# An Inverse-free Truncated Rayleigh-Ritz Method for Sparse Generalized Eigenvalue Problem 

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#### Abstract

This paper considers the sparse generalized eigenvalue problem (SGEP), which aims to find the leading eigenvector with at most $k$ nonzero entries. SGEP naturally arises in many applications in machine learning, statistics, and scientific computing, for example, the sparse principal component analysis (SPCA), the sparse discriminant analysis (SDA), and the sparse canonical correlation analysis (SCCA). In this paper, we focus on the development of a three-stage algorithm named inverse-free truncated Rayleigh-Ritz method (IFTRR) to efficiently solve SGEP. In each iteration of IFTRR, only a small number of matrix-vector products is required. This makes IFTRR well-suited for large scale problems. Particularly, a new truncation strategy is proposed, which is able to find the support set of the leading eigenvector effectively. Theoretical results are developed to explain why IFTRR works well. Numerical simulations demonstrate the merits of IFTRR.


## 1 Introduction

Given a matrix pair $(\widetilde{A}, \widetilde{B})$, where $\widetilde{A}, \widetilde{B}$ are both $p$-by- $p$ symmetric matrices and $\widetilde{B}$ is (semi) positive definite, the sparse generalized eigenvalue problem (sparse GEP, or SGEP) aims to maximize the Rayleigh quotient $\frac{v^{\mathrm{T}} \tilde{A} v}{v^{\mathrm{T}} \tilde{B} v}$ with $v \in \mathbb{R}^{p}$ having no more than $k$ nonzero entries, where $k \ll p$. Mathematically, SGEP can be formulated as the following optimization problem:

$$
\begin{equation*}
\max _{v \in \mathbb{R}^{p}} \frac{v^{\mathrm{T}} \widetilde{A} v}{v^{\mathrm{T}} \widetilde{B} v}, \quad \text { subject to } \quad\|v\|_{0} \leq k \tag{1}
\end{equation*}
$$

where $\|v\|_{0}$ denotes the $\ell_{0}$-norm of $v$, which is the number of nonzero entries of $v$. In many applications, such as sparse principle component analysis (SPCA) (Zou et al., 2006), sparse discriminant analysis (SDA) (Clemmensen et al., 2011), and sparse canonical correlation analysis (SCCA) (Witten et al., 2009) in high dimensional statistical analysis, the matrices $\widetilde{A}$ and $\widetilde{B}$ usually can be decomposed as follows:

$$
\begin{equation*}
\widetilde{A}=A+E, \quad \widetilde{B}=B+F, \tag{2}
\end{equation*}
$$

where $A, B$ are both symmetric, $B$ is positive definite, $E, F$ are symmetric perturbations due to finite sample estimation.

Next, we consider the following two concrete examples of SGEP, which arise from Sparse Fisher's discriminant analysis (SFDA) and SCCA, respectively.

Example 1 Given a data matrix $X \in \mathbb{R}^{n \times p}$ (i.e., $n$ observations with $p$ features), each row belongs to one of $K$ classes. Denote $\mathcal{C}_{k} \subset\{1,2, \ldots, n\}$ the indices of the observations in the $k$-th class, $n_{k}=\left|\mathcal{C}_{k}\right|, \bar{x}_{k}=$ $\sum_{i \in \mathcal{C}_{k}} \frac{X_{(i,))}}{n_{k}}$. Then we may use

$$
\begin{aligned}
\widetilde{\Sigma}_{b} & =\sum_{k=1}^{K} \frac{n_{k} \bar{x}_{k}^{\mathrm{T}} \bar{x}_{k}}{n} \\
\widetilde{\Sigma}_{w} & =\frac{1}{n} \sum_{k=1}^{K} \sum_{i \in \mathcal{C}_{k}}\left(X_{(i,:)}-\bar{x}_{k}\right)^{\mathrm{T}}\left(X_{(i,:)}-\bar{x}_{k}\right),
\end{aligned}
$$

as the estimators for the between class variance $\Sigma_{b}$ and the within class variance $\Sigma_{w}$, respectively. SFDA intends to find a sparse leading discriminant vector $v$ that maximizes $\frac{v^{\mathrm{T}} \widetilde{\Sigma}_{b} v}{v^{\mathrm{T}} \widetilde{\Sigma}_{w} v}$, which can be formulated as an $S G E P$ with $\widetilde{A}=\widetilde{\Sigma}_{b}, \widetilde{B}=\widetilde{\Sigma}_{w}$.

Example 2 Let $X \in \mathbb{R}^{p / 2}$ and $Y \in \mathbb{R}^{p / 2}$ be two random variables, $\Sigma_{x x}, \Sigma_{y y}, \Sigma_{x y}$ be the covariance matrices for $X, Y$, the cross-covariance matrix between $X$ and $Y$, respectively, $\hat{\Sigma}_{x x}, \hat{\Sigma}_{y y}, \hat{\Sigma}_{x y}$ be estimators
for $\Sigma_{x x}, \Sigma_{y y}, \Sigma_{x y}$, respectively. SCCA aims to maximize $v_{x}^{\mathrm{T}} \hat{\Sigma}_{x y} v_{y}$, subject to $v_{x}^{\mathrm{T}} \hat{\Sigma}_{x x} v_{x}=1, v_{y}^{\mathrm{T}} \hat{\Sigma}_{y y} v_{y}=1$, $\left\|v_{x}\right\|_{0} \leq s_{x},\left\|v_{y}\right\|_{0} \leq s_{y}$, where $s_{x}$ and $s_{y}$ are two small integers. Such a problem can be reformulated as an SGEP with $\widetilde{A}=\left[\begin{array}{cc}0 & \hat{\Sigma}_{x y} \\ \hat{\Sigma}_{x y}^{\mathrm{T}} & 0\end{array}\right], \widetilde{B}=\left[\begin{array}{cc}\hat{\Sigma}_{x x} & 0 \\ 0 & \hat{\Sigma}_{y y}\end{array}\right], v=\left[\begin{array}{l}v_{x} \\ v_{y}\end{array}\right]$.

Computational challenges. The SGEP can be computationally challenging. Recall that in our model we have $\widetilde{A}=A+E, \widetilde{B}=B+F$. Denote the eigenvalues and the corresponding eigenvectors of $A v=\lambda B v$ by $\lambda_{1} \geq \lambda_{2} \geq \cdots \geq \lambda_{p}$ and $v_{1}, v_{2}, \ldots, v_{p}$, respectively. We call $\lambda_{1}$ the leading eigenvalue of $(A, B), v_{1}$ the leading eigenvector of $(A, B)$, and $\left(\lambda_{1}, v_{1}\right)$ the leading eigenpair of $(A, B)$. In this paper, the leading eigenvector $v_{1}$ is assumed to be sparse, i.e., $\left\|v_{1}\right\|_{0} \ll p$. Overall, the task of SGEP is essentially to find an approximation of $v_{1}$ via $(\widetilde{A}, \widetilde{B})$, without knowing $E, F$.

Due to finite number of samples, the perturbations $E$ and $F$ may be large, and consequently, the leading eigenvector of $(\widetilde{A}, \widetilde{B})$ may not be a good approximation of the true $v_{\widetilde{\sim}}$. Furthermore, in a high dimensional setting, $\widetilde{A}$ and $\widetilde{B}$ can be both ill-conditioned (or singular), meaning that infinity eigenvalue $\infty$ and indeterminate eigenvalue $0 / 0$ occur. In the presence of rounding-off error, numerical algorithms may fail to detect the singularity due to ill-conditioning. As a result, one may not be able to compute accurate or meaningful eigenvalues and eigenvectors. In fact, the optimization problem (1) is essentially a subset selection problem, which is known to be NP-hard (Moghaddam et al., 2005, 2006).
Here, it is worth mentioning that, when $B=\widetilde{B}=I_{p}$, the problem (1) is reduced to the so-called sparse eigenvalue problem (SEP), also known as sparse principal component analysis (SPCA). Obviously SGEP can be substantially more challenging than SEP (SPCA).
Related work. A variety of numerical methods have been proposed for SEP. Existing algorithms of SEP are mostly optimization approaches, which are based on relaxation, or penalization, or both. The $\ell_{1}$-norm relaxation, inspired by LASSO, is first studied in (Jolliffe et al., 2003) and called SCoTLASS. In (Witten et al., 2009), a penalized matrix decomposition method is proposed for computing a low rank approximation of a matrix, where $\ell_{1}$-norm relaxation is used to encourage sparsity. In (d'Aspremont et al., 2007), a convex relaxation for the $\ell_{1}$ constrained PCA is introduced and solved by semidefinite programming. In (Journée et al., 2010), a generalized power (GPower) method is proposed for SPCA, where $\ell_{0} / \ell_{1}$ penalization is used. In (Luss and Teboulle, 2013), based on the well-known conditional gradient algorithm, a framework called ConGradU is proposed, which unifies a variety of algorithms. In (Yuan and Zhang, 2013), a truncated power method (TPower) is proposed, which adopts the
power method to update the approximate eigenvector, followed by a truncation procedure that keeps a few largest magnitude entries of the approximate eigenvector and truncates the remaining entries to zero. Also, see (d'Aspremont et al., 2008; Moghaddam et al., 2006) for other greedy algorithms proposed for SPCA.
The SGEP, compared with SEP, is less investigated, especially for the large ill-conditioned problems. SEP solvers such as GPower, ConGradU, and TPower only require matrix-vector product (MVP) operations and hence are efficient for large problems. For SGEP, however, those methods are no longer directly applicable. In (Sriperumbudur et al., 2011), SGEP is framed as a difference of convex functions program and solved via a sequence of convex programs where the majorizationminimization method is used. In (Song et al., 2015), SGEP is transformed into a sequence of regular GEP via quadratic minorization functions, and the preconditioned steepest ascent method is used to find the leading eigenpair. In (Safo et al., 2018), a general framework called sparse estimation with linear programming is proposed, where the leading eigenpair of $(\widetilde{A}, \widetilde{B})$ is used to simplify the constraint. In (Tan et al., 2018), the truncated Rayleigh flow method (RIFLE) is proposed, where the approximate eigenvector is updated via fixed step size steepest ascent method, and followed by simple truncation.
Our proposal - IFTRR. We propose an inverse-free truncated Rayleigh-Ritz (IFTRR) method for SGEP. The classical Rayleigh-Ritz method is an approximate algorithm for computing eigenvalue equations (Demmel, 1997; Stewart, 2001). IFTRR has three major steps: first, the approximated eigenvector is updated via an inverse-free generalized eigensolver; second, with the help of the updated eigenvector, a truncation procedure is used to find the support set for the approximate eigenvector in the next iteration; third, a small GEP is solved, and the approximate eigenvector is updated.
In the implementation of IFTRR, only matrix-vector product (MVP) is required, and hence the method is inherently suited for large scale problems. Furthermore, IFTRR is applicable for ill-conditioned or singular $\widetilde{A}, \widetilde{B}$. Additionally, the proposed truncation procedure, which is based on "eigenvalue increment" (see Section 2), is able to find the support set of the leading eigenvector effectively. Our numerical experiments (Section 3) show that IFTRR usually converges in a few iterations.

Notation. The symbol $\otimes$ denotes the Kronecker product. The calligraphic letter $\mathcal{I}$ is usually used to denote an index set, $|\mathcal{I}|$ denotes the cardinality of $\mathcal{I}$, e.g., $\mathcal{I}=\left\{i_{1}, i_{2}, \ldots, i_{s}\right\}$, where $i_{1}, i_{2}, \ldots, i_{s}$ are distinct integers, then $|\mathcal{I}|=s$. Let $a=$ $\left[\alpha_{1}, \alpha_{2}, \ldots, \alpha_{p}\right]^{\mathrm{T}} \in \mathbb{R}^{p}, A=\left[a_{j k}\right] \in \mathbb{R}^{p \times p}, a_{\mathcal{I}}, A_{\mathcal{I}}$
stand for $\left[\alpha_{i_{1}}, \alpha_{i_{2}}, \ldots, \alpha_{i_{s}}\right] \in \mathbb{R}^{s}$ and $\left[a_{i_{j} i_{k}}\right] \in \mathbb{R}^{s \times s}$, respectively. For $w=\left[w_{1}, w_{2}, \ldots, w_{p}\right]^{\mathrm{T}} \in \mathbb{R}^{p}, \operatorname{supp}(w)$ denotes the index set of all nonzero entries of $w$, $\operatorname{supp}(w, k)$ denotes the index set of the $k$ largest magnitude entries of $w$, i.e., $\operatorname{supp}(w) \triangleq\left\{i \mid w_{i} \neq 0\right\}$, $\operatorname{supp}(w, k) \triangleq\left\{i_{1}, \ldots, i_{k}| | w_{i_{1}}\left|\geq\left|w_{i_{2}}\right| \geq \cdots \geq\left|w_{i_{p}}\right|\right\}\right.$. $A_{(j,:)}$ and $A_{(:, k)}$ denote the $j$-th row and $k$-th column of $A$, respectively. $I_{p}$ is the $p \times p$ identity matrix, and $e_{j}$ is its $j$-th column. For symmetric definite matrix pairs $(A, B)$ and $(\widetilde{A}, \widetilde{B})$, we denote $\rho(v)=\frac{v^{\mathrm{T}} A v}{v^{\mathrm{T}} B v}$, $\tilde{\rho}(v)=\frac{v^{\mathrm{T}} \widetilde{A} v}{v^{\mathrm{T}} \tilde{B} v}$. The $i$ th largest eigenvalue of $(A, B)$ is denoted by $\lambda_{i}(A, B)$.

## 2 The Inverse Free Truncated Rayleigh-Ritz Method (IFTRR)

In this section, we present the inverse-free truncated Rayleigh-Ritz (IFTRR) method for solving the sparse generalized eigenvalue problem (SGEP). We first explain the intuition behind the development of the algorithm, before we present the details of the algorithm.

The mechanism of IFTRR is deceivingly simple: given an approximate eigenvector, update the vector via certain eigensolvers, then sparsify the resulting vector via a truncation procedure.

### 2.1 Eigensolvers for Generalized Eigenvalue Problem (GEP)

For large scale generalized eigenvalue problem (GEP) $\widetilde{A} v=\lambda \widetilde{B} v$, where $\widetilde{A}, \widetilde{B} \in \mathbb{R}^{p \times p}$ are symmetric and $\widetilde{B}$ is (semi) positive definite, iterative methods are usually used to compute its a few largest (or smallest) eigenvalues and the corresponding eigenvectors. Simply speaking, these iterative methods consist of two major steps: first, determine a subspace of $\mathbb{R}^{p}$; second, update the approximate eigenpairs via the Rayleigh-Ritz procedure. Some detailed discussions follow.

The subspace. The most popular subspace for the eigenvalue problem is the Krylov subspace. Given a matrix $T \in \mathbb{R}^{p \times p}$ and a nonzero vector $v \in \mathbb{R}^{p}$, the order- $m$ Krylov subspace is defined as

$$
\begin{equation*}
\mathscr{K}_{m}(T, v) \triangleq \operatorname{span}\left\{v, T v, T^{2} v, \ldots, T^{m-1} v\right\} \tag{3}
\end{equation*}
$$

An orthonormal basis of $\mathscr{K}_{m}(T, v)$ can be obtained via the Arnoldi iteration, e.g., (Stewart, 2001, Chapter 5), (Demmel, 1997, Chapter 6). Here we would like to emphasize that since the Arnoldi iteration only requires matrix vector product (MVP) Tv, it is unnecessary to formulate $T$ explicitly and a subroutine that computes $T v$ is sufficient. For GEP, $T$ is usually set as $T=\widetilde{B}^{-1} \widetilde{A}$. As $\widetilde{B}^{-1}$ is involved, the implementation of the MVP $T v$ requires the MVP $u=\widetilde{A} v$ and also solving the linear system $\widetilde{B} z=u$ for $z$. When the matrix size $p$ is
large, it is expensive to solve the linear system $\widetilde{B} z=u$. More importantly, when $\widetilde{B}$ is ill-conditioned (or even singular), solving $\widetilde{B} z=u$ is not only expensive but also prone to large numerical errors. In (Golub and Ye, 2002), Golub and Ye propose to use $\mathscr{K}_{m}(\widetilde{A}-\rho \widetilde{B}, v)$ to solve GEP, where $\rho \in \mathbb{R}$ is a shift. There are also other subspaces that can be used to solve GEP, e.g., the Davidson method (Davidson, 1975) and the JacobiDavidson method (Sleijpen and Van der Vorst, 2000). In this paper, we use the Krylov subspace $\mathscr{K}_{m}(\widetilde{A}-$ $\rho \widetilde{B}, v)$, mainly due to its simplicity, scalability, and most importantly, it is inverse-free, since only MVP $(\widetilde{A}-\rho \widetilde{B}) v$ is required.
The Rayleigh-Ritz procedure. Given an $m$ dimensional subspace $\mathcal{V}_{m}$ of $\mathbb{R}^{p}(m \ll p)$, let $V_{m}$ be an orthonormal basis of $\mathcal{V}_{m}$. The Rayleigh-Ritz procedure has three steps: First, project the GEP $\widetilde{A} v=\lambda \widetilde{B} v$ onto $\mathcal{V}_{m}$, which yields a small GEP $\left(V^{\mathrm{T}} \widetilde{A} V\right) y=\mu\left(V^{\mathrm{T}} \widetilde{B} V\right) y$; Second, solve the eigenpairs $\left(\mu_{i}, y_{i}\right)$ for $i=1, \ldots, m$ of the small GEP; Third, compute $\left(\tilde{\lambda}_{i}, \tilde{v}_{i}\right)=\left(\mu_{i}, V_{m} y_{i}\right)$ for $i=1, \ldots, m$. Then $\left(\tilde{\lambda}_{i}, \tilde{v}_{i}\right)$ 's, often referred to as Ritz pairs, are used as approximate eigenpairs of the original GEP $\widetilde{A} v=\lambda \widetilde{B} v$.

### 2.2 The Truncation Procedure

Let $(\rho, w)$ be a Ritz pair, which is used to approximate the leading eigenpair of $(\widetilde{A}, \widetilde{B})$. In general, $w$ is dense. So, it is natural to sparsify $w$ since we are solving a sparse vector. A popular way to accomplish this task is the so-called truncation, where the entries of $w$ are truncated to zeros except for the first $k$ largest magnitude entries. However, this truncation procedure is found to be potentially misleading (Cadima and Jolliffe, 1995). In this paper, we propose to do the "truncation procedure" as follows:

1. Find a permutation $\left\{i_{1}, i_{2}, \ldots, i_{p}\right\}$ of $\{1,2, \ldots, p\}$ such that $\left|w_{i_{1}}\right| \geq\left|w_{i_{2}}\right| \geq \cdots \geq\left|w_{i_{p}}\right|$.
2. For $s=s_{1}, s_{1}+1, \ldots, s_{2}$, set $\mathcal{J}=\left\{i_{1}, i_{2}, \ldots, i_{s}\right\}$ and compute the leading eigenpair of the small $\operatorname{GEP}\left(\widetilde{A}_{\mathcal{J}}, \widetilde{B}_{\mathcal{J}}\right)$, denoted by $\left(\rho_{s}, z_{s}\right), s_{1}<s_{2}$ are user-prescribed integers.
3. Determine the smallest $s$ such that $\rho_{s_{2}}-\rho_{s} \leq$ tol, where tol $>0$ is a small real number.
4. Set $\mathcal{I}=\left\{i_{1}, i_{2}, \ldots, i_{s}\right\}, \hat{v}_{\mathcal{I}}=z_{s}$ and $\hat{v}_{\mathcal{I}^{c}}=0$.

The above truncation procedure is based on this observation: for any $\mathcal{J} \supseteq \mathcal{I}=\operatorname{supp}\left(v_{1}\right)$, we have

$$
\lambda_{1}=\max _{z \neq 0} \frac{z^{\mathrm{T}} A_{\mathcal{I}} z}{z^{\mathrm{T}} B_{\mathcal{I}} z} \leq \max _{z \neq 0} \frac{z^{\mathrm{T}} A_{\mathcal{J}} z}{z^{\mathrm{T}} B_{\mathcal{J}} z} \leq \max _{z \neq 0} \frac{z^{\mathrm{T}} A z}{z^{\mathrm{T}} B z}=\lambda_{1} .
$$

Thus, $\max _{z \neq 0} \frac{z^{\mathrm{T}} A_{\mathcal{J}} z}{z^{\mathrm{T}} B_{\mathcal{J}} z} \equiv \lambda_{1}$ as long as $\mathcal{J} \supseteq \mathcal{I}$. In other words, when $\mathcal{J}$ is a superset of $\mathcal{I}$, the leading eigenvalue
of $\left(A_{\mathcal{J}}, B_{\mathcal{J}}\right)$ remains a constant. Therefore, for $(\widetilde{A}, \widetilde{B})$, we also expect that when $\mathcal{J}$ contains $\mathcal{I}$ and $|\mathcal{J}| \ll p$, the leading eigenvalue of $\left(\widetilde{A}_{\mathcal{J}}, \widetilde{B}_{\mathcal{J}}\right)$ slightly changes.

Let $\hat{w}_{\mathcal{I}}=w, \hat{w}_{\mathcal{I}^{c}}=0$. We prefer $\hat{v}$ rather than the simple truncated vector $\hat{w}$ simply because

$$
\tilde{\rho}(\hat{v})=\max _{\operatorname{supp}(v) \subset \mathcal{I}} \tilde{\rho}(v) \geq \tilde{\rho}(\hat{w}),
$$

i.e., the target value of $\tilde{\rho}(v)$ at $v=\hat{v}$ is no less than that at $v=\hat{w}$.

In order to compare the simple truncation method with our "eigenvalue increment" method, we take an approximate leading eigenvector $w=\left[w_{1}, \ldots, w_{p}\right]^{\mathrm{T}}$ of $(\widetilde{A}, \widetilde{B})$ from section $3.1(p=1000, n=200, s=6)$. We sort the entries of $w$ such that $\left|w_{i_{1}}\right| \geq \cdots \geq\left|w_{i_{p}}\right|$, and compute $\rho_{s}=\lambda_{1}\left(\widetilde{A}_{\mathcal{J}_{s}}, \widetilde{B}_{\mathcal{J}_{s}}\right)$, where $\mathcal{J}_{s}=\left\{i_{1}, \ldots, i_{s}\right\}$.


Figure 1: Absolute entries vs. eigenvalues.
In Figure 1, we plot the top 25 entries $\left|w_{i_{1}}\right|, \ldots,\left|w_{i_{25}}\right|$ and the 25 eigenvalues $\rho_{1}, \ldots, \rho_{25}$. We can see that there is no obvious gap among $\left|w_{5}\right|, \ldots,\left|w_{18}\right|$, therefore, it is difficult to determine a proper $k$ to do the simple truncation. On the other hand, $\rho_{13}, \ldots, \rho_{25}$ almost remain unchanged, then we may use $\mathcal{I}=\left\{i_{1}, \ldots, i_{13}\right\}$ as the support set for a new approximate eigenvector. In other words, $w_{i_{14}}, \ldots, w_{i_{1000}}$ are truncated to zeros. As a matter of fact, for this example, the true support set of $v_{1}$ is contained in $\left\{i_{1}, \ldots, i_{13}\right\}$.

The above example (and many others) show that our truncation procedure is effective to find the true support set of $v_{1}$. As a result, the proposed algorithm usually converges in a few steps.

### 2.3 Algorithm

We present the IFTRR method in Algorithm 1. Basically, IFTRR consists of three parts: The first part (lines 5 to 7 ) updates the leading eigenvector of ( $\widetilde{A}, \widetilde{B}$ ) via an eigensolver. The second part determines an index set $\mathcal{J}$, which serves as the support of $v^{(t)}$ (lines 8 to 13 ), then compute $v^{(t)}$ (line 17). The third part (line 20) determines $\mathcal{I}$ and compute the final solution $\tilde{v}$ with $\operatorname{supp}(\tilde{v})=\mathcal{I}$. The first two parts generate a
sequence $\left\{\left(\rho^{(t)}, v^{(t)}\right)\right\}_{t}$, and the last part is the final update for the solution. Some implementation details and discussions of the algorithm follow.

```
Algorithm 1 The proposed inverse-free truncated
Rayleigh-Ritz (IFTRR) method.
    Input: \(\widetilde{A}, \widetilde{B}\), an integer \(k\) for sparsity level, an
    integer \(m\) for Krylov subspace dimension, and a
    randomly generated initial guess \(v^{(0)} \in \mathbb{R}^{p}\).
    Output: An approximate solution \(\tilde{v}\) to (1).
    Set \(t=0, \rho^{(0)}=\tilde{\rho}\left(v^{(0)}\right), s_{1}=k\) and \(s_{2}=k+\Delta k\);
    (e.g., \(\Delta k=20\) or 30 .)
    while unconverged and \(t<\) itermax do
        Compute an orthonormal \(Q \in \mathbb{R}^{p \times m}\) such that
    \(\operatorname{span}(Q)=\mathscr{K}_{m}\left(\widetilde{A}-\rho^{(t)} \widetilde{B}, v^{(t)}\right) ;\)
        Solve the leading eigenvector \(\tilde{y}\) of
    \(\left(Q^{\mathrm{T}} \widetilde{A} Q, Q^{\mathrm{T}} \widetilde{B} Q\right) ;\)
        Set \(w=Q \tilde{y}, w=w /\|w\|_{2}\);
        Find a permutation \(\left\{i_{1}, i_{2}, \ldots, i_{p}\right\}\) of
    \(\{1,2, \ldots, p\}\) such that \(\left|w_{i_{1}}\right| \geq\left|w_{i_{2}}\right| \geq \cdots \geq\left|w_{i_{p}}\right|\);
        for \(s=s_{1}, s_{1}+1, \ldots, s_{2}\) do
            Set \(\mathcal{J}=\left\{i_{1}, i_{2}, \ldots, i_{s}\right\}\);
            Solve the leading eigenpair of \(\left(\widetilde{A}_{\mathcal{J}}, \widetilde{B}_{\mathcal{J}}\right)\), de-
    note it by \(\left(\rho_{s}, z_{s}\right)\);
        end for
        Find the smallest \(s \in\left\{s_{1}, s_{1}+1, \ldots, s_{2}\right\}\) such
    that \(\rho_{s_{2}}-\rho_{s} \leq\left(s_{2}-s\right) \times\) tol;
    4: \(\quad\) Set \(\rho^{(t+1)}=\rho_{s}, v_{\mathcal{J}}^{(t+1)}=z_{s} /\left\|z_{s}\right\|_{2}, v_{\mathcal{J}^{c}}^{(t+1)}=0\),
    where \(\mathcal{J}=\left\{i_{1}, i_{2}, \ldots, i_{s}\right\}\);
        Set \(t=t+1\);
    end while
    17: Let \(\mathcal{I}=\operatorname{supp}\left(v^{(t)}, k\right)\), solve the leading eigenvector
    \(z\) of \(\left(\widetilde{A}_{\mathcal{I}}, \widetilde{B}_{\mathcal{I}}\right)\), set \(\tilde{v}_{\mathcal{I}}=z /\|z\|_{2}, \tilde{v}_{\mathcal{I}^{c}}=0\).
```

Convergence test. The maximum number of iterations itermax is set as 100. The algorithm converges if one of the following conditions is satisfied:
(i) $\frac{\left\|\left(\tilde{A}-\rho^{(t)} \widetilde{B}\right) v^{(t)}\right\|_{2}}{\|\tilde{A}\|_{2}+\left|\rho^{(t)}\right|\|\tilde{B}\|_{2}}<\mathrm{tol}_{1}$, where $\mathrm{tol}_{1}$ is a tolerance and is set as 0.01 in our experiments. This condition indicates that $\left(\rho^{(t)}, v^{(t)}\right)$ is a good approximation of an eigenpair of $(\widetilde{A}, \widetilde{B})$.
(ii) $\left|\rho^{(t)}-\rho^{(t-1)}\right|<\mathrm{tol}_{2}$, where $\mathrm{tol}_{2}$ is a prescribed tolerance, say $10^{-3}$. This condition indicates that the value of $\rho^{(t)}$ stagnates, hence we may take $\left\{\rho^{(t)}\right\}$ as a converged sequence.
Solving a sequence of GEPs. At first glance, a sequence of generalized eigenvalue problems needs to be solved on lines 9 to 12 . But notice that

$$
\rho_{s+1}=\max _{z \neq 0} \frac{z^{\mathrm{T}} \widetilde{A}_{\mathcal{J}_{2}} z}{z^{\mathrm{T}} \widetilde{B}_{\mathcal{J}_{2}} z} \geq \frac{\left[\begin{array}{c}
z_{s} \\
0
\end{array}\right]^{\mathrm{T}} \widetilde{A}_{\mathcal{J}_{2}}\left[\begin{array}{c}
z_{s} \\
0
\end{array}\right]}{\left[\begin{array}{c}
z_{s} \\
0
\end{array}\right]^{\mathrm{T}} \widetilde{\mathcal{J}}_{2}\left[\begin{array}{c}
z_{s} \\
0
\end{array}\right]}=\rho_{s},
$$

where $\mathcal{J}_{1}=\left\{i_{1}, i_{2}, \ldots, i_{s}\right\}, J_{2}=\left\{i_{1}, i_{2}, \ldots, i_{s}, i_{s+1}\right\}$. Thus $\left\{\rho_{s}\right\}_{s=s_{1}}^{s_{2}}$ is a non-decreasing sequence and we use
the idea of bisection to find the desired $s$ on line 13 :

```
Set \(a=s_{1}, b=s_{2}\);
Compute \(\rho_{a}, \rho_{b}\);
While \(b-a>1\) do
    Set \(s=\frac{a+b+\bmod (a+b, 2)}{2}\);
    Compute \(\rho_{s}\);
    If \(\rho_{s_{2}}-\rho_{s} \leq \mathrm{tol}\), set \(b=s, \rho_{b}=\rho_{s}\);
    Otherwise, set \(a=s, \rho_{a}=\rho_{s}\).
```


## End while

As a result, there are approximately $\log _{2}\left(s_{2}-s_{1}+1\right)$ small GEPs rather than $s_{2}-s_{1}+1$.
Dealing with ill-conditioning. When $\widetilde{B}$ is singular, $\widetilde{B}_{\mathcal{J}}$ can also be singular. As a result, infinity or indeterminate eigenvalues, which are sensitive to perturbations (Bai et al., 2000), occur, then it will be difficult to determine which eigenpair is the leading one. In our implementation, we use the following procedure as a cure for singular $\widetilde{B}_{\mathcal{J}}$ : First, compute the QR decomposition of $\widetilde{B}_{\mathcal{J}}$ with column pivoting (Van Loan and Golub, 2012, Chapter 5.4.2) $\widetilde{B}_{\mathcal{J}} \Pi=U R$, where $\Pi$ is a permutation matrix, $U$ is an orthogonal matrix and $R$ is upper triangular with its diagonal entries non-negative and non-increasing; Then let tol ${ }_{3}>0$ be a user given threshold, say $\mathrm{tol}_{3}=10^{-9}$. Whenever $R_{(i, i)}<\mathrm{tol}_{3} \times R_{(1,1)}$, we remove the corresponding index in $\mathcal{J}$. For the resulting $\mathcal{J}, \widetilde{B}_{\mathcal{J}}$ is good conditioned.

Table 1: Computational complexity of Algorithm 1. See the next paragraph "Computational complexity. for the explanation of "-".

| Line No. | OPERATION | COMPLEXITY |
| :---: | :---: | :---: |
| 5 | MVP | - |
| 5 | ORTHOGONALIZATION | $\mathcal{O}\left(m^{2} p\right)$ |
| 6 | EIGENVALUE PROB. | $\mathcal{O}\left(m^{3}\right)$ |
| 8 | SORTING | $\mathcal{O}(p \log p)$ |
| 11,17 | EIGENVALUE PROB. | $\mathcal{O}\left(s^{3}\right)$ |

Computational complexity. In Table 1, we list the computational complexity of the major steps of the IFTRR method. The symbol "-" means the computational complexity is different case by case: (1) when $\widetilde{A}$ and $\widetilde{B}$ are available, the operation $\left(\widetilde{A}-\rho^{(t)} \widetilde{B}\right) v$ requires $\mathcal{O}\left(m p^{2}\right)$ FLOPS if $\widetilde{A}$ and $\widetilde{B}$ are dense, $\mathcal{O}(m(\operatorname{nnz}(\widetilde{A})+$ $\operatorname{nnz}(\widetilde{B})))$ FLOPS if $\widetilde{A}$ and $\widetilde{B}$ are sparse; (2) when $\widetilde{A}$ and $\widetilde{B}$ are unavailable directly, the operations $\widetilde{A} v$ and $\widetilde{B} v$ are carried out via a data matrix $X \in \mathbb{R}^{n \times p}$, then the operation $\left(\widetilde{A}-\rho^{(t)} \widetilde{B}\right) v$ in general requires $\mathcal{O}(m n p)$ FLOPS if $\widetilde{A}$ and $\widetilde{B}$ are dense, $\mathcal{O}(m \mathrm{nnz}(X))$ FLOPS if $X$ are sparse. ${ }^{1}$ Since $s \ll p$ and $m \ll p$, the overall

[^0]complexity of IFTRR is dominated by line 5 .

### 2.4 Convergence

Before the study of the convergence, we give some definitions and preliminary lemmas.
The angle between two vectors $x, y \in \mathbb{R}^{p}$ is defined as $\theta(x, y) \triangleq \arccos \frac{\left|x^{\mathrm{T}} y\right|}{\|x\|\|y\|}$. Define the Crawford number for a definite-symmetric matrix pair $(A, B)$ as

$$
c(A, B) \triangleq \min _{\|x\|_{2}=1} \sqrt{\left(x^{\mathrm{T}} A x\right)^{2}+\left(x^{\mathrm{T}} B x\right)^{2}} .
$$

The following lemma tells that when $(A, B)$ is slightly perturbed, the changes of eigenvalues are small.

Lemma 1 (Van Loan and Golub, 2012, Theorem 8.7.3) Suppose $(A, B)$ is a symmetric-definite pair with eigenvalues $\lambda_{1} \geq \lambda_{2} \geq \cdots \geq \lambda_{p}, E$ and $F$ are symmetric p-by-p matrices that satisfy

$$
\epsilon=\sqrt{\|E\|_{2}^{2}+\|F\|_{2}^{2}}<c(A, B)
$$

Then $(A+E, B+F)$ is also a symmetric-definite pair with eigenvalues $\tilde{\lambda}_{1} \geq \tilde{\lambda}_{2} \geq \cdots \geq \tilde{\lambda}_{p}$ that satisfy
$\left|\arctan \left(\lambda_{i}\right)-\arctan \left(\tilde{\lambda}_{i}\right)\right| \leq \arctan (\epsilon / c(A, B))$,

$$
\text { for } \quad i=1,2, \ldots, p .
$$

Let $\left(\lambda^{(t)}, u^{(t)}\right)$ be the current guess of the largest eigenpair of $(A, B)$ and $Q_{t} \in \mathbb{R}^{p \times m}$ be an orthonormal basis for $\mathscr{K}_{m}\left(A-\lambda^{(t)} B, u^{(t)}\right)$. Then $\left(\lambda^{(t+1)}, u^{(t+1)}\right)$ can be obtained via the Rayleigh-Ritz procedure. Specifically, let $(\omega, y)$ be the largest eigenpair of $\left(Q_{t}^{\mathrm{T}} A Q_{t}, Q_{t}^{\mathrm{T}} B Q_{t}\right)$, then $\lambda^{(t+1)}=\omega, u^{t+1}=Q_{t} y$. By (Golub and Ye, 2002, Theorem 3.4), we have the following lemma.

Lemma 2 Let the eigenvalues of $A-\lambda^{(t)} B$ be $\sigma_{p} \leq$ $\cdots \leq \sigma_{2}<\sigma_{1}$. Assume $\lambda_{2}<\lambda^{(t)}<\lambda_{1}$. Then

$$
\lambda_{1}-\lambda^{(t+1)} \leq\left(\lambda_{1}-\lambda^{(t)}\right) \epsilon_{m}^{2}+\mathcal{O}\left(\left(\lambda_{1}-\rho^{(t)}\right)^{\frac{3}{2}}\right)
$$

where $\epsilon_{m}=\min _{p \in \mathcal{P}_{m}, p\left(\sigma_{1}\right)=1} \max _{i \neq 1}\left|p\left(\sigma_{i}\right)\right| \leq 2\left(\frac{1-\sqrt{\psi}}{1+\sqrt{\psi}}\right)^{m}$
with $\mathcal{P}_{m}$ denoting the set of all polynomials of degree not greater than $m, \psi=\frac{\sigma_{1}-\sigma_{2}}{\sigma_{1}-\sigma_{q}}$.

Let $\rho^{(t)}, v^{(t)}$ be obtained via Algorithm 1. Denote $\mathcal{J}_{t}=\operatorname{supp}\left(v^{(t)}\right)$. Here, we consider an alternative way to update $\rho^{(t)}, v^{(t)}$ :
(i) Compute an orthonormal basis for $\mathscr{K}_{m}\left(\widetilde{A}_{\mathcal{J}_{t+1}}-\rho^{(t)} \widetilde{B}_{\mathcal{J}_{t+1}}, v_{\mathcal{J}_{t+1}}^{(t)}\right)$, denote it as $Q_{\mathcal{J}_{t+1}}$;
$\mathbf{1}_{n}=[1, \ldots, 1]^{\mathrm{T}} \in \mathbb{R}^{n}, \bar{x}=\left[\bar{x}_{1}, \ldots, \bar{x}_{p}\right]^{\mathrm{T}}, \bar{x}_{i}$ is the mean of the $i$-th column of $X$. Then MVP $u=C v$ is computed as $w=X v-\left(\bar{x}^{\mathrm{T}} v\right) \mathbf{1}_{n}, u=\frac{1}{n}\left(X^{\mathrm{T}} w-\left(\mathbf{1}_{n}^{\mathrm{T}} w\right) \bar{x}\right)$, which requires $\mathcal{O}(n p)$ if $X$ is dense, and $\mathcal{O}(n n z(X))$ if $X$ is sparse.
(ii) Solve the largest eigenpair of $\left(Q_{\mathcal{J}_{t+1}}^{\mathrm{T}} \widetilde{A}_{\mathcal{J}_{t+1}} Q_{\mathcal{J}_{t+1}}, Q_{\mathcal{J}_{t+1}}^{\mathrm{T}} \widetilde{B}_{\mathcal{J}_{t+1}} Q_{\mathcal{J}_{t+1}}\right)$, and denote it by ( $\omega, y$ );
(iii) Set $\hat{\rho}^{(t+1)}=\omega, \hat{v}_{\mathcal{J}_{t+1}}^{(t+1)}=Q_{\mathcal{J}_{t+1}} y, \hat{v}_{\mathcal{J}_{t+1}^{c}}^{(t+1)}=0$.

Note that the above Rayleigh-Ritz procedure is only for the purpose of analyzing the convergence, is not applicable in practice since $\mathcal{J}_{t+1}$ is unknown. Also note that the existence of $Q_{\mathcal{J}_{t+1}}$ implicitly requires that $m \leq\left|\mathcal{J}_{t+1}\right|$, meaning that the dimension of the Krylov subspace should not exceed sparsity level of the approximate eigenvector.

By Lemma 2, we have the following result.
Lemma 3 Let $\mathcal{J}_{t}=\operatorname{supp}\left(v^{(t)}\right), \ell=\left|\mathcal{J}_{t+1}\right|$, the eigenvalues of $\left(\widetilde{A}_{\mathcal{J}_{t+1}}, \widetilde{B}_{\mathcal{J}_{t+1}}\right)$ be $\lambda_{1, t+1} \geq \cdots \geq \lambda_{\ell, t+1}$, the eigenvalues of $\widetilde{A}_{\mathcal{J}_{t+1}}-\rho^{(t)} \widetilde{B}_{\mathcal{J}_{t+1}}$ be $\sigma_{\ell} \leq \cdots \leq \sigma_{2}<\sigma_{1}$. Assume $\lambda_{2, t+1}<\rho^{(t)}<\lambda_{1, t+1}$. Then

$$
\begin{aligned}
\lambda_{1, t+1}-\hat{\rho}^{(t+1)} \leq\left(\lambda_{1, t+1}\right. & \left.-\rho^{(t)}\right) \epsilon_{m}^{2} \\
& +\mathcal{O}\left(\left(\lambda_{1, t+1}-\rho^{(t)}\right)^{\frac{3}{2}}\right)
\end{aligned}
$$

where $\epsilon_{m}$ is the same as in Lemma 2.
Recall that $\rho^{(t+1)}$ is the largest eigenvalue of $\left(\widetilde{A}_{\mathcal{J}}, \widetilde{B}_{\mathcal{J}}\right), \quad \hat{\rho}^{(t+1)} \quad$ is the largest eigenvalue of $\left(Q_{\mathcal{J}_{t+1}}^{\mathrm{T}} \widetilde{A}_{\mathcal{J}_{t+1}} Q_{\mathcal{J}_{t+1}}, Q_{\mathcal{J}_{t+1}}^{\mathrm{T}} \widetilde{B}_{\mathcal{J}_{t+1}} Q_{\mathcal{J}_{t+1}}\right)$, and $\mathcal{J}_{t+1} \subset \mathcal{J}$. Then we have
Lemma 4 It holds that $\rho^{(t+1)} \geq \hat{\rho}^{(t+1)}$.
Define

$$
\begin{align*}
& \eta_{s}^{(2)} \triangleq \max _{|\mathcal{J}| \leq s} \lambda_{2}\left(\widetilde{A}_{\mathcal{J}}, \widetilde{B}_{\mathcal{J}}\right)  \tag{4a}\\
& \eta_{s, \ell}^{(1)} \triangleq \max _{\substack{|\mathcal{J}| \leq s \\
\left|\mathcal{J} \cap \operatorname{supp}\left(v_{1}\right)\right| \leq \ell}} \lambda_{1}\left(\widetilde{A}_{\mathcal{J}}, \widetilde{B}_{\mathcal{J}}\right) . \tag{4b}
\end{align*}
$$

Combining Lemmas 3 and 4, we have
Theorem 1 Let $\mathcal{J}_{t}=\operatorname{supp}\left(v^{(t)}\right), s=\sup _{t}\left|\mathcal{J}_{t}\right|$ and $k=\left|\operatorname{supp}\left(v_{1}\right)\right|$. For any $\mathcal{J} \subset[p]$ with $|\mathcal{J}|=s$, denote the eigenvalues of $\widetilde{A}_{\mathcal{J}}-\rho^{(t)} \widetilde{B}_{\mathcal{J}}$ by $\sigma_{1, \mathcal{J}}>\sigma_{2, \mathcal{J}} \geq \cdots \geq$ $\lambda_{s, \mathcal{J}}$,

$$
\psi_{*}=\min _{|\mathcal{J}|=s} \frac{\sigma_{1, \mathcal{J}}-\sigma_{2, \mathcal{J}}}{\sigma_{1, \mathcal{J}}-\sigma_{s, \mathcal{J}}}, \quad \epsilon_{*}=2\left(\frac{1-\sqrt{\psi_{*}}}{1+\sqrt{\psi_{*}}}\right)^{m}
$$

If $\eta_{s, k-1}^{(1)} \geq \rho^{(t)}>\eta_{s}^{(2)}$ and $\left|\mathcal{J}_{t} \cap \operatorname{supp}\left(v_{1}\right)\right|<k$, then there exists a $\lambda_{1, t+1} \in\left(\rho^{(t)},+\infty\right)$ such that

$$
\begin{aligned}
\lambda_{1, t+1}-\rho^{(t+1)} \leq\left(\lambda_{1, t+1}\right. & \left.-\rho^{(t)}\right) \epsilon_{*}^{2} \\
& +\mathcal{O}\left(\left(\lambda_{1, t+1}-\rho^{(t)}\right)^{\frac{3}{2}}\right)
\end{aligned}
$$

Asymptotically,

$$
\rho^{(t+1)} \gtrsim \rho^{(t)}+\left(\lambda_{1, t+1}-\rho^{(t)}\right)\left(1-\epsilon_{*}^{2}\right)
$$

Remark 1 Let $s>k=\left|\operatorname{supp}\left(v_{1}\right)\right|$. Assuming that for any $|\mathcal{J}| \leq s,\left\|\widetilde{A}_{\mathcal{J}}-A_{\mathcal{J}}\right\|^{2}+\left\|\widetilde{B}_{\mathcal{J}}-B_{\mathcal{J}}\right\|^{2}$ is small, by Lemma 1, we know that $\lambda_{i}\left(\widetilde{A}_{\mathcal{J}}, \widetilde{B}_{\mathcal{J}}\right) \approx$ $\lambda_{i}\left(A_{\mathcal{J}}, B_{\mathcal{J}}\right)$, for all $i=1,2, \ldots, s$. By interlacing property (e.g., (Van Loan and Golub, 2012, Theorem 8.1.7)), $\lambda_{2}\left(A_{\mathcal{J}}, B_{\mathcal{J}}\right) \leq \lambda_{2}$. Therefore, we have

$$
\eta_{s}^{(2)} \lesssim \lambda_{2}<\lambda_{1} \approx \eta_{s, k}^{(1)}
$$

i.e., the gap between $\eta_{s}^{(2)}$ and $\eta_{s, k}^{(1)}$ is larger than that between $\lambda_{2}$ and $\lambda_{1}$. In fact, in practice, the former is much larger than the latter.

Remark 2 Let $k=\left|\operatorname{supp}\left(v_{1}\right)\right|$. Intuitively, we also expect a gap between $\eta_{s, k-1}^{(1)}$ and $\eta_{s, k}^{(1)}$, the larger the gap is, the easier the problem is. Otherwise, when the gap is sufficiently small, the problem has two "solutions": one is approximately $v_{1}$, the other is $v^{\prime}$ such that $\tilde{\rho}\left(v^{\prime}\right)=\eta_{s, k-1}^{(1)} ;$ they are both sparse, and $\tilde{\rho}\left(v_{1}\right) \approx \tilde{\rho}\left(v^{\prime}\right)$. In addition, notice that $\left\|v^{\prime}\right\|_{0}=k-1<k=\left\|v_{1}\right\|_{0}$, consequently, we can not expect to find good approximation of the true solution $v_{1}$, since $v^{\prime}$ is a "better" solution, in the sense that it is sparser and $\tilde{\rho}\left(v_{1}\right) \approx \tilde{\rho}\left(v^{\prime}\right)$.

Theorem 1 tells that as long as $\operatorname{supp}\left(v_{1}\right)$ is not a subset of $\mathcal{J}_{t}$ and $\rho^{(t)}>\eta_{s}^{(2)},\left\{\rho^{(t)}\right\}_{t}$ is asymptotically nondecreasing. Theorem 2 below tells that once $\rho^{(t)}$ is larger than $\eta_{s, k-1}^{(1)}, \operatorname{supp}\left(v_{1}\right)$ is a subset of $\mathcal{J}_{t}$.

Theorem 2 If $\rho^{(t)}>\eta_{s, k-1}^{(1)}$ with $k=\left|\operatorname{supp}\left(v_{1}\right)\right|$, then $\operatorname{supp}\left(v_{1}\right) \subset \mathcal{J}_{t}$.

The following theorem tells that when $\operatorname{supp}\left(v_{1}\right) \subset$ $\operatorname{supp}\left(v^{(t)}\right)$, then $\rho^{(t)}$ is close to $\lambda_{1}$ and $\theta\left(v^{(t)}, v_{1}\right)$ is small, i.e., they are approximations of $\lambda_{1}$ and $v_{1}$.

Theorem 3 Let $\mathcal{J}_{t}=\operatorname{supp}\left(v^{(t)}\right)$. Denote $c_{\mathcal{J}}=$ $c\left(A_{\mathcal{J}_{t}}, B_{\mathcal{J}_{t}}\right), E_{\mathcal{J}}=\widetilde{A}_{\mathcal{J}_{t}}-A_{\mathcal{J}_{t}}, F_{\mathcal{J}}=\widetilde{B}_{\mathcal{J}_{t}}-B_{\mathcal{J}_{t}}$, and $\epsilon_{\mathcal{J}}=\sqrt{\left\|E_{\mathcal{J}}\right\|_{2}^{2}+\left\|F_{\mathcal{J}}\right\|_{2}^{2}}$. Assume $\operatorname{supp}\left(v_{1}\right) \subset \mathcal{J}_{t}$.
(a) If $\epsilon_{\mathcal{J}}<c_{\mathcal{J}}$, then

$$
\left|\arctan \left(\rho^{(t)}\right)-\arctan \left(\lambda_{1}\right)\right| \leq \arctan \left(\epsilon_{\mathcal{J}} / c_{\mathcal{J}}\right)
$$

(b) Furthermore, if $\left|\rho^{(t)}\right| \epsilon_{\mathcal{J}}<c_{\mathcal{J}}$ and $\rho^{(t)}$ is simple, then

$$
\sin \theta\left(v^{(t)}, v_{1}\right) \leq \frac{\left\|\widetilde{B}_{\mathcal{J}_{t}}\right\|_{2} \delta+\sqrt{1+\mu^{2}} \epsilon_{\mathcal{J}}}{g}=\mathcal{O}\left(\epsilon_{\mathcal{J}}\right)
$$

where $g$ is the smallest nonzero singular value of $\widetilde{A}_{\mathcal{J}_{t}}-$ $\rho^{(t)} \widetilde{B}_{\mathcal{J}_{t}}, \delta=\frac{\left(1+\left(\rho^{(t)}\right)^{2}\right) \epsilon_{\mathcal{J}}}{c_{\mathcal{J}}-\left|\rho^{(t)}\right| \epsilon_{\mathcal{J}}}$.

## 3 Numerical Experiments

To illustrate the behavior of the IFTRR method and compare it with existing methods for the SGEP, this section presents some numerical experiments.

### 3.1 Sparse Canonical Correlation Analysis

Recall Example 2. In our simulations, we set $\Sigma_{x x}=$ $\Sigma_{y y}=I_{5} \otimes D, D=\left[d_{j l}\right] \in \mathbb{R}^{p / 10 \times p / 10}$ is a Toeplitz matrix with $d_{j l}=0.8^{|j-l|}$. Let $v_{x}^{*}$ be collinear with $\sum_{j=1}^{s / 2} e_{5 j-4}$ and $\left(v_{x}^{*}\right)^{\mathrm{T}} \Sigma_{x x} v_{x}^{*}=1$, where $s$ is a small even integer. Set $v_{y}^{*}=v_{x}^{*}, \Sigma_{x y}=0.9 \times \Sigma_{x x} v_{x}^{*}\left(v_{y}^{*}\right)^{\mathrm{T}} \Sigma_{y y}$ (low rank case), or $\Sigma_{x y}=0.9 \times \Sigma_{x x} v_{x}^{*}\left(v_{y}^{*}\right)^{\mathrm{T}} \Sigma_{y y}+0.1 \times$ $\Sigma_{x x} V_{x}^{*}\left(V_{y}^{*}\right)^{\mathrm{T}} \Sigma_{y y}$ (approximate low rank case), wher $\epsilon$ $V_{x}^{*}, V_{y}^{*}$ are random matrices such that $\left(V_{x}^{*}\right)^{\mathrm{T}} \Sigma_{x x} V_{x}^{*}=$ $I_{p / 2},\left(V_{y}^{*}\right)^{\mathrm{T}} \Sigma_{y y} V_{y}^{*}=I_{p / 2}$.
We perform the IFTRR method for 200 times under the following settings:

1. Low rank $\Sigma_{x y}, p=1000, s=6$, different numbers of samples $n=100,200,300,400$;
2. Low rank $\Sigma_{x y}, p=1000, n=400$, different num bers of sparsity levels $s=6,10,14,18$;
3. Same as setting 1 except that $\Sigma_{x y}$ is approximatє low rank;
4. Same as setting 2 except that $\Sigma_{x y}$ is approximate low rank.
5. Low rank $\Sigma_{x y}, s=6, p=5000$, different numbers of samples $n=2000,4000, \ldots, 10000$;
6. Low rank $\Sigma_{x y}, s=6, n=4000$, different numbers of features $p=2000,4000, \ldots, 10000$.

The performance of the method is evaluated in terms of the angle between $v_{1}=\left[\begin{array}{c}v_{x}^{*} \\ v_{y}^{*}\end{array}\right]$ and the computed $\tilde{v}$, and also success rate - we say the returned $\tilde{v}$ is a $\operatorname{success}$ if $\operatorname{supp}\left(v_{1}\right)=\operatorname{supp}(\tilde{v})$. The results are reported in Figures 2 and 3. We can see from these figures that (i) for reasonable large $n, \tilde{v}$ (returned by the IFTRR method) is a good approximation of $v_{1}$, the larger $n$ is, the smaller the angle is, and the larger the success rate is; (ii) for different sparsity levels $s, \tilde{v}$ is also a good approximation of $v_{1}$, the smaller $s$ is, the smaller the angle is, and the larger the success rate is; (iii) the results for the low rank case are better than that for the approximate low rank case. The above numerical results indicate that the IFTRR method gives a better result when the number of samples is sufficiently large and the leading eigenvector $v_{1}$ is sufficiently sparse.

In Figure 4, we give the boxplots of the CPU time for settings 5 and 6 . We can see that with a fixed number of features, the CPU time increases almost linearly with respect to the number of samples; with a fixed number of samples, the CPU time increases almost linearly with respect to the number of features. This confirms that the computational cost of the IFTRR method is dominated by MVP, which is $\mathcal{O}(n p)$.


Figure 2: Accuracy and success rate, low rank case, from left to right, settings 1 to 2 .


Figure 3: Accuracy and success rate, approximate low rank case, from left to right, settings 3 to 4.


Figure 4: CPU time, from left to right, settings 5 to 6 .

### 3.2 Sparse Fisher's Discriminant Analysis

Recall Example 1. In our simulations, for $k=$ $1,2, \ldots, K$, we set $\bar{x}_{k j}=\frac{2 k-2}{K+2}$ for $j=2,4, \ldots, 40$, $\bar{x}_{k j}=0$ otherwise. The data matrix $X$ is generated via $X_{(:, i)} \sim N\left(\bar{x}_{k}, \Sigma\right)$ for $i \in \mathcal{C}_{k}$, where $\Sigma=I_{5} \otimes D$, $D=\left[d_{j l}\right] \in \mathbb{R}^{p / 5 \times p / 5}$ is a Toeplitz matrix with $d_{j l}=0.8^{|j-l|}$.

Table 2: Results of Misclassification error and number of selected features.

|  | $K$ | GLMNEt | D(M)SDA | RIFLE | IFTRR |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Err. | 2 | 32 | 29 | 15 | $\mathbf{1 4}(4)$ |
| Feat. |  | 88 | 105 | 42 | $42(1)$ |
| Err. | 4 | 495 | 247 | 192 | $\mathbf{1 0 3 ( 1 1 )}$ |
| Feat. |  | 54 | 102 | 42 | $42(1)$ |

Fix $p=500$, for $K=2,4$, using 400 training samples, we perform GLMNET (Friedman et al., 2010),

DSDA/MSDA (Mai et al., 2015, 2012), RIFLE (Tan et al., 2018) and the IFTRR method. The results are then used to classify 1000 test samples, the misclassification error (denoted by Err.) and number of selected features (denoted by Feat.) are recorded. Err. and Feat. are averaged over 200 independently generated datasets and reported in Table 2. There the number in the brackets is the corresponding standard error, and all numbers are rounded to the nearest integers. Table 2 shows that for $K=2$, the misclassification errors of RIFLE and the IFTRR method are comparable and lower than the other two methods; and for $K=4$, the IFTRR method has the lowest misclassification error.

### 3.3 Sparse Sliced Inverse Regression

Consider the sparse sliced inverse regression for the model $Y=f\left(v_{1}^{\mathrm{T}} X, \ldots, v_{k}^{\mathrm{T}} X, \epsilon\right)$, where $Y$ is a univariate response, $X$ is $d$-dimensional covariates, $\epsilon$ is the stochastic error independent of $X, f$ is the link function, which is unknown. Under regularity conditions, the subspace spanned by $v_{1}, \ldots, v_{k}$ can be identified via solving an SGEP with $\widetilde{A}=\hat{\Sigma}_{\mathbb{E}(X \mid Y)}, \widetilde{B}=\hat{\Sigma}_{x}$, where $\hat{\Sigma}_{x}$ is the sample covariance matrix of $X, \hat{\Sigma}_{\mathbb{E}(X \mid Y)}$ is the sample covariance matrix of the conditional expectation $\mathbb{E}(X \mid Y)$, which is $\hat{\Sigma}_{\mathbb{E}(X \mid Y)}=\hat{\Sigma}_{x}-\frac{1}{n_{1}+n_{2}} \sum_{k=1}^{2} n_{k} \hat{\Sigma}_{x, k}$, where $n_{k}$ is the number of samples for class $k, \hat{\Sigma}_{x, k}$ is the sample covariance matrix for class $k$, for $k=1,2$. See (Chen et al., 2010; Li, 1991, 2007; Tan et al., 2018) and reference therein for more details.

Let $v^{(t)}$ be an approximate solution to SGEP. $X v^{(t)}$ is usually used as a predictor. Here we may also use the indices for the nonzero entries of $v^{(t)}$ to select the features, and the features can be ranked by ordering the absolute values of the nonzero entries of $v^{(t)}$. Now we compare our method with feature selection methods - relieff, mutinffs, fsv and fisher, which are all available in the Feature Selection Library (Roffo, 2017; Roffo and Melzi, 2016; Roffo et al., 2017, 2015). The datasets are all downloaded from scikit-feature feature selection repository. Each dataset is randomly partitioned into a training set and a test set, and the test set size is approximately $0.2 n$. A support vector machine (SVM) classifier is trained using the training set with only the selected features and then used to predict on the test set. The average accuracy (averaged over 10 independent runs) is plotted in Figure 5. We can see that our method is comparable with the other four methods for the first 5 datasets, outperforms the other four methods for the last dataset.

## 4 Conclusion

We have proposed the IFTRR method to solve the SGEP. The IFTRR method has the following advantages: Since only the MVP is required, the method is


Figure 5: Accuracy vs. number of features.
suited for large scale problem; A cure is incorporated into the IFTRR method, which makes it applicable for ill-conditioned or singular coefficient matrices $\widetilde{A}$, $\widetilde{B}$; Based on "eigenvalue increment", a new truncation procedure is proposed, which is able to find the support set of the leading eigenvector effectively, as a result, the IFTRR method usually converges in a few iterations. Numerical simulations show that the IFTRR method is effective and efficient, especially when the matrix size is large and the leading eigenvector is very sparse.
There are several future research topics for the IFTRR method. First, can we extend the IFTRR method to compute multiple leading sparse eigenvectors? Computing several leading eigenvectors one by one seems simple, how to compute them simultaneously is uneasy since the orthogonalization procedure, which is required for computing several eigenvectors simultaneously, usually destroys the sparsity. Second, how to truncate the eigenvector to ensure some structured sparsity, say group sparsity as in the group LASSO. Third, based on the IFTRR method, a general framework for solving SGEP can be obtained - eigensolver + truncation. Various eigensolvers together with certain truncation procedure can be tried to solve the SGEP. Which is the best choice, how is the convergence? More studies towards these directions are apparently required.

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## Supplementary Materials

## A. Proof of Theorem 1

Proof. Let $\lambda_{i, t+1}$ be the $i$ th largest eigenvalue of $\left(\widetilde{A}_{\mathcal{J}_{t+1}}, \widetilde{B}_{\mathcal{J}_{t+1}}\right)$, $\hat{\rho}^{(t+1)}$ be the same as in Lemma 3. By the definition of $\eta_{s}^{(2)}$, we know that $\eta_{s}^{(2)} \geq \lambda_{2, t+1}$. Together with $\rho^{(t)}>\eta_{s}^{(2)}$, we have $\rho^{(t)}>\lambda_{2, t+1}$. On the other hand, using $\left|\mathcal{J}_{t} \cap \operatorname{supp}\left(v_{1}\right)\right|<k$, we know that $\rho^{(t)} \leq \eta_{s, k-1}^{(1)}$. Then by Lemma 3 , we have

$$
\lambda_{1, t+1}-\hat{\rho}^{(t+1)} \leq\left(\lambda_{1, t+1}-\rho^{(t)}\right) \epsilon_{m}^{2}+\mathcal{O}\left(\left(\lambda_{1, t+1}-\rho^{(t)}\right)^{\frac{3}{2}}\right),
$$

where $\epsilon_{m}$ is the same as in Lemma 2. By the definition of $\epsilon_{*}$, we know that $\epsilon_{*} \geq \epsilon_{m}$, it follows that

$$
\lambda_{1, t+1}-\hat{\rho}^{(t+1)} \leq\left(\lambda_{1, t+1}-\rho^{(t)}\right) \epsilon_{*}^{2}+\mathcal{O}\left(\left(\lambda_{1, t+1}-\rho^{(t)}\right)^{\frac{3}{2}}\right),
$$

Now using Lemma 4, we get the conclusion.

## B. Proof of Theorem 2

Proof. Noticing that $\left|\operatorname{supp}\left(v^{(t)}\right)\right| \leq s$, using the definition of $\eta_{s, \ell}^{(1)}$, we know that if $\rho^{(t)}>\eta_{s, k-1}^{(1)}$, then

$$
\left|\operatorname{supp}\left(v^{(t)}\right) \cap \operatorname{supp}\left(v_{1}\right)\right|=k=\left|\operatorname{supp}\left(v_{1}\right)\right| .
$$

The conclusion follows immediately.

## C. Proof of Theorem 3

In order to show Theorem 3, we need the following lemmas.
Lemma 5 Suppose $(A, B)$ is a symmetric-definite pair. Let $E, F$ be two symmetric matrices with $\epsilon=$ $\sqrt{\|E\|_{2}^{2}+\|F\|_{2}^{2}}<c(A, B)$. Let $(\lambda, x)$ and $(\tilde{\lambda}, \tilde{x})$ be the leading eigenpairs of $(A, B)$ and $(A+E, B+F)$, respectively. Suppose $\tilde{\lambda}$ is simple, and denote the smallest nonzero singular value of $(A+E)-\tilde{\lambda}(B+F)$ by $g$. If $|\tilde{\lambda}| \epsilon<c(A, B)$, then

$$
\sin \theta(x, \tilde{x}) \leq \frac{\|B\|_{2} \delta+\sqrt{1+\tilde{\lambda}^{2}} \epsilon}{g}
$$

where

$$
\begin{equation*}
\delta=\frac{\left(1+\tilde{\lambda}^{2}\right) \epsilon}{c(A, B)-|\tilde{\lambda}| \epsilon} . \tag{5}
\end{equation*}
$$

Proof. First, since $\epsilon<c(A, B)$, by Lemma $1,(A+E, B+F)$ is a definite pair and

$$
\begin{equation*}
\arctan (\tilde{\lambda})-\arctan (\epsilon / c(A, B)) \leq \arctan (\lambda) \leq \arctan (\tilde{\lambda})+\arctan (\epsilon / c(A, B)) . \tag{6}
\end{equation*}
$$

Using $|\tilde{\lambda}| \epsilon<c(A, B)$, we know that $\arctan (\epsilon / c(A, B))<\arctan (1 /|\tilde{\lambda}|)=\frac{\pi}{2}-\arctan (|\tilde{\lambda}|)$, which implies that the left hand side and righthand side of (6) are larger than $-\frac{\pi}{2}$ and smaller than $\frac{\pi}{2}$, respectively. Then it follows from (6) that

$$
\frac{\tilde{\lambda} c(A, B)-\epsilon}{c(A, B)+\tilde{\lambda} \epsilon} \leq \lambda \leq \frac{\tilde{\lambda} c(A, B)+\epsilon}{c(A, B)-\tilde{\lambda} \epsilon}
$$

Therefore,

$$
\begin{equation*}
|\tilde{\lambda}-\lambda| \leq \frac{\left(1+\tilde{\lambda}^{2}\right) \epsilon}{c(A, B)-|\tilde{\lambda}| \epsilon}=\delta . \tag{7}
\end{equation*}
$$

Second, without loss of generosity, we set $\|x\|_{2}=\|\tilde{x}\|_{2}=1$, let $r=[(A+E)-\tilde{\lambda}(B+F)] x$. Direct calculations give rise to

$$
\begin{align*}
\|r\|_{2} & =\|(A-\tilde{\lambda} B) x+(E-\tilde{\lambda} F) x\|_{2} \leq\|(A-\lambda B) x\|_{2}+|\tilde{\lambda}-\lambda|\|B x\|_{2}+\|(E-\tilde{\lambda} F) x\|_{2} \\
& \leq\|B\|_{2} \delta+\|E\|_{2}+|\tilde{\lambda}|\|F\|_{2} \leq\|B\|_{2} \delta+\sqrt{1+\tilde{\lambda}^{2}} \epsilon \tag{8}
\end{align*}
$$

On the other hand, the spectral decomposition of $(A+E)-\tilde{\lambda}(B+F)$ can be given by $(A+E)-\tilde{\lambda}(B+$ $F)=V \operatorname{diag}\left(0, \gamma_{2}, \ldots, \gamma_{p}\right) V^{\mathrm{T}}$, where $V=\left[\tilde{x}, V_{2}\right]$ is orthogonal, $0>\gamma_{2} \geq \cdots \geq \gamma_{p}$ are the eigenvalues of $(A+E)-\tilde{\lambda}(B+F)$. Here we used the assumption that $\tilde{\lambda}$ is simple. Then it follows that

$$
\begin{equation*}
V_{2}^{\mathrm{T}} r=V_{2}^{\mathrm{T}}[(A+E)-\tilde{\lambda}(B+F)] x=\Gamma_{2} V_{2}^{\mathrm{T}} x \tag{9}
\end{equation*}
$$

where $\Gamma_{2}=\operatorname{diag}\left(\gamma_{2}, \ldots, \gamma_{p}\right)$. Using (8) and (9), we get

$$
\sin \theta(x, \tilde{x})=\left\|V_{2}^{\mathrm{T}} x\right\|_{2}=\left\|\Gamma_{2}^{-1} V_{2}^{\mathrm{T}} r\right\|_{2} \leq \frac{\|r\|_{2}}{\left|\gamma_{2}\right|} \leq \frac{\|B\|_{2} \delta+\sqrt{1+\tilde{\lambda}^{2}} \epsilon}{g}
$$

which completes the proof.
Proof of Theorem 3. Notice that $\left(\lambda_{1},\left(v_{1}\right)_{\mathcal{J}_{t}}\right)$ and $\left(\rho^{(t)},\left(v^{(t)}\right) \mathcal{J}_{t}\right)$ are the leading eigenpairs of $\left(A_{\mathcal{J}_{t}}, B_{\mathcal{J}_{t}}\right)$ and $\left(\widetilde{A}_{\mathcal{J}_{t}}, \widetilde{B}_{\mathcal{J}_{t}}\right)$, respectively. Then (a) and (b) follow from Lemma 1 and Lemma 5 , respectively. This completes the proof.


[^0]:    ${ }^{1}$ For example, consider $X \in \mathbb{R}^{n \times p}$, where $n$ is the number of observations and $p$ is the number of features. The sample correlation matrix is $C=\frac{1}{n}\left(X-\mathbf{1}_{n} \bar{x}^{\mathrm{T}}\right)^{\mathrm{T}}\left(X-\mathbf{1}_{n} \bar{x}^{\mathrm{T}}\right)$, where

