

Supplementary Material for Unsupervised Discriminative Feature Selection With $\ell_{2,0}$ -Norm Constrained Sparse Projection

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I. NOTATIONS

TABLE I: Summary of Notations

Notations	Descriptions
n	Number of samples
d	Number of features
c	Number of clusters
m	Reduced dimensionality
k	Number of selected features
$\mathbf{1}_n$	Vector with all n elements as one
$\mathbf{I}_{n \times n}$	Identity matrix with size $n \times n$
\mathbb{R}	Set of real numbers
\mathbb{Z}^+	Set of positive integers
$\text{Tr}(\mathbf{X})$	Trace of square matrix $\mathbf{X} \in \mathbb{R}^{n \times n}$
$\text{rank}(\mathbf{X})$	Rank of matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$
\mathbf{x}_i	The i -th column of matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$
\mathbf{x}^i	The i -th row of matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$
x_{ij}	The (ij) -th element of matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$
\mathbf{X}^\top	Transpose of matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$
\mathbf{X}^\dagger	Moore-Penrose inverse of matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$
$\{\lambda_i(\mathbf{X})\}_{i=1}^n$	Eigenvalues of \mathbf{X} , ordered in descending order
$\ \mathbf{X}\ _F = \sqrt{\text{Tr}(\mathbf{X}^\top \mathbf{X})}$	Frobenius norm of matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$
$\ \mathbf{X}\ _{p,q} = \left(\sum_{i=1}^n \ \mathbf{x}^i\ _p^q \right)^{1/q}$	$\ell_{p,q}$ -norm of matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$
$\ \mathbf{X}\ _1 = \max_{j \in [1,d]} \sum_{i=1}^n x_{ij} $	1-norm of matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$
$\ \mathbf{X}\ _\infty = \max_{i \in [1,n]} \sum_{j=1}^d x_{ij} $	Infinity norm of matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$

II. THE WORKFLOW OF SPDFS

The workflow of SPDFS is illustrated in Fig. 1.

III. CLARIFIED EXPRESSION OF EQ. (14)

For clarity, we present a more detailed and explicit derivation of Eq. (14) below.

$$\begin{aligned}
 & \sum_{i=1}^n \sum_{j=1}^c y_{ij}^r \|\mathbf{W}^\top \mathbf{x}_i - \mathbf{W}^\top \mathbf{u}_j\|_2^2 \\
 &= \sum_{i=1}^n \sum_{j=1}^c f_{ij} (\mathbf{x}_i^\top \mathbf{W} \mathbf{W}^\top \mathbf{x}_i - 2\mathbf{x}_i^\top \mathbf{W} \mathbf{W}^\top \mathbf{u}_j + \mathbf{u}_j^\top \mathbf{W} \mathbf{W}^\top \mathbf{u}_j) \\
 &= \text{Tr}(\mathbf{W}^\top \mathbf{X} \text{diag}(\mathbf{F}\mathbf{1}) \mathbf{X}^\top \mathbf{W}) - \sum_{j=1}^c \frac{\mathbf{f}_j^\top \mathbf{X}^\top \mathbf{W} \mathbf{W}^\top \mathbf{X} \mathbf{f}_j}{\mathbf{f}_j^\top \mathbf{1}} \\
 &= \text{Tr}(\mathbf{W}^\top \mathbf{X} (\text{diag}(\mathbf{F}\mathbf{1}) - \mathbf{F} \text{diag}(\mathbf{F}^\top \mathbf{1})^{-1} \mathbf{F}^\top) \mathbf{X}^\top \mathbf{W}) \\
 &= \text{Tr}(\mathbf{W}^\top \mathbf{X} (\mathbf{D} - \mathbf{G}) \mathbf{X}^\top \mathbf{W})
 \end{aligned}$$

$$\begin{aligned}
 &= \text{Tr}(\mathbf{W}^\top \mathbf{X} \mathbf{L} \mathbf{X}^\top \mathbf{W}) \\
 &= \text{Tr}(\mathbf{W}^\top \mathbf{S}_m \mathbf{W}), \tag{1}
 \end{aligned}$$

where $\mathbf{S}_m = \mathbf{X} \mathbf{L} \mathbf{X}^\top$, and $\mathbf{L} = \mathbf{D} - \mathbf{G} = \text{diag}(\mathbf{F}\mathbf{1}) - \mathbf{F} \text{diag}(\mathbf{F}^\top \mathbf{1})^{-1} \mathbf{F}^\top$ is indeed the Laplacian matrix in graph theory. To see why, we analyse its two components, \mathbf{D} and \mathbf{G} , separately. First, $\mathbf{G} = \mathbf{F} \text{diag}(\mathbf{F}^\top \mathbf{1})^{-1} \mathbf{F}^\top$ serves as a normalized similarity matrix, capturing the pairwise similarity among samples while incorporating class importance normalization. Second, given the definition of the degree matrix, $\mathbf{D} = \text{diag}(\mathbf{G}\mathbf{1})$. By direct derivation, we have $\mathbf{D} = \text{diag}(\mathbf{F}\mathbf{1})$.

IV. PRACTICAL AND EFFICIENT CHOICE OF γ

In problem (16), $\mathbf{S}_d = \gamma \mathbf{I} - \mathbf{S}_o$, where $\mathbf{S}_o = \mathbf{S}_m - \alpha \mathbf{S}_t$. γ is large enough to ensure \mathbf{S}_d is positive semi-definite. Theoretically, γ can be set to the largest eigenvalue of \mathbf{S}_o , i.e., $\lambda_{\max}(\mathbf{S}_o)$. However, computing $\lambda_{\max}(\mathbf{S}_o)$ via eigenvalue decomposition is computationally expensive. Instead, for the square matrix \mathbf{S}_o , the 1-norm $\|\mathbf{S}_o\|_1$ and infinity norm $\|\mathbf{S}_o\|_\infty$ provide efficient upper bounds on $\lambda_{\max}(\mathbf{S}_o)$ without requiring explicit eigenvalue computation [2]. Since \mathbf{S}_o is symmetric, $\|\mathbf{S}_o\|_1 = \|\mathbf{S}_o\|_\infty$, making them equivalent choices for γ and ensuring computational efficiency.

V. AN EXAMPLE OF MATRIX A

To clarify the description of matrix $\mathbf{A} \in \{0, 1\}^{d \times k}$ in Section IV-A1, we provide an example. Suppose there are $d = 6$ inputs, and we select $k = 3$ with row indices $\mathbf{q} = [2, 4, 5]$. According to the definition of the operator $\Omega_d^k(\mathbf{q})$, the corresponding row-selection matrix \mathbf{A} is:

$$\mathbf{A} = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}.$$

From this example, we see that \mathbf{A} is a sparse matrix with k columns, each containing exactly one 1 at the row index specified by \mathbf{q} , which implies that $\mathbf{A}^\top \mathbf{1}_d = \mathbf{1}_k$.

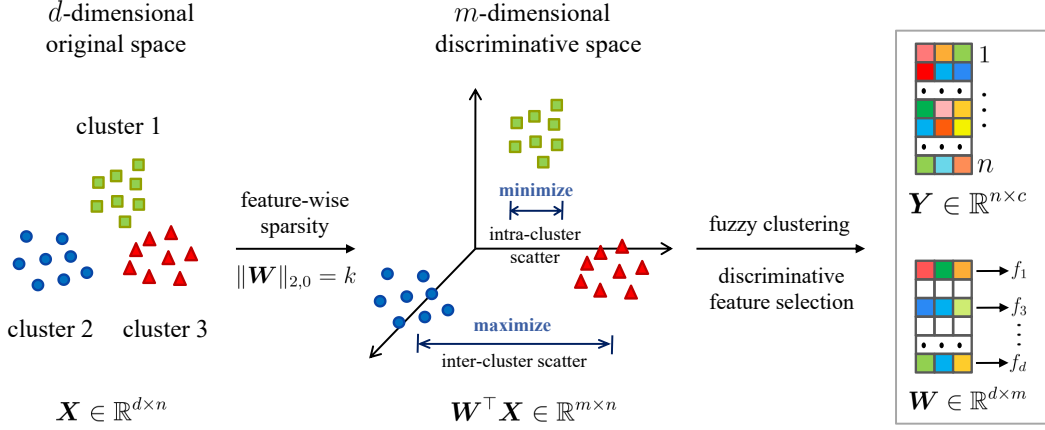


Fig. 1: Illustration of the SPDFS workflow. Guided by the principle of supervised LDA, SPDFS jointly performs fuzzy c -means membership learning $Y \in \mathbb{R}^{n \times c}$ and PCA projection learning $W \in \mathbb{R}^{d \times m}$ under an $\ell_{2,0}$ -norm constraint $\|W\|_{2,0} = k$ for feature-wise sparsity, enabling discriminative feature selection in an unsupervised manner.

Algorithm 3: Solve Problem (6).

Input: $X \in \mathbb{R}^{d \times n}$, $S_d \in \mathbb{R}^{d \times d}$, d, k, m, r .
Initialization: Initialize Y_0 and M_0 by Eq. (5), and initialize W_0 randomly.
while not converge do
 Update α by Eq. (9).
 while not converge do
 Update M by Eq. (11).
 Update W by Algorithm 2.
 Update Y by Eq. (26).
 end while
end while
Output: $W \in \mathbb{R}^{d \times m}$, $Y \in \mathbb{R}^{n \times c}$, $M \in \mathbb{R}^{m \times c}$.

VI. RELATIONSHIP BETWEEN S_m AND S_w

In problem (36), S_w is the intra-cluster scatter matrix in LDA, given by $S_w = \sum_{j=1}^c \sum_{y_{ij}=1} \|\mathbf{x}_i - \bar{\mathbf{x}}_j\|_2^2 = (X - XY(Y^\top Y)^{-1}Y^\top)(X - XY(Y^\top Y)^{-1}Y^\top)^\top = X(I - Y(Y^\top Y)^{-1}Y^\top)X^\top$. In fact, this structure can be directly observed from Eq. (1). Specifically, when $r = 1$, we have $f_{ij} = y_{ij}^\top = y_{ij}$, leading to $S_m = XLYX^\top = X(\text{diag}(Y\mathbf{1}) - Y\text{diag}(Y^\top \mathbf{1})^{-1}Y^\top)X^\top$. Since Y satisfies $\sum_{j=1}^c y_{ij} = 1$ and $y_{ij} \in \{0, 1\}$, it follows that $S_m = X(I - Y(Y^\top Y)^{-1}Y^\top)X^\top = S_w$. This reveals the relationship between S_m and S_w . That is, when $r = 1$, we have $S_m = S_w$.

VII. CORRECTION TO ALGORITHM 3

The pseudocode for Algorithm 3 in the main text of the published article inadvertently missed a line, specifically the optimization step for variable M . The complete Algorithm 3 is provided here as a supplement.

VIII. CORRECTION TO THE PROOF OF THEOREM 6

The proof of Theorem 6 in the main text has been revised for clarity and completeness. The updated version presented

here provides a more accurate and complete presentation of the proof.

Proof. We begin with problem (31), which can be equivalently expressed as follows:

$$\min_{\text{Tr}(W^\top S_t W) = C} \frac{\text{Tr}(W^\top S_m W)}{\text{Tr}(W^\top S_t W)}. \quad (2)$$

Observe that this trace ratio formulation can be rewritten as: $\frac{\text{Tr}(W^\top S_m W)}{\text{Tr}(W^\top S_t W)} = \frac{\sum_{i=1}^m \mathbf{w}_i^\top S_m \mathbf{w}_i}{\sum_{i=1}^m \mathbf{w}_i^\top S_t \mathbf{w}_i}$. Suppose that $\frac{\mathbf{w}_1^\top S_m \mathbf{w}_1}{\mathbf{w}_1^\top S_t \mathbf{w}_1}$ is the minimum among the set $\left\{ \frac{\mathbf{w}_i^\top S_m \mathbf{w}_i}{\mathbf{w}_i^\top S_t \mathbf{w}_i} \right\}_{i=1}^m$. By Lemma 2, we have $\frac{\mathbf{w}_1^\top S_m \mathbf{w}_1}{\mathbf{w}_1^\top S_t \mathbf{w}_1} \leq \frac{\text{Tr}(W^\top S_m W)}{\text{Tr}(W^\top S_t W)}$. Since \mathbf{w}_* is defined as $\mathbf{w}_* = \arg \min_{\mathbf{w}} \frac{\mathbf{w}^\top S_m \mathbf{w}}{\mathbf{w}^\top S_t \mathbf{w}}$, it follows that for any W , $\frac{\mathbf{w}_*^\top S_m \mathbf{w}_*}{\mathbf{w}_*^\top S_t \mathbf{w}_*} \leq \frac{\mathbf{w}_1^\top S_m \mathbf{w}_1}{\mathbf{w}_1^\top S_t \mathbf{w}_1} \leq \frac{\text{Tr}(W^\top S_m W)}{\text{Tr}(W^\top S_t W)}$. When each column of W is equal to \mathbf{w}_* , i.e., $\mathbf{w}_i = \mathbf{w}_*$ for all $i \in [1, m]$, the equality in $\frac{\mathbf{w}_*^\top S_m \mathbf{w}_*}{\mathbf{w}_*^\top S_t \mathbf{w}_*} \leq \frac{\text{Tr}(W^\top S_m W)}{\text{Tr}(W^\top S_t W)}$ holds. Thus, the minimum value of $\frac{\text{Tr}(W^\top S_m W)}{\text{Tr}(W^\top S_t W)}$ is achieved at $\frac{\mathbf{w}_*^\top S_m \mathbf{w}_*}{\mathbf{w}_*^\top S_t \mathbf{w}_*}$. To satisfy the constraint $\text{Tr}(W^\top S_t W) = C$, an optimal solution to problem (31) is $W_* = [c_1 \mathbf{w}_*, c_2 \mathbf{w}_*, \dots, c_m \mathbf{w}_*]$, which is a trivial solution since all columns are multiples of the same vector \mathbf{w}_* , making the rank of W_* at most 1, under the assumption that \mathbf{w}_* is the unique solution. If \mathbf{w}_* is not unique, then each column of the optimal W_* lies within the subspace spanned by the solutions of \mathbf{w}_* . Here, $\{c_i\}_{i=1}^m$ are arbitrary constants chosen such that $\text{Tr}(W_*^\top S_t W_*) = C$. This completes the proof. \square

IX. THE PROOF OF THEOREM 1

Proof. Suppose \mathbf{x}_* is the globally optimal solution to problem (7), with the corresponding globally minimal objective value α_* . This implies that $\frac{h(\mathbf{x}_*)}{p(\mathbf{x}_*)} = \alpha_*$. Consequently, $\forall \mathbf{x} \in \mathcal{S}$, we have $\frac{h(\mathbf{x})}{p(\mathbf{x})} \geq \alpha_*$. Since $p(\mathbf{x}) > 0$, it follows that $h(\mathbf{x}) - \alpha_* p(\mathbf{x}) \geq 0$. Moreover, noting that $h(\mathbf{x}_*) - \alpha_* p(\mathbf{x}_*) = 0$, we conclude that $\min_{\mathbf{x} \in \mathcal{S}} (h(\mathbf{x}) - \alpha_* p(\mathbf{x})) = 0$. Now, define the function $f(\alpha) = \min_{\mathbf{x} \in \mathcal{S}} (h(\mathbf{x}) - \alpha p(\mathbf{x}))$. Then, we have $f(\alpha_*) = 0$. This completes the proof. \square

X. THE PROOF OF THEOREM 2

Proof. In Algorithm 1, we observe from lines 1–2 that $h(\mathbf{x}_t) - \alpha_t p(\mathbf{x}_t) = 0$ and $h(\mathbf{x}_{t+1}) - \alpha_t p(\mathbf{x}_{t+1}) \leq h(\mathbf{x}_t) - \alpha_t p(\mathbf{x}_t)$. Accordingly, it follows that $h(\mathbf{x}_{t+1}) - \alpha_t p(\mathbf{x}_{t+1}) \leq 0$, which implies $\frac{h(\mathbf{x}_{t+1})}{p(\mathbf{x}_{t+1})} \leq \alpha_t = \frac{h(\mathbf{x}_t)}{p(\mathbf{x}_t)}$. This indicates that Algorithm 1 guarantees the objective function of problem (7) is non-increasing at each iteration until convergence.

According to Theorem 1, the global minimum of the objective in problem (7) corresponds to the root of the function $f(\alpha)$. It is well known that Newton's method is widely regarded as an effective algorithm for root-finding under standard regularity conditions. According to line 2 of Algorithm 1, let $f(\alpha_t) = h(\mathbf{x}_{t+1}) - \alpha_t p(\mathbf{x}_{t+1})$, then the derivative is $f'(\alpha_t) = -p(\mathbf{x}_{t+1})$. Applying the Newton's update rule, we obtain

$$\alpha_{t+1} = \alpha_t - \frac{f(\alpha_t)}{f'(\alpha_t)} = \alpha_t - \frac{h(\mathbf{x}_{t+1}) - \alpha_t p(\mathbf{x}_{t+1})}{-p(\mathbf{x}_{t+1})} = \frac{h(\mathbf{x}_{t+1})}{p(\mathbf{x}_{t+1})},$$

which coincides with line 1 of Algorithm 1. Therefore, the iterative scheme in Algorithm 1 is equivalent to applying Newton's method to find the root of $f(\alpha)$. According to [1], Newton's method enjoys a quadratic convergence rate under standard regularity conditions. This completes the proof. \square

XI. THE PROOF OF REMARK 1

Proof. According to problems (16) and (22), we have

$$\begin{aligned} f(\mathbf{W}_t) &= \text{Tr}(\mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_t), \\ g(\mathbf{W}_t | \mathbf{W}_t) &= \text{Tr}\left(\mathbf{W}_t^\top \left(\mathbf{S}_d \mathbf{W}_t (\mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_t)^\dagger \mathbf{W}_t^\top \mathbf{S}_d\right) \mathbf{W}_t\right). \end{aligned} \quad (3) \quad (4)$$

It is straightforward to verify that $f(\mathbf{W}_t) = g(\mathbf{W}_t | \mathbf{W}_t)$ since $\mathbf{P} = \mathbf{P}\mathbf{P}^\dagger \mathbf{P}$ for any matrix \mathbf{P} .

Since \mathbf{S}_d is positive semi-definite, it admits a factorization $\mathbf{S}_d = \mathbf{Q}\mathbf{Q}^\top$. Denote the following matrices:

$$\Upsilon = \mathbf{Q}^\top \mathbf{W}_t (\mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_t)^\dagger \mathbf{W}_t^\top \mathbf{Q}, \quad (5)$$

$$\Psi = \mathbf{Q}^\top \mathbf{W} \mathbf{W}^\top \mathbf{Q}. \quad (6)$$

Then, the function $g(\mathbf{W} | \mathbf{W}_t)$ can be rewritten as

$$\begin{aligned} g(\mathbf{W} | \mathbf{W}_t) &= \text{Tr}\left(\mathbf{W}^\top \left(\mathbf{S}_d \mathbf{W}_t (\mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_t)^\dagger \mathbf{W}_t^\top \mathbf{S}_d\right) \mathbf{W}\right) \\ &= \text{Tr}(\Upsilon \Psi). \end{aligned} \quad (7)$$

According to Theorems 4.3.53 and 1.3.22 [2], and noting that $\lambda_i(\Psi) \geq 0$ for all $i \in [1, m]$, we obtain

$$\text{Tr}(\Upsilon \Psi) \leq \sum_{i=1}^d \lambda_i(\Upsilon) \lambda_i(\Psi) \leq \sum_{i=1}^m \lambda_i(\Psi). \quad (8)$$

Since $\text{rank}(\Psi) \leq \text{rank}(\mathbf{W}) = m$, we have $\sum_{i=1}^m \lambda_i(\Psi) = \text{Tr}(\Psi)$. That is, $\text{Tr}(\Upsilon \Psi) \leq \text{Tr}(\Psi) = \text{Tr}(\mathbf{W}^\top \mathbf{S}_d \mathbf{W}) = f(\mathbf{W})$. In summary, we have $g(\mathbf{W} | \mathbf{W}_t) \leq f(\mathbf{W})$. This completes the proof. \square

XII. THE PROOF OF THEOREM 3

According to [3], we provide the proof of Theorem 3 below.

Proof. Recall that Remark 1 demonstrates that the surrogate problem (22) for optimizing \mathbf{W} meets the condition (20) required by the majorize-minimization (MM) framework [4], [5]. Let $\tilde{\mathbf{W}}_{t+1} = \arg \max_{\mathbf{W}} g(\mathbf{W} | \mathbf{W}_t)$, according to Eq. (21), the following inequality holds:

$$f(\tilde{\mathbf{W}}_{t+1}) \geq g(\tilde{\mathbf{W}}_{t+1} | \mathbf{W}_t) \geq g(\mathbf{W}_t | \mathbf{W}_t) = f(\mathbf{W}_t). \quad (9)$$

According to Eq. (3) and inequality (9), we have

$$\text{Tr}(\mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_t) \leq \text{Tr}(\tilde{\mathbf{W}}_{t+1}^\top \mathbf{S}_d \tilde{\mathbf{W}}_{t+1}). \quad (10)$$

Given $\tilde{\mathbf{W}}_{t+1} = \mathbf{A}_{t+1} \tilde{\mathbf{B}}_{t+1}$ and $\mathbf{W}_{t+1} = \mathbf{A}_{t+1} \mathbf{B}_{t+1}$. According to problem (23), \mathbf{B}_{t+1} maximizes its objective in the $(t+1)$ -th iteration, then we have

$$\begin{aligned} \text{Tr}(\tilde{\mathbf{W}}_{t+1}^\top \mathbf{S}_d \tilde{\mathbf{W}}_{t+1}) &= \text{Tr}(\tilde{\mathbf{B}}_{t+1}^\top \mathbf{A}_{t+1}^\top \mathbf{S}_d \mathbf{A}_{t+1} \tilde{\mathbf{B}}_{t+1}) \\ &\leq \text{Tr}(\mathbf{B}_{t+1}^\top \mathbf{A}_{t+1}^\top \mathbf{S}_d \mathbf{A}_{t+1} \mathbf{B}_{t+1}) \\ &= \text{Tr}(\mathbf{W}_{t+1}^\top \mathbf{S}_d \mathbf{W}_{t+1}). \end{aligned} \quad (11)$$

According to inequalities (10) and (11), we have

$$\text{Tr}(\mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_t) \leq \text{Tr}(\mathbf{W}_{t+1}^\top \mathbf{S}_d \mathbf{W}_{t+1}). \quad (12)$$

This indicates that Algorithm 2 ensures the objective of problem (16) remains non-decreasing with each iteration. Then we aim to prove that if $\mathbf{W}_t \neq \mathbf{W}_{t+1}$, then $\text{Tr}(\mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_t) \neq \text{Tr}(\mathbf{W}_{t+1}^\top \mathbf{S}_d \mathbf{W}_{t+1})$. This result demonstrates the ascent property of Algorithm 2, namely, $\text{Tr}(\mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_t) < \text{Tr}(\mathbf{W}_{t+1}^\top \mathbf{S}_d \mathbf{W}_{t+1})$.

Note that if $\mathbf{W}_t \neq \mathbf{W}_{t+1}$, then $\mathbf{A}_t \neq \mathbf{A}_{t+1}$, since $\mathbf{W} = \mathbf{A}\mathbf{B}$ and \mathbf{B} is formed by the leading m eigenvectors of $(\mathbf{A}^\top \mathbf{S}_d \mathbf{A})$. Therefore, suppose that there exists $\mathbf{A}_t \neq \mathbf{A}_{t+1}$ such that $\text{Tr}(\mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_t) = \text{Tr}(\mathbf{W}_{t+1}^\top \mathbf{S}_d \mathbf{W}_{t+1})$. Then the equality in inequality (8) holds. According to the equality condition in Theorem 4.3.53 [2], the matrices $\mathbf{Q}^\top \mathbf{W}_t (\mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_t)^\dagger \mathbf{W}_t^\top \mathbf{Q}$ and $\mathbf{Q}^\top \mathbf{W}_{t+1} \mathbf{W}_{t+1}^\top \mathbf{Q}$ are simultaneously diagonalizable. Assuming that \mathbf{S}_d is full rank, we have that $\Omega_t = \mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_t$ is diagonal. Define $\Phi_t = \mathbf{Q}^\top \mathbf{W}_t \Omega_t^{-1/2}$, then

$$\mathbf{Q}^\top \mathbf{W}_t (\mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_t)^\dagger \mathbf{W}_t^\top \mathbf{Q} = \mathbf{Q}^\top \mathbf{W}_t \Omega_t^{-1} \mathbf{W}_t^\top \mathbf{Q} = \Phi_t \Phi_t^\top, \quad (13)$$

$$\Phi_t^\top \Phi_t = \Omega_t^{-1/2} \mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_t \Omega_t^{-1/2} = \Omega_t^{-1/2} \Omega_t \Omega_t^{-1/2} = \mathbf{I}_{m \times m}. \quad (14)$$

From the simultaneously diagonalizable property and Theorem 1.3.22 [2], it follows that

$$\begin{aligned} \mathbf{Q}^\top \mathbf{W}_{t+1} \mathbf{W}_{t+1}^\top \mathbf{Q} &= \Phi_t \Omega_{t+1} \Phi_t^\top \\ &= \mathbf{Q}^\top \mathbf{W}_t \Omega_t^{-1/2} \Omega_{t+1} \Omega_t^{-1/2} \mathbf{W}_t^\top \mathbf{Q}. \end{aligned} \quad (15)$$

Based on Eq. (15), we have

$$\begin{aligned} &\mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_{t+1} \mathbf{W}_{t+1}^\top \mathbf{S}_d \mathbf{W}_t \\ &= \mathbf{W}_t^\top \mathbf{Q} (\mathbf{Q}^\top \mathbf{W}_{t+1} \mathbf{W}_{t+1}^\top \mathbf{Q}) \mathbf{Q}^\top \mathbf{W}_t \\ &= \mathbf{W}_t^\top \mathbf{Q} \mathbf{Q}^\top \mathbf{W}_t \Omega_t^{-1/2} \Omega_{t+1} \Omega_t^{-1/2} \mathbf{W}_t^\top \mathbf{Q} \mathbf{Q}^\top \mathbf{W}_t \end{aligned}$$

$$= \Omega_t \Omega_{t+1}. \quad (16)$$

We now consider the objective of the surrogate problem (22), leading to

$$\begin{aligned} & \text{Tr} \left(\mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_{t+1} (\mathbf{W}_{t+1}^\top \mathbf{S}_d \mathbf{W}_{t+1})^\dagger \mathbf{W}_{t+1}^\top \mathbf{S}_d \mathbf{W}_t \right) \\ &= \text{Tr} \left(\mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_{t+1} \Omega_{t+1}^{-1} \mathbf{W}_{t+1}^\top \mathbf{S}_d \mathbf{W}_t \right) \\ &= \text{Tr} \left(\mathbf{W}_t^\top \mathbf{Q} \mathbf{Q}^\top \mathbf{W}_{t+1} \Omega_{t+1}^{-1} \mathbf{W}_{t+1}^\top \mathbf{Q} \mathbf{Q}^\top \mathbf{W}_t \right) \\ &= \text{Tr} \left(\mathbf{Q}^\top \mathbf{W}_{t+1} \Omega_{t+1}^{-1} \mathbf{W}_{t+1}^\top \mathbf{Q} \mathbf{Q}^\top \mathbf{W}_t \mathbf{W}_t^\top \mathbf{Q} \right) \\ &= \text{Tr} (\Upsilon_{t+1} \Psi_t). \end{aligned} \quad (17)$$

From Eq. (17), inequality (8), and Theorem 4.3.53 [2], we obtain

$$\begin{aligned} & \text{Tr} \left(\mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_{t+1} \Omega_{t+1}^{-1} \mathbf{W}_{t+1}^\top \mathbf{S}_d \mathbf{W}_t \right) \\ & \leq \text{Tr} \left(\mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_t \right) = \text{Tr} (\Omega_t). \end{aligned} \quad (18)$$

Let $\Gamma = \mathbf{W}_{t+1}^\top \mathbf{S}_d \mathbf{W}_t \mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_{t+1} \in \mathbb{R}^{m \times m}$ and $\mathbf{U} = \Omega_{t+1}^{-1} \in \mathbb{R}^{m \times m}$, then based on Theorem 4.3.53 [2], we have

$$\begin{aligned} & \text{Tr} \left(\mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_{t+1} \Omega_{t+1}^{-1} \mathbf{W}_{t+1}^\top \mathbf{S}_d \mathbf{W}_t \right) \\ &= \text{Tr} (\Gamma \mathbf{U}) \geq \sum_{i=1}^m \lambda_i(\Gamma) \lambda_{m-i+1}(\mathbf{U}). \end{aligned} \quad (19)$$

Note that $\lambda_{m-i+1}(\mathbf{U}) = \lambda_i(\Omega_{t+1})^{-1}$, and by Eq. (16) and Theorem 1.3.22 [2], we get

$$\sum_{i=1}^m \lambda_i(\Gamma) \lambda_{m-i+1}(\mathbf{U}) = \sum_{i=1}^m \frac{\lambda_i(\Omega_t \Omega_{t+1})}{\lambda_i(\Omega_{t+1})} = \text{Tr} (\Omega_t). \quad (20)$$

Combining inequalities (18), (19) and Eq. (20), we conclude that $\text{Tr} \left(\mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_{t+1} \Omega_{t+1}^{-1} \mathbf{W}_{t+1}^\top \mathbf{S}_d \mathbf{W}_t \right) = \text{Tr} (\Omega_t)$. According to Theorem 4.3.53 [2], the equality in inequality (19) implies that Γ and \mathbf{U} are simultaneously diagonalizable. From Eq. (16), we know that $\Gamma = \mathbf{W}_{t+1}^\top \mathbf{S}_d \mathbf{W}_t \mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_{t+1} = \Omega_t \Omega_{t+1}$, which implies that $\mathbf{W}_{t+1}^\top \mathbf{S}_d \mathbf{W}_t = \Omega_t^{1/2} \Omega_{t+1}^{1/2}$ is diagonal. Recall that $\Phi_t = \mathbf{Q}^\top \mathbf{W}_t \Omega_t^{-1/2}$ and $\Phi_{t+1} = \mathbf{Q}^\top \mathbf{W}_{t+1} \Omega_{t+1}^{-1/2}$, then we have

$$\begin{aligned} \Phi_t^\top \Phi_t &= \Omega_t^{-1/2} \mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_t \Omega_t^{-1/2} = \mathbf{I}_{m \times m}, \\ \Phi_{t+1}^\top \Phi_{t+1} &= \Omega_{t+1}^{-1/2} \mathbf{W}_{t+1}^\top \mathbf{S}_d \mathbf{W}_{t+1} \Omega_{t+1}^{-1/2} = \mathbf{I}_{m \times m}, \\ \Phi_{t+1}^\top \Phi_t &= \Omega_{t+1}^{-1/2} \mathbf{W}_{t+1}^\top \mathbf{S}_d \mathbf{W}_t \Omega_t^{-1/2} = \mathbf{I}_{m \times m}. \end{aligned} \quad (21)$$

Thus, we conclude that $\Phi_t = \Phi_{t+1}$, which implies that $\mathbf{S}_d \mathbf{W}_t \Omega_t^{-1/2} = \mathbf{S}_d \mathbf{W}_{t+1} \Omega_{t+1}^{-1/2}$. Since \mathbf{S}_d is full rank, it follows that $\mathbf{W}_t \Omega_t^{-1/2} = \mathbf{W}_{t+1} \Omega_{t+1}^{-1/2}$. Therefore, we conclude that $\mathbf{A}_t = \mathbf{A}_{t+1}$, since the operation $\Omega^{-1/2}$ does not affect the sparsity pattern of \mathbf{W} . This leads to a contradiction with our initial assumption.

The above analysis establishes the non-decreasing property of the sequence $\{\text{Tr}(\mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_t)\}_{t \in \mathbb{Z}^+}$. Note that $\text{Tr}(\mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_t)$ is upper bounded by $\text{Tr}(\mathbf{S}_d)$. Therefore, the sequence will eventually converge after a finite number of iterations. Moreover, we have shown that if $\mathbf{W}_t \neq \mathbf{W}_{t+1}$, then $\text{Tr}(\mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_t) < \text{Tr}(\mathbf{W}_{t+1}^\top \mathbf{S}_d \mathbf{W}_{t+1})$. Therefore, by the contrapositive, if the objective value converges, i.e., $\text{Tr}(\mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_t) = \text{Tr}(\mathbf{W}_{t+1}^\top \mathbf{S}_d \mathbf{W}_{t+1})$, then it must be that $\mathbf{W}_t = \mathbf{W}_{t+1}$ and $\mathbf{A}_t = \mathbf{A}_{t+1}$. Consequently, the sequence $\{\mathbf{W}_t\}_{t \in \mathbb{Z}^+}$ converges to a fixed point $\widehat{\mathbf{W}}$, and as $\mathbf{W}_t \rightarrow \widehat{\mathbf{W}}$,

we have $\text{Tr}(\mathbf{W}_t^\top \mathbf{S}_d \mathbf{W}_t) \rightarrow \text{Tr}(\widehat{\mathbf{W}}^\top \mathbf{S}_d \widehat{\mathbf{W}})$. This completes the proof. \square

XIII. THE PROOF OF LEMMA 1

According to [3], we provide the proof of Lemma 1 below.

Proof. Let $\mathbf{S}_d = \mathbf{S}_d^m + \mathbf{S}_d^c$. We then have the following derivation:

$$\begin{aligned} & \text{Tr}(\mathbf{W}_*^\top \mathbf{S}_d \mathbf{W}_*) \\ &= \max_{\mathbf{W}^\top \mathbf{W} = \mathbf{I}_{m \times m}, \|\mathbf{W}\|_{2,0} = k} \text{Tr}(\mathbf{W}^\top (\mathbf{S}_d^m + \mathbf{S}_d^c) \mathbf{W}) \\ &\leq \max_{\substack{\mathbf{W}^\top \mathbf{W} = \mathbf{I}_{m \times m}, \\ \|\mathbf{W}\|_{2,0} = k}} \text{Tr}(\mathbf{W}^\top \mathbf{S}_d^m \mathbf{W}) + \max_{\substack{\mathbf{W}^\top \mathbf{W} = \mathbf{I}_{m \times m}, \\ \|\mathbf{W}\|_{2,0} = k}} \text{Tr}(\mathbf{W}^\top \mathbf{S}_d^c \mathbf{W}) \\ &\leq \text{Tr}(\mathbf{W}_m^\top \mathbf{S}_d^m \mathbf{W}_m) + \max_{\mathbf{W}^\top \mathbf{W} = \mathbf{I}_{m \times m}} \text{Tr}(\mathbf{W}^\top \mathbf{S}_d^c \mathbf{W}) \\ &\leq \text{Tr}(\mathbf{W}_m^\top \mathbf{S}_d^m \mathbf{W}_m) + \sum_{i=m+1}^{2m} \lambda_i(\mathbf{S}_d), \end{aligned} \quad (22)$$

from which it follows that

$$\frac{\text{Tr}(\mathbf{W}_m^\top \mathbf{S}_d^m \mathbf{W}_m)}{\text{Tr}(\mathbf{W}_*^\top \mathbf{S}_d \mathbf{W}_*)} \geq 1 - \frac{\sum_{i=m+1}^{2m} \lambda_i(\mathbf{S}_d)}{\text{Tr}(\mathbf{W}_*^\top \mathbf{S}_d \mathbf{W}_*)}. \quad (23)$$

Furthermore, we have the following two observations:

$$\begin{aligned} \text{Tr}(\mathbf{W}_*^\top \mathbf{S}_d \mathbf{W}_*) &\stackrel{(a)}{\geq} \max_{\mathbf{W}^\top \mathbf{W} = \mathbf{I}_{m \times m}, \|\mathbf{W}\|_{2,0} = m} \text{Tr}(\mathbf{W}^\top \mathbf{S}_d \mathbf{W}) \\ &\stackrel{(b)}{\geq} \frac{m}{d} \text{Tr}(\mathbf{S}_d) = \frac{m}{d} \sum_{i=1}^d \lambda_i(\mathbf{S}_d), \end{aligned} \quad (24)$$

$$\begin{aligned} \text{Tr}(\mathbf{W}_*^\top \mathbf{S}_d \mathbf{W}_*) &\stackrel{(c)}{\geq} \max_{\mathbf{W}^\top \mathbf{W} = \mathbf{I}_{m \times m}, \|\mathbf{W}\|_{2,0} = k} \text{Tr}(\mathbf{W}^\top \mathbf{S}_d^m \mathbf{W}) \\ &\stackrel{(d)}{\geq} \frac{k}{d} \sum_{i=1}^d \lambda_i(\mathbf{S}_d^m) = \frac{k}{d} \sum_{i=1}^m \lambda_i(\mathbf{S}_d), \end{aligned} \quad (25)$$

where (a) holds because $m \leq k$, and (c) holds since \mathbf{S}_d is positive semi-definite. Inequality (b) holds since $k = m$, implying that the problem on the left side of (b) achieves its global optimum via Algorithm 2. Inequality (d) holds because $\text{rank}(\mathbf{S}_d^m) = m$, and thus the problem on the left side of (d) also achieves its global optimum via Algorithm 2.

Let $z = \min\{\text{rank}(\mathbf{S}_d), 2m\}$, $c_1 = \frac{\sum_{i=m+1}^z \lambda_i(\mathbf{S}_d)}{\sum_{i=1}^m \lambda_i(\mathbf{S}_d)}$, and $c_2 = \frac{\sum_{i=m+1}^d \lambda_i(\mathbf{S}_d)}{\sum_{i=1}^d \lambda_i(\mathbf{S}_d)}$. Combining inequalities (23), (24), (25), we obtain

$$1 \geq \frac{\text{Tr}(\mathbf{W}_m^\top \mathbf{S}_d^m \mathbf{W}_m)}{\text{Tr}(\mathbf{W}_*^\top \mathbf{S}_d \mathbf{W}_*)} \geq 1 - \min \left\{ \frac{d \cdot c_1}{k}, \frac{d \cdot c_2}{m} \right\}. \quad (26)$$

Since \mathbf{S}_d is positive semi-definite, we have

$$\begin{aligned} \text{Tr}(\mathbf{W}_m^\top \mathbf{S}_d \mathbf{W}_m) &= \text{Tr}(\mathbf{W}_m^\top \mathbf{S}_d^m \mathbf{W}_m) + \text{Tr}(\mathbf{W}_m^\top \mathbf{S}_d^c \mathbf{W}_m) \\ &\geq \text{Tr}(\mathbf{W}_m^\top \mathbf{S}_d^m \mathbf{W}_m). \end{aligned} \quad (27)$$

Combining inequalities (26) and (27), we obtain $\varepsilon \leq \min\{(d \cdot c_1/k), (d \cdot c_2/m)\}$. Moreover, according to Theorem 4.3.53 [2], we have

$$\text{Tr}(\mathbf{W}_m^\top \mathbf{S}_d \mathbf{W}_m) \geq \sum_{i=d-m+1}^d \lambda_i(\mathbf{S}_d) \geq m \cdot \lambda_d(\mathbf{S}_d). \quad (28)$$

Let $\kappa = \lambda_1(\mathbf{S}_d)/\lambda_d(\mathbf{S}_d)$, then by Ky Fan's Theorem [6], we obtain

$$\begin{aligned} \text{Tr}(\mathbf{W}_*^\top \mathbf{S}_d \mathbf{W}_*) &\leq \max_{\mathbf{W}^\top \mathbf{W} = \mathbf{I}_{m \times m}} \text{Tr}(\mathbf{W}^\top \mathbf{S}_d \mathbf{W}) = \sum_{i=1}^m \lambda_i(\mathbf{S}_d) \\ &\leq m \cdot \lambda_1(\mathbf{S}_d) = m \cdot \kappa \cdot \lambda_d(\mathbf{S}_d). \end{aligned} \quad (29)$$

Combing inequalities (28) and (29), we obtain $\varepsilon \leq 1 - \kappa^{-1}$. Furthermore, we have

$$\begin{aligned} \text{Tr}(\mathbf{W}_m^\top \mathbf{S}_d \mathbf{W}_m) &\geq \text{Tr}(\mathbf{W}_m^\top \mathbf{S}_d^m \mathbf{W}_m) \\ &\geq \frac{k}{d} \text{Tr}(\mathbf{S}_d^m) \geq \frac{k}{d} \sum_{i=1}^m \lambda_i(\mathbf{S}_d). \end{aligned} \quad (30)$$

According to inequality (29), we have

$$\text{Tr}(\mathbf{W}_*^\top \mathbf{S}_d \mathbf{W}_*) \leq \sum_{i=1}^m \lambda_i(\mathbf{S}_d). \quad (31)$$

Combing inequalities (30) and (31), we obtain $\varepsilon \leq 1 - k/d$. In summary, we conclude that $\varepsilon \leq \min\{(d \cdot c_1/k), (d \cdot c_2/m), 1 - \kappa^{-1}, 1 - k/d\}$. This completes the proof. \square

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