}^T\bar{\mathbf{R}}\mathbf{z} + \bar{\mathbf{c}}^T\mathbf{z} + \bar{v}},\ s.t.\ \|\mathbf{z}\|_0 \le q \qquad (5)$$

where $\bar{\mathbf{Q}} = \mathbf{A}_{BB} + \theta\mathbf{I}$, $\bar{\mathbf{p}} = \mathbf{A}_{BN}\mathbf{x}_N - \theta\mathbf{x}_B^t$, $\bar{w} = \frac{1}{2}\mathbf{x}_N^T\mathbf{A}_{NN}\mathbf{x}_N + \frac{\theta}{2}\|\mathbf{x}_B^t\|_2^2$, $\bar{\mathbf{R}} = \mathbf{C}_{BB}$, $\bar{\mathbf{c}} = \mathbf{C}_{BN}\mathbf{x}_N$, , $\bar{v} = \frac{1}{2}\mathbf{x}_N^T\mathbf{C}_{NN}\mathbf{x}_N$, $q = s - \|\mathbf{x}_N\|_0$.

Problem (5) is equally NP-hard due to the combinatorial constraint $\|\mathbf{z}\|_0 \le q$. Inspired by [29], we develop an exhaustive combinatorial search algorithm to solve it. Specifically, we consider to solve the following optimization problem:

$$\min_{\mathbf{z}\in\mathbb{R}^k} p(\mathbf{z}),\ s.t.\ \mathbf{z}_K = 0$$

where K has $\sum_{i=0}^q C_k^i$ possible choices for the coordinates. We systematically enumerate the full binary tree for K to obtain all possible candidate solutions for $\mathbf{z}$ and then pick the best one that leads to the lowest objective value as the optimal solution. In other words, we need to solve a quadratic fractional programming problem with $m = k - |K|$ variables, as follows:

$$\min_{\mathbf{y}\in\mathbb{R}^m} \mathcal{L}(\mathbf{y}) \triangleq \frac{u(\mathbf{y})}{q(\mathbf{y})} \triangleq \frac{\frac{1}{2}\mathbf{y}^T\mathbf{Q}\mathbf{y} + \mathbf{p}^T\mathbf{y} + w}{\frac{1}{2}\mathbf{y}^T\mathbf{R}\mathbf{y} + \mathbf{c}^T\mathbf{y} + v}, \qquad (6)$$

The optimal solution can be computed as $\mathbf{z}_K = \mathbf{0}$, $\mathbf{z}_{\bar{\mathbf{K}}} = \mathbf{y}$ with $\bar{\mathbf{K}} = \{1, 2, ..., k\} \setminus K$. Therefore, if we find the global optimal solution of (6), we find the global optimal solution of (5) as well.

The non-convex problem in (6) is challenging. For solving it, we present two methods, namely a bisection search method and a coordinate descent method, which are of independent research interest.

5.1. A Bisection Search Method

This subsection presents a bisection search method for finding the global optimal solution of Problem (6).

We now discuss the relationship between this fractional programming problem and the following parametric programming problem [10]:

$$\mathcal{J}(\alpha) = 0,\ \text{with } \mathcal{J}(\alpha) \triangleq \min_{\mathbf{y}} u(\mathbf{y}) - \alpha q(\mathbf{y}) \qquad (7)$$

The minimum of this problem equals to α^* if and only if $\min_{\mathbf{y}} h(\mathbf{y}) - \alpha g(\mathbf{y})$ is 0 for $\alpha = \alpha^*$.

The following theorem sheds some theoretic lights for the original non-convex problem in (6).

Theorem 1. *We have the following results. (i) The objective value for the optimal solution in Program (6) is sandwiched as:* $\lambda_{\min}(\mathbf{Z}) \le \min_{\mathbf{y}} J(\mathbf{y}) < \lambda_{\min}(\mathbf{O})$, *with* $\mathbf{O} \triangleq \mathbf{R}^{-1/2}\mathbf{Q}\mathbf{R}^{-1/2}$, $\gamma \triangleq 2v - \|\mathbf{R}^{-1/2}\mathbf{c}\|_2^2 > 0$, $\mathbf{g} \triangleq \mathbf{R}^{-1/2}\mathbf{p} - \mathbf{R}^{-1/2}\mathbf{Q}\mathbf{R}^{-1}\mathbf{c}$, $\delta \triangleq \mathbf{c}^T\mathbf{R}^{-1}\mathbf{Q}\mathbf{R}^{-1}\mathbf{c} - 2\mathbf{c}^T\mathbf{R}^{-1}\mathbf{p} + 2w$, *and* $\mathbf{Z} \triangleq \begin{pmatrix} \mathbf{O} & \mathbf{g}/\sqrt{\gamma} \\ \mathbf{g}^T/\sqrt{\gamma} & \delta/\gamma \end{pmatrix}$. *(ii) Let* $\mathbf{O} = \mathbf{U}diag(\mathbf{d})\mathbf{U}^T$ *be the eigenvalue decomposition of* $\mathbf{O}$. *The function* $\mathcal{J}(\alpha)$ *can be rewritten as*

$$\mathcal{J}(\alpha) = \frac{1}{2}\delta - \frac{1}{2}\alpha\gamma - \frac{1}{2}\sum_i^m \frac{\mathbf{a}_i^2}{\mathbf{d}_i - \alpha},\ \textit{with } \mathbf{a} = \mathbf{U}^T\mathbf{g} \qquad (8)$$

and it is monotonically decreasing on the range $\lambda_{\min}(\mathbf{Z}) \le \alpha < \lambda_{\min}(\mathbf{O})$. *The optimal solution can be computed as* $\mathbf{y}^* = \mathbf{R}^{-1/2}(\mathbf{u}^* - \mathbf{R}^{-1/2}\mathbf{c})$, *with* $\mathbf{u}^* = -(\mathbf{O} - \alpha^*\mathbf{I})^{-1}\mathbf{g}$ *and* α^* *being the unique root of the equation* $\mathcal{J}(\alpha) = 0$ *on the range* $\lambda_{\min}(\mathbf{Z}) \le \alpha < \lambda_{\min}(\mathbf{O})$.

Proof. (i) Firstly, it is not hard to notice that Program (6) is equivalent to the following problem:

$$\begin{aligned}
&\min_{\mathbf{y}} \mathcal{L}(\mathbf{y}) \\
=&\min_{\mathbf{d}} \frac{\frac{1}{2}(\mathbf{R}^{-1/2}\mathbf{d})^T\mathbf{Q}(\mathbf{R}^{-1/2}\mathbf{d}) + \mathbf{p}^T(\mathbf{R}^{-1/2}\mathbf{d}) + w}{\frac{1}{2}(\mathbf{R}^{-1/2}\mathbf{d})^T\mathbf{R}(\mathbf{R}^{-1/2}\mathbf{d}) + \mathbf{c}^T(\mathbf{R}^{-1/2}\mathbf{d}) + v} \\
=&\min_{\mathbf{d}} \frac{\frac{1}{2}\mathbf{d}^T\mathbf{O}\mathbf{d} + \mathbf{d}^T(\mathbf{R}^{-1/2}\mathbf{p}) + w}{\frac{1}{2}\|\mathbf{d}\|_2^2 + \mathbf{d}^T(\mathbf{R}^{-1/2}\mathbf{c}) + v} \\
=&\min_{\mathbf{d}} \frac{\frac{1}{2}\mathbf{d}^T\mathbf{O}\mathbf{d} + \mathbf{d}^T(\mathbf{R}^{-1/2}\mathbf{p}) + w}{\frac{1}{2}\|\mathbf{d} + \mathbf{R}^{-1/2}\mathbf{c}\|_2^2 + v - \frac{1}{2}\|\mathbf{R}^{-1/2}\mathbf{c}\|_2^2} \\
=&\min_{\mathbf{u}} \frac{\frac{1}{2}\mathbf{u}^T\mathbf{O}\mathbf{u} + \mathbf{u}^T\mathbf{g} + \frac{1}{2}\delta}{\frac{1}{2}\|\mathbf{u}\|_2^2 + \frac{1}{2}\gamma}, \qquad (9)
\end{aligned}$$

where the first step uses the variable substitution that $\mathbf{y} = \mathbf{R}^{-1/2}\mathbf{d}$; the third step uses the transformation that $\mathbf{u} = \mathbf{d} + \mathbf{R}^{-1/2}\mathbf{c}$. Note that the denominator is always strictly positive for all decision variables, we have $\frac{1}{2}\mathbf{y}^T\mathbf{R}\mathbf{y} + \mathbf{c}^T\mathbf{y} + v$, $\forall\mathbf{y}$. Setting $\mathbf{y} = \mathbf{0}$, we obtain $\frac{\gamma}{2} > 0$. We naturally obtain the upper for $\min_{\mathbf{y}} \mathcal{L}(\mathbf{y})$:

$$\begin{aligned}
&\min_{\mathbf{y}} \mathcal{L}(\mathbf{y}) \\
=&\min_{\mathbf{u},\eta=\sqrt{\gamma}} \frac{\frac{1}{2}\mathbf{u}^T\mathbf{O}\mathbf{u} + \frac{1}{\sqrt{\gamma}}\mathbf{u}^T\mathbf{g}\eta + \frac{\delta}{2\gamma}\eta^2}{\frac{1}{2}\|\mathbf{u}\|_2^2 + \frac{1}{2}\eta^2} \\
\ge&\min_{\mathbf{u},\eta} \frac{\frac{1}{2}\mathbf{u}^T\mathbf{O}\mathbf{u} + \frac{1}{\sqrt{\gamma}}\mathbf{u}^T\mathbf{g}\eta + \frac{\delta}{2\gamma}\eta^2}{\frac{1}{2}\|\mathbf{u}\|_2^2 + \frac{1}{2}\eta^2} \\
=&\min_{\mathbf{u},\eta} \frac{\frac{1}{2}\left[\mathbf{u}^T \mid \eta^T\right]^T\mathbf{Z}\left[\mathbf{u}^T \mid \eta^T\right]}{\frac{1}{2}\|\mathbf{u}\|_2^2 + \frac{1}{2}\eta^2} = \lambda_{\min}(\mathbf{Z}),
\end{aligned}$$

where the first inequality uses the fact that $\min_{\mathbf{x}} f(\mathbf{x}) \leq \min_{\mathbf{x}\in\Psi} f(\mathbf{x})$ for all $f(\cdot)$ and Ψ. We now derive the upper bound of $\min_{\mathbf{y}}\ \mathcal{L}(\mathbf{y})$. Since the objective function $\mathcal{J}(\alpha)$ is always bounded, there must exist α with $\mathbf{Q} - \alpha\mathbf{R} \succ 0$, such that the value of $\mathbf{y}$ minimizing the function $(u(\mathbf{y}) - \alpha q(\mathbf{y}))$. Therefore, we have $\mathbf{Q} - \alpha\mathbf{R} \succ 0 \Rightarrow \mathbf{Q} - \alpha\mathbf{R}^{1/2}\mathbf{I}\mathbf{R}^{1/2} \succ 0 \Rightarrow \mathbf{R}^{-1/2}\mathbf{Q}\mathbf{R}^{-1/2} - \alpha\mathbf{I} \succ 0 \Rightarrow \alpha < \lambda_{\min}(\mathbf{O})$.

(ii) Using the result of (9), we can rewrite $\mathcal{J}(\alpha)$ as:

$$\begin{aligned}\mathcal{J}(\alpha) &= \min_{\mathbf{u}} \tfrac{1}{2}\mathbf{u}^T\mathbf{O}\mathbf{u} + \mathbf{u}^T\mathbf{g} + \tfrac{1}{2}\delta - \alpha\left(\tfrac{1}{2}\|\mathbf{u}\|_2^2 + \tfrac{1}{2}\gamma\right)\\ &= \min_{\mathbf{u}} \tfrac{1}{2}\mathbf{u}^T(\mathbf{O} - \alpha I)\mathbf{u} + \mathbf{u}^T\mathbf{g} + \tfrac{1}{2}\delta - \tfrac{\alpha\gamma}{2}.\end{aligned}$$

Solving the quadratic optimization with respect to $\mathbf{u}$ we have $\mathbf{u}^* = -(\mathbf{O} - \alpha\mathbf{I})\mathbf{g}$. Thus, we can repress $\mathcal{J}(\alpha)$ as: $\mathcal{J}(\alpha) = -\frac{1}{2}\mathbf{g}^T(\mathbf{O} - \alpha I)^{-1}\mathbf{g} + \frac{1}{2}\delta - \frac{\alpha\gamma}{2}$. Since it holds that $\mathbf{g}^T(\mathbf{O} - \alpha I)^{-1}\mathbf{g} = \mathbf{g}^T\mathbf{U}^T\mathrm{diag}(1 \div (\mathbf{d} - \alpha))\mathbf{U}\mathbf{g}$, we obtain (8). Noticing that the first-order and second-order gradient of $\mathcal{J}(\alpha)$ with respect to α can be computed as: $\mathcal{J}'(\alpha) = -\frac{1}{2}\sum_i^m(\frac{\mathbf{a}_i}{\mathbf{d}_i - \alpha})^2 - \frac{\gamma}{2}$, $\mathcal{J}''(\alpha) = -\sum_i^m(\mathbf{a}_i^2/(\mathbf{d}_i - \alpha)^3)$ and $\gamma > 0$, we obtain $\mathcal{J}'(\alpha) < 0$ and $\mathcal{J}''(\alpha) \leq 0$. Thus, the function $\mathcal{J}(\alpha)$ is concave and monotonically decreasing on the range $\lambda_{\min}(\mathbf{Z}) \leq \alpha < \lambda_{\min}(\mathbf{O})$, and there exists a unique root of the equation $\mathcal{J}(\alpha) = 0$ on the range $\lambda_{\min}(\mathbf{Z}) \leq \alpha < \lambda_{\min}(\mathbf{O})$.

□

Based on Theorem 1, we now present a bisection method for solving Problem (6). For notation convenience, we define $\underline{\alpha} \triangleq \lambda_{\min}(\mathbf{Z})$ and $\overline{\alpha} \triangleq \lambda_{\max}(\mathbf{O}) - \epsilon$, where ϵ denotes the machine precision parameter which is sufficiently small. Due to the monotonically decreasing property of $\mathcal{J}(\alpha)$, we can solve (8) by checking where the sign of the left-hand side changes. Specifically, we consider the following three cases for $\mathcal{J}(\alpha)$ on the range $\underline{\alpha} \leq \alpha \leq \overline{\alpha}$: **(a)** $\mathcal{J}(\underline{\alpha}) \geq \mathcal{J}(\overline{\alpha}) \geq 0$, **(b)** $0 \geq \mathcal{J}(\underline{\alpha}) \geq \mathcal{J}(\overline{\alpha})$, and **(c)** $\mathcal{J}(\underline{\alpha}) \geq 0 \geq \mathcal{J}(\overline{\alpha})$. For case $(\mathbf{a})$ and $(\mathbf{b})$, we can directly return $\overline{\alpha}$ and $\underline{\alpha}$ as the optimal solution, respectively. We now consider case $(\mathbf{c})$. By the Rolle mean value theorem, there always exists an $\alpha^* \in [\underline{\alpha}, \overline{\alpha}]$ such that $\mathcal{J}(\alpha^*) = 0$. Thus, one can define and initialize the lower bound $lb = \underline{\alpha}$ and the upper bound $ub = \overline{\alpha}$ and then perform the following loop until the optimal solution $\alpha^* = mid$ with $\mathcal{J}(mid) \approx 0$ is found: $\{mid = (lb + ub)/2,\ \text{if}(\mathcal{J}(mid) > 0)\ lb = mid;\ \text{else}\ ub = mid;\}$. Such a bisection scheme is guaranteed to find the optimal solution within $\mathcal{O}(\log_2((\overline{\alpha} - \underline{\alpha})/\varepsilon))$ iteration that $ub \leq lb + \varepsilon$ [6].

Remarks. (i) To the best of our knowledge, this is the first algorithm for unconstrained quadratic fractional programming with global optimal guarantee. Although the classical Dinkelbach's method [10] can solve our problem, it only finds a stationary solution for the non-convex problem. Our results are based on the monotone property of the associated parametric programming problem in a restricted domain. **(ii)** The matrix $\mathbf{O}$ is a $n \times n$ principal sub-matrix of $\mathbf{Z}$. Using theorem 4.3.17 in [12], it always holds that $\boldsymbol{\lambda}_1(\mathbf{Z}) \leq \boldsymbol{\lambda}_1(\mathbf{O}) \leq \boldsymbol{\lambda}_2(\mathbf{Z}) \leq ... \leq \boldsymbol{\lambda}_n(\mathbf{Z}) \leq \boldsymbol{\lambda}_{n-1}(\mathbf{O}) \leq \boldsymbol{\lambda}_n(\mathbf{Z})$, where $\boldsymbol{\lambda}(\mathbf{X})$ denotes the eigenvalues of $\mathbf{X}$ in increasing order. Thus, the bound for the α^* is tight.

5.2. A Coordinate Descent Method

This subsection presents a simple coordinate descent method [27, 13, 14, 28, 20] for solving (6). Although it can not guarantee to find the global optimal solution to (6), it has many merits. (i) It is able to incorporate additional bound constraints. (ii) It is numerically robust and does not require additional eigenvalue solvers. (iii) It is guaranteed to converge a coordinate-wise minimum point for our specific quadratic fractional programming problem (see Proposition 1 below).

To illustrate the merits of the coordinate descent method, we consider incorporating the bound constraint on the solution by $\bar{L} \leq \mathbf{x} \leq \bar{U}$ into the sparse optimization problem in (1) and our decomposition method [2]. Our methods for finding the working set and strategies for handling the NP-hard ℓ_0 norm directly follow and what one needs is to replace (6) and solve the following problem:

$$\min_{\mathbf{y}\in\mathbb{R}^m}\ \mathcal{L}(\mathbf{y}) \triangleq \frac{\frac{1}{2}\mathbf{y}^T\mathbf{Q}\mathbf{y} + \mathbf{p}^T\mathbf{y} + w}{\frac{1}{2}\mathbf{y}^T\mathbf{R}\mathbf{y} + \mathbf{c}^T\mathbf{y} + v},\ s.t.\ \hat{L} \leq \mathbf{y} \leq \hat{U} \quad (10)$$

for some constants $\hat{L}$ and $\hat{U}$. The coordinate descent method iteratively picks a coordinate $i \in \{1, 2, ..., m\}$ and solves the following one dimensional subproblem based on its current solution $\mathbf{y}^j$ with $j = 0, 1, ...\infty$:

$$\beta^* = \arg\min_{\beta}\ \mathcal{L}(\mathbf{y}^j + \beta\mathbf{e}_i),\ s.t.\ \hat{L} \leq \mathbf{y}_i^j + \beta \leq \hat{U} \quad (11)$$

where j is the iteration counter for the coordinate descent algorithm. Problem (11) reduces to the one-dimensional subproblem as in (4) with suitable parameters. In every iteration j, once the optimal solution β^* in (11) is found, the intermediate solution for (10) is updated via $\mathbf{y}_i^{j+1} \Leftarrow \mathbf{y}_i^j + \beta^*$. There are several ways and orders to decide which coordinates to update in the literature. (i) Cyclic order strategy runs all coordinates in cyclic order, i.e. $1 \rightarrow 2 \rightarrow 3 \rightarrow ... \rightarrow m \rightarrow 1$ at each iteration. (ii) Random sampling strategy randomly select one coordinate to update (sample with replacement). (iii) Gauss-Southwell pick coordinate i such that $i = \arg\max_{1\leq t\leq m} |\bar{\boldsymbol{\nabla}}\mathcal{L}(\mathbf{x}^j)|_t$, with $\bar{\boldsymbol{\nabla}}\mathcal{L}(\mathbf{x}) \in \mathbb{R}^m$ being the projected gradient of $\mathcal{L}$ at $\mathbf{x}$ [21]: $\bar{\boldsymbol{\nabla}}\mathcal{L}(\mathbf{x})_i = \begin{cases}\boldsymbol{\nabla}\mathcal{L}(\mathbf{x})_i, & \hat{L} < \mathbf{x}_i < \hat{U};\\ \max(0, \boldsymbol{\nabla}\mathcal{L}(\mathbf{x})_i), & \mathbf{x}_i = \hat{U};\\ \min(0, \boldsymbol{\nabla}\mathcal{L}(\mathbf{x})_i), & \mathbf{x}_i = \hat{L};\end{cases}$ and $\boldsymbol{\nabla}\mathcal{L}(\mathbf{x})$ being the gradient of $\boldsymbol{\nabla}\mathcal{L}$ at $\mathbf{x}$. Note that $\bar{\boldsymbol{\nabla}}\mathcal{L}(\mathbf{x}^*) = \mathbf{0}$ implies $\mathbf{x}^*$ is a first-order stationary point.

[2] This is useful in sparse non-negative PCA [2].

We now present our convergence result of our coordinate descent method for solving (10), which is an extension of Theorem 4.1 in [27].

Proposition 1. *When the cyclic order strategy is used, coordinate descent method is guaranteed to converge to a stationary point $\mathbf{y}^*$ of Problem (10). In addition, any stationary point $\mathbf{y}^*$ is also a global coordinate-wise minimum of Problem (10) that $\mathbf{y}_i^* = \arg\min_{\hat{L}\leq\alpha\leq\hat{U}} \mathcal{L}(\mathbf{y}_i^* + \alpha\mathbf{e}_i),\ \forall\alpha, i$.*

Proof. (i) First, we prove that the non-convex problem in (11) only contains one unique optimal solution. This can be proven by contradiction. We first omit the bound constraint since it does not effect the uniqueness of the optimal solution. Problem (11) reduces to the following one-dimensional quadratic fractional problem: $\min_\beta\ (\frac{1}{2}a\beta^2 + b\beta + c)/(\frac{1}{2}r\beta^2 + s\beta + t)$ with suitable parameters $a,\ b,\ c,\ r,\ s,\ t$. Assume that there exists two optimal solutions x and y to this problem that leads to the same objective value ϑ. According to the first-order and second-order optimal condition [10, 31], we have: $(a - \vartheta r)x = -b + \vartheta s,\ (a - \vartheta r)y = -b + \vartheta s,\ (a - \vartheta r) > 0$, which leads to the following contraction: $\frac{\vartheta s - b}{a - \vartheta r} = x \neq y = \frac{\vartheta s - b}{a - \vartheta r}$. Therefore, Problem (11) only contains one unique solution.

(ii) Note that $\mathcal{L}(\mathbf{y})$ is continuous and $\{\mathcal{L}(\mathbf{y}^j)\}$ converges monotonically. Assuming that it converges to $\mathcal{L}^*$ with $\lim_{j\to\infty}\mathcal{L}(\mathbf{y}^j) = \mathcal{L}^*$, we obtain that $\forall\alpha,\ i = 1, .., m$:

$$\mathcal{L}^* = \mathcal{L}(\mathbf{y}^{j-1}) = \mathcal{L}(\mathbf{y}^j) \leq \mathcal{L}(\mathbf{y}^{j-1} + \alpha\mathbf{e}_i). \tag{12}$$

Therefore, the right-handed side in (12) attains it minimum at both 0 and $(\mathbf{y}^j)_i - (\mathbf{y}^{j-1})_i$. Combining with the fact that the subproblem only contains one unique global solution, we have $(\mathbf{y}^{j-1})_i = (\mathbf{y}^j)_i$. Since the coordinate i is picked using cyclic order, we have: $\mathbf{y}^{j-1} = \mathbf{y}^j = \mathbf{y}^*$ and $\mathbf{y}^*$ is a coordinate-wise minimum point.

□

Remarks. (i) One remarkable feature of the non-convex problem in (10) is that its associated one-dimensional subproblem in (11) only contains one unique optimal solution. This is different from the work of [20] where their one-dimensional subproblem may have multiple optimal solutions and cause divergence for coordinate descent method. **(ii)** Coordinate descent method is guaranteed to produce a coordinate-wise stationary point which is stronger than the full gradient projection method. Note that any coordinate-wise stationary point $\mathbf{x}^*$ that $\mathbf{x}_i^* = \arg\min_{\hat{L}\leq\alpha\leq\hat{U}} \mathcal{L}(\mathbf{x}_i^* + \alpha\mathbf{e}_i),\ \forall\alpha, i$ also satisfies the first-order optimal condition with $\overline{\boldsymbol{\nabla}}\mathcal{L}(\mathbf{x}^*) = 0$. However, the reverse is not true. This implies that our coordinate descent method can exploit possible higher order derivatives to escape saddle points for the non-convex problem.

6. Convergence Analysis of Algorithm 1

This section presents the convergence analysis of Algorithm 1. The following sufficient decrease condition is useful.

Lemma 2. ***(Sufficient Decrease Condition)*** *Suppose $\{f(x^t)\}_{t=0}^\infty$ is generated by Algorithm 1, it holds that: $f(\mathbf{x}^{t+1}) - f(\mathbf{x}^t) \leq \frac{-\theta\|\mathbf{x}^{t+1} - \mathbf{x}^t\|_2^2}{\mathbf{x}^{t+1}\mathbf{C}\mathbf{x}^{t+1}}$.*

Proof. We let B be the working set in the t-th iteration and $N \triangleq \{1, 2, ..., n\} \setminus B$. Since we solve Problem (2) in the t-th iteration, we have $(h(\mathbf{x}_B, \mathbf{x}_N^t) + \frac{\theta}{2}\|\mathbf{x}_B - \mathbf{x}_B^t\|_2^2)\ /\ g(\mathbf{x}_B, \mathbf{x}_N^t) \leq (h(\mathbf{z}, \mathbf{x}_N^t) + \frac{\theta}{2}\|\mathbf{z} - \mathbf{x}_B^t\|_2^2)\ /\ g(\mathbf{z}, \mathbf{x}_N^t),\ \forall\mathbf{z} \in \mathbb{R}^k$ and $\mathbf{x}_N^{t+1} = \mathbf{x}_N^t$. Letting $\mathbf{z} = \mathbf{x}_B^t$, we have: $-\frac{\mathbf{x}^t\mathbf{A}\mathbf{x}^t}{\mathbf{x}^t\mathbf{C}\mathbf{x}^t} \leq -\frac{\mathbf{x}^{t+1}\mathbf{A}\mathbf{x}^{t+1} + \sigma\|\mathbf{x}^{t+1} - \mathbf{x}^t\|_2^2}{\mathbf{x}^{t+1}\mathbf{C}\mathbf{x}^{t+1}}$. In addition, using the structure of $f(\cdot)$, we obtain: $f(\mathbf{x}^{t+1}) - f(\mathbf{x}^t) = \frac{\mathbf{x}^{t+1}\mathbf{A}\mathbf{x}^{t+1}}{\mathbf{x}^{t+1}\mathbf{C}\mathbf{x}^{t+1}} - \frac{\mathbf{x}^t\mathbf{A}\mathbf{x}^t}{\mathbf{x}^t\mathbf{C}\mathbf{x}^t} \leq \frac{-\theta\|\mathbf{x}^{t+1} - \mathbf{x}^t\|_2^2}{\mathbf{x}^{t+1}\mathbf{C}\mathbf{x}^{t+1}}$. Thus, we finish the proof of this lemma.

□

Remarks: The proximal term in the numerator in (2) is necessary for our non-convex optimization problem since it guarantees sufficient decrease condition which is important for convergence.

Now we present our main theorem.

Theorem 2. ***Convergence Properties of Algorithm 1.*** *Assume that the subproblem in (2) is solved globally and there exists a constant σ such that $\mathbf{x}^t\mathbf{C}\mathbf{x}^t \geq \sigma > 0,\ \forall\mathbf{x}^t$. Let $\{f(\mathbf{x}^t)\}_{t=0}^\infty$ be the sequence generated by Algorithm 1. We have the following results. (i) When random strategy is used to find the working set, we have $\lim_{t\to\infty}\mathbb{E}[\|\mathbf{x}^{t+1} - \mathbf{x}^t\|] = 0$ and Algorithm 1 converges to the block-k stationary point in expectation. (ii) When swapping strategy is used to find the working set with $k \geq 2$, we have $\lim_{t\to\infty}\|\mathbf{x}^{t+1} - \mathbf{x}^t\| = 0$ and Algorithm 1 converges to the block-2 stationary point deterministically.*

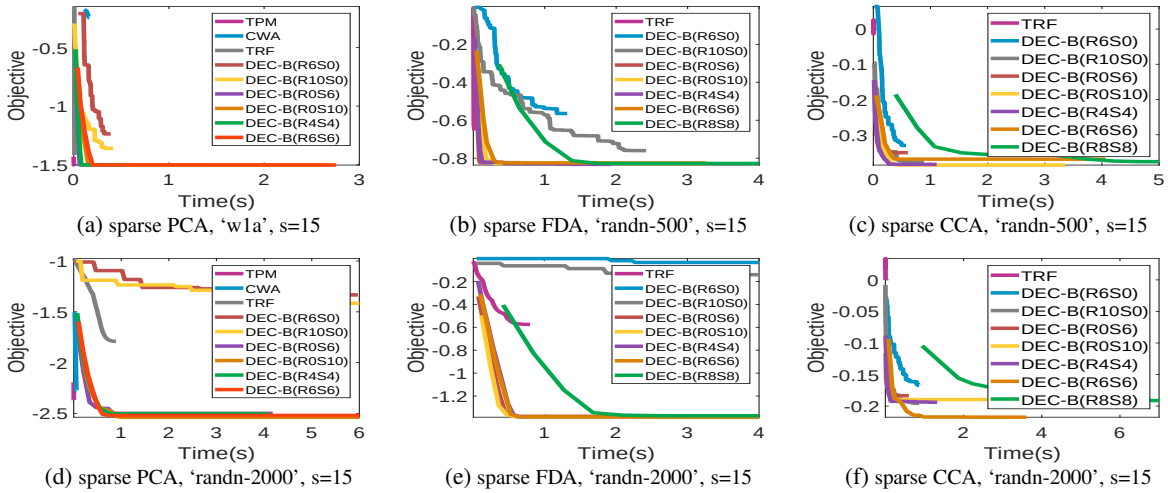
Proof. For notation simplicity, we define $f^k \triangleq f(\mathbf{x}^k)$ and $f^* \triangleq f(\mathbf{x}^*)$, where $\mathbf{x}^*$ denotes the stationary point. (i) Taking the expectation of B for the sufficient descent inequality in Lemma 2, we have $\mathbb{E}[f^{t+1} \mid \mathbf{x}^t] \leq f^t - \mathbb{E}[\mu\|\mathbf{x}^{t+1} - \mathbf{x}^t\|_2^2 \mid \mathbf{x}^t]$ with $\mu \triangleq \theta/\sigma$. Summing this inequality over $i = 0, 1, ..., t-1$, we have:

$$\mu\textstyle\sum_{i=0}^t \mathbb{E}[\|\mathbf{x}^{i+1} - \mathbf{x}^i\|_2^2 \mid \mathbf{x}^i] \leq f(\mathbf{x}^0) - f(\mathbf{x}^t). \tag{13}$$

Using the fact that $f^* \leq f^t$, we obtain:

$$\begin{aligned} & \mu\textstyle\sum_{i=0}^t \mathbb{E}[\|\mathbf{x}^{i+1} - \mathbf{x}^i\|_2^2 \mid \mathbf{x}^i] \leq f^0 - f^* \\ \Rightarrow\quad & \min_{i=1,...,t}\mathbb{E}[\|\mathbf{x}^{i+1} - \mathbf{x}^i\|_2^2 \mid \mathbf{x}^i] \leq \tfrac{f^0 - f^*}{t\mu}. \end{aligned}$$

Therefore, we have $\lim_{t\to\infty}\mathbb{E}[\|\mathbf{x}^{t+1} - \mathbf{x}^t\| \mid \mathbf{x}^t] = 0$. We now prove the rest of this statement by contradiction. We assume Algorithm 1 does not converge to the



(a) sparse PCA, 'w1a', s=15 (b) sparse FDA, 'randn-500', s=15 (c) sparse CCA, 'randn-500', s=15

(d) sparse PCA, 'randn-2000', s=15 (e) sparse FDA, 'randn-2000', s=15 (f) sparse CCA, 'randn-2000', s=15

Figure 1 Convergence behavior of different methods for sparse PCA (left column), sparse FDA (middle column), and CCA (right column).

block-k stationary point. Using Definition 1, in expectation there exists a block of coordinates B such that $\mathbf{x}_B^t \notin \arg\min_{\mathbf{z}} h(\mathbf{z}, \mathbf{x}_N^t)/g(\mathbf{z}, \mathbf{x}_N^t)$. Therefore, we obtain: $\mathbf{x}_B^t \notin \arg\min_{\mathbf{z}} (h(\mathbf{z}, \mathbf{x}_N^t) + 0.5\theta\|\mathbf{z} - \mathbf{x}_N^t\|_2^2)/g(\mathbf{z}, \mathbf{x}_N^t)$. However, according to the fact that $\mathbf{x}_N^t = \mathbf{x}_N^{t+1}$ and step S2 in Algorithm 1, we have $\mathbf{x}_B^{t+1} \in \arg\min_{\mathbf{z}} (h(\mathbf{z}, \mathbf{x}_N^t) + 0.5\theta\|\mathbf{z} - \mathbf{x}_N^t\|_2^2)/g(\mathbf{z}, \mathbf{x}_N^t)$. Hence, we have $\mathbf{x}_B^t \neq \mathbf{x}_B^{t+1}$. This contradicts with the fact that $\mathbf{x}^t = \mathbf{x}^{t+1}$ as $t \to \infty$. We conclude that $\mathbf{x}^t$ converges to the block-k stationary point. (ii) Using similar strategy for deriving (i), we have $\lim_{t\to\infty} \|\mathbf{x}^{t+1} - \mathbf{x}^t\| = 0$. We now prove that Algorithm 1 convergence to a block-2 stationary point $\mathbf{x}^*$. Since Algorithm 1 is monotonically non-increasing and converges to a stationary point $\mathbf{x}^*$ such that no decrease is made, we have $\mathbf{D}_{i,j} \geq 0$ for (3). Therefore, it holds that $\min_\alpha f(\mathbf{x}^* + \alpha\mathbf{e}_i - (\mathbf{x}^*)_j\mathbf{e}_j) \geq f(\mathbf{x}^*)$, $\forall i \in \bar{\mathcal{S}}(\mathbf{x}^*)$, $j \in \bar{\mathcal{Z}}(\mathbf{x}^*)$. We have the following result: $f(\mathbf{x}^*) \leq f(\mathbf{x}^* + \mathbf{d}), \forall \mathbf{d}$ with $\|\mathbf{d} - \mathbf{x}^*\|_0 = 2$. Therefore, $\mathbf{x}^*$ is a block-2 stationary point. □

7. Experiments

This section demonstrates the efficacy of the proposed decomposition algorithm by considering three important applications (i.e. sparse FDA, sparse CCA, and sparse PCA) on synthetic and real-world data sets. All codes are implemented in MATLAB on an Intel 3.20GHz CPU with 8 GB RAM.

• **Data sets**. (i) We consider four real-world data sets: 'a1a', 'w1a', 'w2a', and 'madelon'. We randomly select a subset of examples from the original data sets [3]. The size of the data sets used in our experiments are 2000×119, 2000×300, 2000×300, 2000×112, respectively. (ii) We also use a similar method as [5] to generate synthetic Gaussian random data sets. Specifically, we produce the feature matrix $\mathbf{X} \in \mathbb{R}^{m\times d}$ and the label vector $\mathbf{y} \in \mathbb{R}^m$ as follows: $\mathbf{X} = \text{randn}(m, d)$, $\mathbf{y} = \text{sign}(\text{randn}(m, 1))$, where $\text{randn}(m, d)$ is a function that returns a standard Gaussian random matrix of size $m \times d$ and sign is a signum function. We fix $m = 300$ and consider different values for $d = \{100, 500, 1500, 2000\}$. We denote the data sets as 'randn-d'.

Based on $\mathbf{X}$ and $\mathbf{y}$, we generate the matrix $\mathbf{A}$ and $\mathbf{C}$ in Problem (1) for different applications (See Section 2). Note that the resulting size of the sparse generalized eigenvalue problem for sparse PCA, sparse FDA and sparse CCA are d, d and $d + m$, respectively. We vary the sparsity $s \in \{4, 8, 12, ..., 40\}$ and report the objective values for Problem (1).

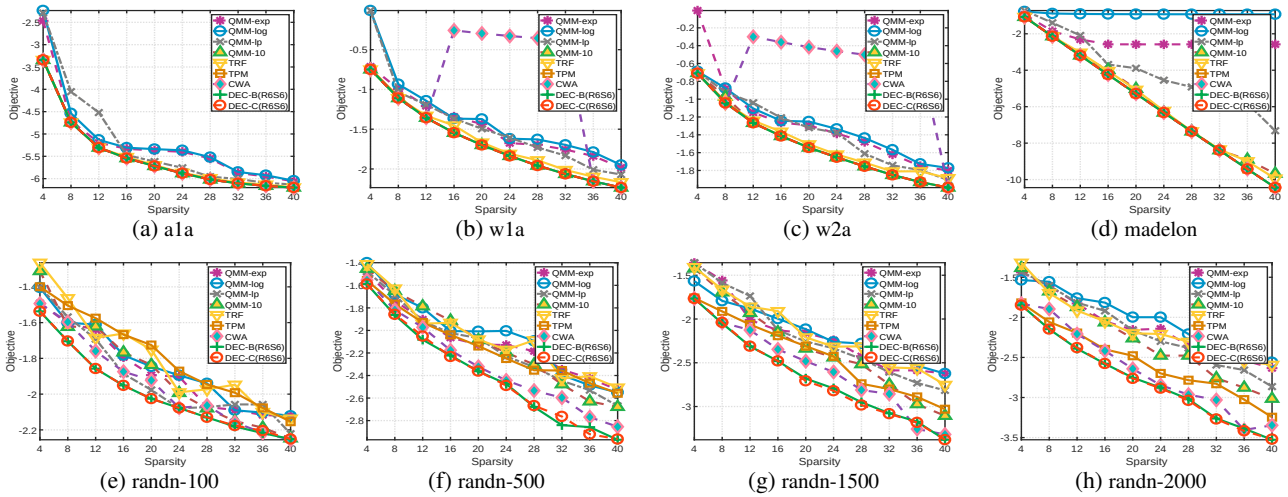
• **Compared Methods**. We introduce the following methods for comparison. **(a)** Truncated Power Method (TPM) [30] [4] considers an iterative procedure that greedily decreases the objective while maintaining the desired sparsity for the intermediate solutions by hard-thresholding truncation. **(b)** Coordinate-Wise Algorithm (CWA) [3, 5] [5] iteratively performs an optimization step with respect to two coordinates, where the coordinates that need to be altered are chosen to be the ones that produce the maximal decrease among all possible alternatives. **(c)** Truncated Rayleigh Flow (TRF) [25] iteratively updates the solution using the gradient of the generalized Rayleigh quotient and performs a truncation operation to achieve sparsity. **(d)** Quadratic Majorization Method (QMM) [23] [6] approximate the ℓ_0-norm by a continuous surrogate function and iteratively ma-

[3] https://www.csie.ntu.edu.tw/~cjlin/libsvm/

[4] code: sites.google.com/site/xtyuan1980/

[5] code: sites.google.com/site/amirbeck314/

[6] code: https://junxiaosong.github.io/



(a) a1a (b) w1a (c) w2a (d) madelon

(e) randn-100 (f) randn-500 (g) randn-1500 (h) randn-2000

Figure 2 Accuracy of different methods on different data sets for sparse PCA problem with varying the cardinalities.

jorizes the surrogate function by a quadratic separable function, which at each iteration reduces to a regular generalized eigenvalue problem. Using different smooth non-convex approximation functions, they develop different versions of QMM (QMM-exp, QMM-log, QMM-ℓ_p, QMM-ℓ_0). Since they only solve a regularized problem and fail to control the sparsity of the solution, we use a simple bisection search to find the best regulation parameter and report the lowest objective value after hard thresholding. **(e)** The proposed decomposition method (denoted as DEC). We use DEC-B(Ri-Sj) and DEC-C(Ri-Sj) to denote our method based on a **B**isection search method and a **C**oordinate descent method, respectively, along with selecting i coordinate using **R**andom strategy and j coordinates using the **S**wapping strategy. Hence, the working set contains at most $i + j$ coordinates. We set $\theta = 10^{-5}$ for our method. We keep a record of the relative changes of the objective function values by $r_t = (f(\mathbf{x}^t) - f(\mathbf{x}^{t+1}))/f(\mathbf{x}^t)$. We let Algorithm 1 algorithms run up to T iterations and stop them at iteration $t < T$ if mean$([r_{t-\min(t,M)+1},\ r_{t-min(t,M)+2}, ..., r_t]) \leq \epsilon$. The defaults values of ϵ, M, and T are 10^{-5}, 50 and 1000, respectively.

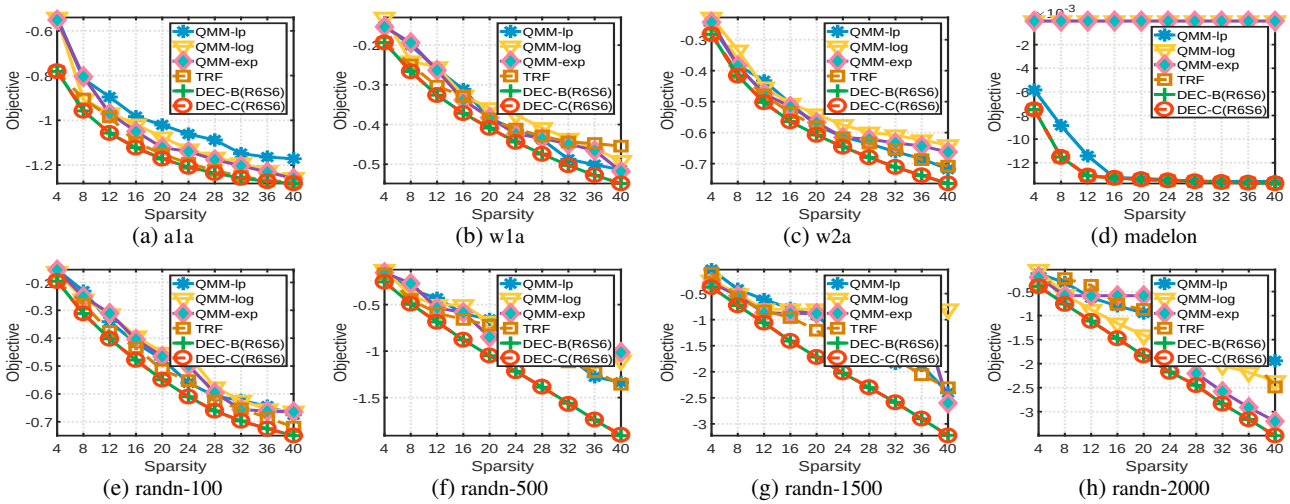
We remark that both (a) and (b) are only designed for sparse PCA with $\mathbf{C} = \mathbf{I}$. We do not compare with the DC programming algorithms [24, 26] since it fails to control the sparsity of the solution and results in worse accuracy than QMM (see [23]).

• **Convergence Behavior**. We demonstrate the convergence behavior for different methods in Figure 1. We do not include the results of QMM since it fails to control the sparsity of the solution. Due to space limitation, we only report the result of DEC-B in this set of experiments, and we have the following observations. (i) The methods {TPM, CWA, TRF} converge within one second and they are faster than DEC. However, they get stuck into poor local minima and result in much worse accuracy than DEC. (ii) The objective values of DEC stabilize after less than 5 seconds, which means it has converged, and the decrease of the objective value is negligible afterwards. This implies that one may use a looser stopping criterion without sacrificing accuracy. (iii) DEC-B(R6S0) and DEC-B(R8S8) converge very slow, and it seems that DEC-B(R6S6) finds a good trade-off between efficiency and effectiveness. (iv) DEC-B(R10S0) achieves a lower objective value than DEC-B(R6S0). This is reasonable since larger k in the block-k notation implies stronger stationary point. (v) {DEC-B(R6S0), DEC-B(R10S0)} achieve much larger objective values than {DEC-B(R0S6), DEC-B(R0S10)}, which implies that the swapping strategy plays an indispensable role in our decomposition algorithm.

• **Experimental Results**. We demonstrate the experimental results for sparse PCA, sparse FDA, and sparse CCA in Figure 2, 3 and 4, respectively. Several conclusions can be drawn. (i) CWA generally outperforms {TPM, TRF, QMM}. (ii) CWA is not stable and generates much worse result for 'w1a' and 'w2a'. (iii) The proposed method DEC still outperforms CWA and achieves the lowest value of objective function. (iv) Both DEC-B and DEC-C perform similarly. This is because coordinate descent method finds a desirable solution for the quadratic fractional programming problem.

8. Conclusions

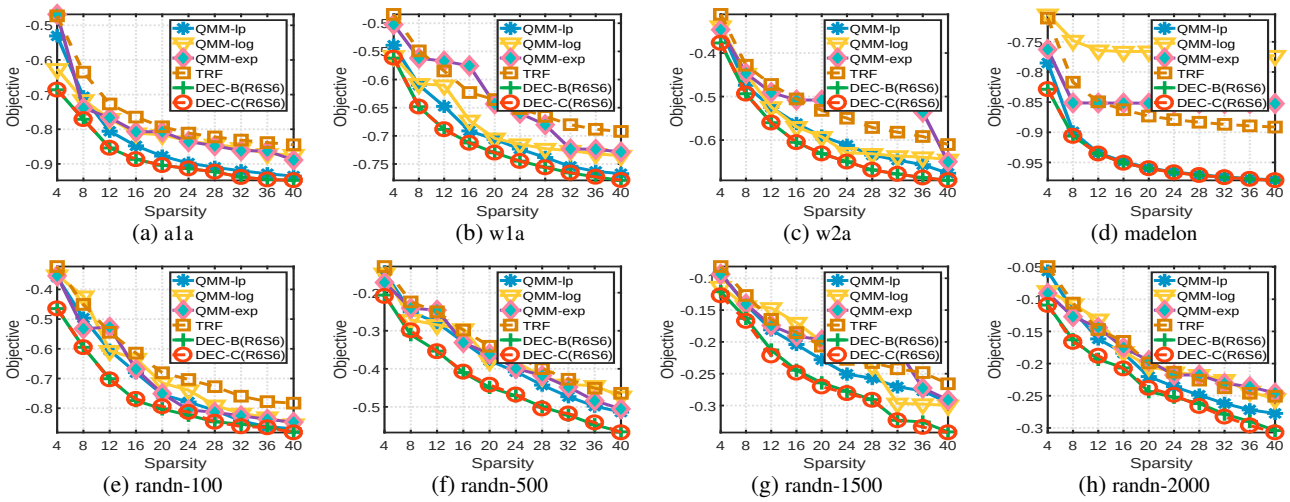
This paper presents an effective decomposition algorithm for solving the sparse generalized eigenvalue problem. Although the problem is NP-hard, we consider a decomposition algorithm to solve it. Extensive experiments on synthetic data and real-world data have shown that our method achieves state-of-the-art performance.



(a) a1a (b) w1a (c) w2a (d) madelon

(e) randn-100 (f) randn-500 (g) randn-1500 (h) randn-2000

Figure 3: Accuracy of different methods on different data sets for sparse FDA problem with varying cardinalities.



(a) a1a (b) w1a (c) w2a (d) madelon

(e) randn-100 (f) randn-500 (g) randn-1500 (h) randn-2000

Figure 4: Accuracy of different methods on different data sets for sparse CCA problem with varying cardinalities.

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