Spherical Principal Component Analysis

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Abstract

Principal Component Analysis (PCA) is one of the most important methods to handle high dimensional data. However, most of the studies on PCA aim to minimize the loss after projection, which usually measure the Euclidean distance, though in some fields, angle distance is known to be more important and critical for analysis. In this paper, we propose a method by adding constraints on factors to unify the Euclidean distance and angle distance. However, due to the nonconvexity of the objective and constraints, the optimized solution is not easy to obtain. We propose an alternating linearized minimization method to solve it with provable convergence rate and guarantee. Experiments on synthetic data and real-world datasets have validated the effectiveness of our method and demonstrated its advantages over state-of-art clustering methods.

1 Introduction

In many real-world applications such as text categorization and face recognition, the dimensions of data are usually very high. Dealing with high-dimensional data is computationally expensive while noise or outliers in the data can increase dramatically as the dimension increases. Dimension reduction is one of the most important and effective methods to handle high dimensional data [4, 17, 20]. Among the dimension reduction methods, Principal Component Analysis (PCA) is one of the most widely used methods due to its simplicity and effectiveness.

PCA is a statistical procedure that uses an orthogonal transformation to convert a set of correlated variables into a set of linearly uncorrelated principal directions. Usually the number of principal directions is less than or equal to the number of original variables. This transformation is defined in such a way that the first principal direction has the largest possible variance (that is, accounts for as much of the variability in the data as possible), and each succeeding direction has the highest variance under the constraint that it is orthogonal to the preceding directions. The resulting vectors are an uncorrelated orthogonal basis set.

When data points lie in a low-dimensional manifold and the manifold is linear or nearly-linear, the low-dimensional structure of data can be effectively captured by a linear subspace spanned by the principal PCA directions.

More specifically, let \( X = [x_1 \cdots x_n] \in \mathbb{R}^{m \times n} \) be \( n \) data points in \( m \)-dimensional space while \( U = [u_1 \cdots u_r] \in \mathbb{R}^{m \times r} \) contains the principal directions and \( V = [v_1 \cdots v_n] \in \mathbb{R}^{r \times n} \) contains the principal components (data projects along the principal directions). Generally speaking, there can be two formulations for PCA:

- **Covariance-based approach**, which computes the covariance matrix \( C = \sum_{i=1}^{n} (x_i - \bar{x})(x_i - \bar{x})^\top = XX^\top \).
  Here we assume the data are already centered, i.e., \( \bar{x} = 0 \), and we drop the factor \( \frac{1}{n-1} \) which does not affect \( U \).
  The principal directions are obtained as:

  \[
  \maximize_{U^\top U = I} \text{tr}(U^\top XX^\top U). \tag{1}
  \]

- **Matrix low-rank approximation-based approach**. Let \( X \approx UV \), we solve:

  \[
  \minimize_{U^\top U = I} \|X - UV\|_F^2 = \sum_{i,j} |X_{ij} - (UV)_{ij}|^2. \tag{2}
  \]

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2 Motivation

In Eq. (2), the objective function measures the gap between original data $X$ and approximation after projection $UV$, which is based on squared Euclidean distance measurements and treat each feature as equally important. However, in the real world, there are some given datasets which are preprocessed to be normalized and different features may have various significance. Thus distance-based measurement method may yield poor results. On the other side, similarity-based measurement methods such as angle distance have been proved to be more efficient in some applications, including information retrieval [18], signal processing [8], metric learning [15], etc.. Though one can calculate the similarity after projection, still this appears to be more or less awkward and inefficient. Thus, deriving some methods which can directly measure angle distance from PCA is vitally important. However, to our best knowledge, it has not been studied yet.

Motivated by the above observations and a previous work [19], in this paper we propose a spherically-PCA model which can unify the Euclidean distance and angle distance. By noticing that larger angle in the sphere in Fig. 1 also has larger Euclidean distance, we can add the normalization constraint to the component matrix, where the norm of each column in $V$ is 1 to guarantee the spherical distribution of components:

$$\begin{align*}
\min_{U \in \mathbb{R}^{m \times r}, V \in \mathbb{R}^{r \times n}} & \quad \|X - UV\|_F^2 = \sum_{i,j} [X_{ij} - (UV)_{ij}]^2 \\
\text{s.t.} & \quad U \in \mathbb{U}, V \in \mathbb{V}
\end{align*}$$

(3)

where we define:

$$\begin{align*}
\mathbb{U} & := \{U : U^T U = I\}, \\
\mathbb{V} & := \{V : \|v_j\| = 1 \text{ } \forall j\}
\end{align*}$$

(4)

where $\| \cdot \|$ denotes $\ell_2$ norm for vectors and denotes the spectral norm for matrices. Suppose the component is spherically distributed, then the Euclidean distance between $v_i$ and $v_j$ is:

$$\begin{align*}
\|v_i - v_j\|^2 & = \|v_i\|^2 + \|v_j\|^2 - 2 \langle v_i, v_j \rangle \\
& = \|v_i\|^2 + \|v_j\|^2 - 2 \frac{\langle v_i, v_j \rangle}{\|v_i\|\|v_j\|} \\
& = 2 - 2 \cos(\theta), \theta \in [0, \pi]
\end{align*}$$

(5)
which is equivalent to angle distance that bigger angle \( \theta \) will result in larger Euclidean distance, and vice versa.

Remark 2.1. In traditional PCA, without the normalization constraint on each column of \( \mathbf{v} \), the optimized solution to Eq. (2) can barely satisfy the spherical distribution. Since \( r \) is usually less than \( m \), PCA will lose some component more or less, thus \( \mathbf{x}_i \neq \mathbf{U} \mathbf{v}_i \) and usually \( \| \mathbf{x}_i \| \neq \| \mathbf{U} \mathbf{v}_i \| \) (they may be equal, but it barely happens) . We have \( \| \mathbf{x}_i \|^2 = 1 \) for normalized data and if \( \| \mathbf{v}_i \|^2 = 1 \) then \( \| \mathbf{U} \mathbf{v}_i \|^2 = \text{tr} ( \mathbf{v}_i^\top \mathbf{U}^\top \mathbf{U} \mathbf{v}_i ) = \text{tr} ( \mathbf{v}_i^\top \mathbf{v}_i ) = \| \mathbf{v}_i \|^2 = 1 \), which leads a contradiction, thus the constraint on \( \mathbf{V} \) is necessary to guarantee our motivation.

3 Formulation And Algorithm

3.1 Objective Function with Proximal Term

We first denote:

\[ h(\mathbf{U}, \mathbf{V}) = \| \mathbf{X} - \mathbf{U} \mathbf{V} \|^2_F = \sum_{j=1}^{n} \| \mathbf{x}_j - \mathbf{U} \mathbf{v}_j \|^2 \quad s.t. \quad \mathbf{U} \in \mathcal{U}, \mathbf{V} \in \mathcal{V} \]  

(6)

By noting the nonconvexity of Eq. (3), where no closed solution exists, we propose an alternating minimization method to get the optimized solution as: given \( k \)th iterate of \( \mathbf{V} \) variable \( \mathbf{V}(k) = [\mathbf{v}_1(k) \cdots \mathbf{v}_n(k)] \),

\[
\mathbf{U}(k+1) = \arg \min_{\mathbf{U} \in \mathcal{U}} \| \mathbf{X} - \mathbf{U} \mathbf{V}(k) \|^2_F;
\]

\[
\mathbf{v}_j(k+1) = \arg \min_{\| \mathbf{v} \|=1} \| \mathbf{x}_j - \mathbf{U}(k+1) \mathbf{v} \|^2_2, \quad \forall j \quad (7)
\]

Note that when the constraints \( \mathbf{U} \in \mathcal{U}, \mathbf{V} \in \mathcal{V} \), the problem (6) is known as the nonconvex matrix factorization problems, which have been well-studied \([12, 25]\). This work focus on develop efficient and provable algorithm to deal with (6) with the constraints \( \mathbf{U} \in \mathcal{U}, \mathbf{V} \in \mathcal{V} \). Note that the proximal algorithm recently has been successfully applied to a wide variety of situations: convex optimization, nonmonotone operators \([6, 10]\) with various applications to nonconvex programming. It was first introduced by Rockafellar \([16]\) as an approximation regularization method in convex optimization and in the study of variational inequalities associated to maximal monotone operators.

Considering the fact that the objective function in Eq. (3) is nonconvex w.r.t. \( \mathbf{U} \) and \( \mathbf{V} \), and the constraint on \( \mathbf{U} \) and \( \mathbf{V} \) are also nonconvex, we consider adding proximal term and optimize the solution as: with the alternating linearized minimization solutions becomes:

\[
\mathbf{U}(k+1) = \arg \min_{\mathbf{U} \in \mathcal{U}} \langle \mathbf{U} - \mathbf{U}(k), \nabla h(\mathbf{U}(k), \mathbf{V}(k)) \rangle + \frac{\mu}{2} \| \mathbf{U} - \mathbf{U}(k) \|^2_F;
\]

\[
\mathbf{v}_j(k+1) = \arg \min_{\| \mathbf{v} \|=1} \langle \mathbf{v} - \mathbf{v}_j(k), \nabla \mathbf{v}_j h(\mathbf{U}(k+1), \mathbf{V}(k)) \rangle + \frac{\lambda}{2} \| \mathbf{v} - \mathbf{v}_j(k) \|^2, \quad \forall j \quad (8)
\]

Remark 3.1. We add the proximal term to make the new updating solution will not be too far from the previous step to avoid drastic changes. One can see that when the proximal term regularization parameters \( \mu, \lambda \) are sufficiently large, they will dominate the objective function. Moreover, we can take the linearized minimization as to minimize the objective with Taylor expansion by making use of first order (linear) information.

3.2 Proposed Algorithm

Given the alternating minimization objective in Eq. (8), now we turn to provide detailed (closed) updating algorithm,

We first derive the solution for \( \mathbf{U} \) and before that we give a useful lemma that is similar to \([22, \text{Theorem 1}]\) and \([23, \text{Theorem 1}]\):

Lemma 3.1. maximize_{\mathbf{U} \in \mathcal{U}} \text{tr}(\mathbf{U}^\top \mathbf{M}) is given by \( \mathbf{U} = \mathbf{A} \mathbf{B}^\top \), where \([\mathbf{A}, \mathbf{\Sigma}, \mathbf{B}] = \text{svd}(\mathbf{M})\).

Proof. On one hand, we have:

\[
\text{tr}(\mathbf{U}^\top \mathbf{M}) = \text{tr}(\mathbf{U}^\top \mathbf{A} \mathbf{\Sigma} \mathbf{B}^\top) = \text{tr}(\mathbf{P} \mathbf{\Sigma}),
\]

(9)
Algorithm 1 Alternating Linearized Minimization for Problem Eq. (6)

Input: data $X \in \mathbb{R}^{m \times n}$, rank of factors $r$, regularization parameters $\lambda, \mu$, number of iterations $K$

Initialization: $U(0) \in \mathbb{R}^{m \times r}$, $V(0) \in \mathbb{R}^{r \times n}$

for $k = 1, \ldots, K$

- Optimize $U(k)$ via Eq. (11)
- Optimize $V(k)$ via Eq. (12) for $j = 1, \ldots, n$

end

Output: $U(K)$ and $V(K)$

where $P = B^\top U^\top A$ is an orthogonal matrix since

$$PP^\top = (B^\top U^\top A)(B^\top U^\top A)^\top = I.$$ 

Thus every element including the diagonal of $P$ is no larger than 1. Then we have:

$$\text{tr}(P\Sigma) \leq \text{tr}(\Sigma)$$ (10)

On the other hand, when $U = AB^\top$, we have

$$\text{tr}(U^\top M) = \text{tr}(BA^\top A\Sigma B^\top) = \Sigma.$$ 

Thus $U = AB^\top$ is the optimized solution to maximize the objective.

Accordingly, we have:

$$U(k + 1) = \arg\min_{U^\top U = I} \langle U - U(k), \nabla_U h(U(k), V(k)) \rangle + \frac{\mu}{2} \| U - U(k) \|^2_F$$

$$= \arg\max_{U^\top U = I} \langle U, M(k) \rangle = YZ^\top$$ (11)

where $M(k) := 2(X - U(k)V(k))V(k)^\top + \mu U(k)$ and $Y, Z$ is obtained from $[Y, \Sigma, Z] = \text{svd}(M(k))$.

Then we compute $V(k + 1)$:

$$v_j(k + 1) = \arg\min_{\| v \| = 1} \langle v - v_j(k), \nabla_v h(U(k + 1), V(k)) \rangle + \frac{\lambda}{2} \| v - v_j(k) \|^2$$

$$= \arg\max_{\| v \| = 1} \langle v, q \rangle$$

$$= \frac{q}{\| q \|}, \text{ for } j = 1, \ldots, n,$$ (12)

where $q := 2U(k + 1)^\top x_j + (\lambda - 2)v_j(k)$.

4 Convergence Analysis

In the following case, we let $U$ and $V$ be as defined in Eq. (4), and show the convergence of our proposed algorithm in the last section.

To begin with, we first show that $h(U, V)$ has Lipschitz continuous gradient at $U \in \mathbb{U}, V \in \mathbb{V}$, which will be very useful for the following convergence analysis.

Proposition 4.1. $h(U, V)$ has Lipschitz continuous gradient at $U \in \mathbb{U}, V \in \mathbb{V}$, where $U$ and $V$ are defined in Eq. (4). That is, there exists a constant $L_c$ such that

$$\| \nabla h(U, V) - \nabla h(U', V') \|_F \leq L_c \| (U, V) - (U', V') \|_F$$ (13)

for all $U, U' \in \mathbb{U}$ and $V, V' \in \mathbb{V}$. Here $L_c > 0$ is referred to as the Lipschitz constant.
Proof of Proposition 4.1. It is equivalent to show $|\nabla^2 h(U, V)| \leq L_c$ for all $U \in \mathbb{U}, V \in \mathbb{V}$. Standard computations give the Hessian quadrature form $[\nabla^2 h(U, V)](\Delta, \Delta)$ for any $\Delta = \begin{bmatrix} \Delta U \\ \Delta V \end{bmatrix} \in \mathbb{R}^{(n+m) \times r}$ (where $\Delta U \in \mathbb{R}^{m \times r}$ and $\Delta V \in \mathbb{R}^{r \times n}$) as

$$[\nabla^2 h(U, V)](\Delta, \Delta) = \|\Delta U V + U \Delta V\|^2_F + 2\langle UV - X, \Delta U \Delta V \rangle$$

which gives:

$$\|\nabla^2 h(U, V)\| = \maximize_{\|\Delta\|_F = 1} \|\nabla^2 h(U, V)](\Delta, \Delta)\|
\leq \maximize_{\|\Delta\|_F = 1} \|\Delta U V + U \Delta V\|^2_F + 2\|UV - X, \Delta U \Delta V\|
$$

(15)

where the inequality follows from $\|\langle A, B\rangle\| \leq \|A\|_F \|B\|_F$ and $\|CD\|_F \leq \|C\|_F \|D\|_F$. Due to the constraints on $U$ and $V$, we have $\|U\|^2_F = \text{tr}(U^T U) = \text{tr}(I) = r, \|V\|^2_F = \sum_{j=1}^n \|v_j\|^2 = n$. \hfill \square

To analyse the convergence, we rewrite Eq. (6) as

$$\minimize_{U, V} f(U, V) = h(U, V) + \delta_U(U) + \delta_V(V),$$

where

$$\delta_U(U) = \begin{cases} 0, & U \in \mathbb{U} \\ \infty, & U \notin \mathbb{U} \end{cases}$$

is the indicator function of the set $\mathbb{U}$ and therefore nonsmooth, so is $\delta_V(V)$.

The following result establishes that the subsequence convergence property of the proposed algorithm, i.e., the sequence generated by Algorithm 1 is bounded and any of its limit point is a critical point of Eq. (16).

Theorem 4.1 (Subsequence convergence). Let $\{W(k)\}_{k \geq 0} = \{(U(k), V(k))\}_{k \geq 0}$ be the sequence generated by Algorithm 1 with constant step size $\lambda, \mu > L_c$. Then the sequence $\{W(k)\}_{k \geq 0}$ is bounded and obeys the following properties:

(P1): Sufficient decrease:

$$f(W(k-1)) - f(W(k)) \geq \frac{\min(\lambda, \mu) - L_c}{2} \|W(k) - W(k-1)\|^2_F,$$

which implies that

$$\lim_{k \to \infty} \|W(k-1) - W(k)\|_F = 0.$$  (18)

(P2): The sequence $\{f(W(k))\}_{k \geq 0}$ is convergent.

(P3): For any convergent subsequence $\{W(k')\}$, its limit point $W^*$ is a critical point of $f$ and

$$\lim_{k' \to \infty} f(W(k')) = \lim_{k \to \infty} f(W(k)) = f(W^*).$$

Proof of Theorem 4.1. Before proving Theorem 4.1, we give out some necessary definition.

Definition 4.1. [3] Let $f : \mathbb{R}^d \to (-\infty, \infty]$ be a proper and lower semi-continuous function, whose domain is defined as

$$\text{dom } f := \{ u \in \mathbb{R}^n : f(u) < \infty \}.$$  

The (Fréchet) subdifferential $\partial f$ of $f$ at $u$ is defined by

$$\partial f(u) = \left\{ z \in \mathbb{R}^d : \liminf_{v \to u} \frac{f(v) - f(u) - \langle z, v - u \rangle}{\|v - u\|} \geq 0 \right\}.$$
for any $u \in \text{dom } h$ and $\partial f(u) = \emptyset$ if $u \notin \text{dom } f$.

We say $u$ is a limiting critical point, or simply a critical point of $f$ if

$$0 \in \partial f(u).$$

We now turn to prove Theorem 4.1.

- **Showing (P1):** First note that for all $k$, according to our alternating minimization method, we always have $\delta_{U}(U(k)) = \delta_{V}(V(k)) = 0$ and thus $f(W(k)) = h(W(k))$.

  Since $h(U, V)$ has Lipschitz continuous gradient at $U \in U, V \in V$ with Lipschitz gradient $L_{c}$ and $\lambda > L_{c}$, we define $h_{L_{c}}(U, U', V)$ as proximal regularization of $h(U, V)$ linearized at $U', V$:

$$h(U', V) + \langle \nabla_{U} h(U', V), U - U' \rangle + \frac{L_{c}}{2} \|U - U'\|_{F}^{2},$$

By the definition of Lipschitz continuous gradient and Taylor expansion, we have

$$h(U, V) \leq h_{L_{c}}(U, U', V). \tag{20}$$

Also by the definition of proximal map, we get:

$$U(k) = \arg\min_{U} \delta_{U}(U) + \frac{\mu}{2} \|U - U(k - 1)\|_{F}^{2} + \langle \nabla_{U} h(U(k - 1), V(k - 1)), U - U(k - 1) \rangle \tag{21}$$

and hence we take $U(k) = U$, which implies that

$$\delta_{U}(U(k)) + \frac{\mu}{2} \|U(k) - U(k - 1)\|_{F}^{2} + \langle \nabla_{U} h(U(k - 1), V(k - 1)), U(k) - U(k - 1) \rangle \leq \delta_{U}(U(k - 1)) \tag{22}$$

Combining Eq. (20) and Eq. (22), we have:

$$h(U(k), V(k - 1)) + \delta_{U}(U(k))$$

$$\leq h(U(k - 1), V(k - 1)) + \langle \nabla_{U} h(U(k - 1), V(k - 1)), U(k) - U(k - 1) \rangle + \frac{L_{c}}{2} \|U(k) - U(k - 1)\|_{F}^{2} + \delta_{U}(U(k - 1))$$

$$\leq h(U(k - 1), V(k - 1)) + \frac{L_{c}}{2} \|U(k) - U(k - 1)\|_{F}^{2} + \delta_{U}(U(k - 1)) - \frac{\mu}{2} \|U(k) - U(k - 1)\|_{F}^{2}$$

$$= h(U(k - 1), V(k - 1)) + \delta_{U}(U(k - 1)) - \frac{\mu - L_{c}}{2} \|U(k) - U(k - 1)\|_{F}^{2}, \tag{23}$$

Similarly, we have

$$h(U(k), V(k)) - h(U(k), V(k - 1)) + \delta_{V}(V(k)) - \delta_{V}(V(k - 1)) \leq -\frac{\lambda - L_{c}}{2} \|V(k) - V(k - 1)\|_{F}^{2} \tag{24}$$

which together with the above equation gives Eq. (17). Now repeating Eq. (17) for all $k$ will give

$$(\min(\lambda, \mu) - L_{c}) \sum_{k=1}^{\infty} \|W(k) - W(k - 1)\|_{F}^{2} \leq f(W(0)), \tag{25}$$

which gives Eq. (18).

**Remark 4.1.** In our proposed algorithm, since in every update, our solution is closed while satisfying the constraints, thus in fact $\delta_{U}$ and $\delta_{V}$ are 0, and $\infty$ is never achieved.
• **Showing (P2):** It follows from Eq. (16) that \( \{f(W(k))\}_{k \geq 0} \) is a decreasing sequence. Due to the fact that \( f \) is lower bounded as \( f(W(k)) \geq 0 \) for all \( k \), we conclude that \( \{f(W(k))\}_{k \geq 0} \) is convergent.

• **Showing (P3):** Since \( U(k') \in U, V(k') \in V \) for all \( k' \) and both of the sets \( U \) and \( V \) are closed, we have \( U^* \in U, V^* \in V \). Since \( h \) is continuous, we have

\[
\lim_{k' \to \infty} f(W(k')) = \lim_{k' \to \infty} h(U(k'), V(k')) + \delta_U(U(k')) + \delta_V(V(k')) = f(W^*)
\]

which together with the fact that \( \{f(W(k))\}_{k \geq 0} \) is convergent gives Eq. (18).

To show \( W^* \) is a critical point, we first consider Eq. (21) and the optimality condition yields:

\[
\nabla_U h(U(k-1), V(k-1)) + \mu(U(k) - U(k-1)) + \partial\delta_U(U(k)) = 0.
\]

Similarly, we have

\[
\nabla_V h(U(k), V(k-1)) + \lambda(V(k) - V(k-1)) + \partial\delta_V(V(k)) = 0.
\]

Now, define

\[
A_k := \nabla_U h(U(k), V(k)) + \partial\delta_U(U(k)),
B_k := \nabla_V h(U(k), V(k)) + \partial\delta_V(V(k)).
\]

Thus, we have

\[
A_k \in \partial_U f(U(k), V(k)), B_k \in \partial_V f(U(k), V(k)).
\]

It follows from the above that

\[
\lim_{k \to \infty} \|A_k\|_F \leq \lim_{k \to \infty} \|\nabla_U h(U(k), V(k)) - \nabla_U h(U(k-1), V(k-1))\|_F + \mu\|U(k) - U(k-1)\|_F
\leq \lim_{k \to \infty} (L_c + \mu)\|W(k) - W(k-1)\|_F = 0.
\]

Similarly, we have:

\[
\lim_{k \to \infty} \|B_k\|_F \leq \lim_{k \to \infty} (L_c + \lambda)\|W(k) - W(k-1)\|_F = 0.
\]

Then we have:

\[
\text{dist}(0, \partial f(W(k))) \leq (2L_c + \mu + \lambda)\|W(k) - W(k-1)\|_F
\]

Owing to the closedness properties of \( \partial f(W(k')) \), we finally obtain

\( 0 \in \partial f(W^*) \).

Thus, \( W^* \) is a critical point of \( f \).

\[\blacksquare\]

**Theorem 4.2 (Sequence convergence).** The sequence \( \{W(k)\}_{k \geq 0} \) generated by Algorithm 1 with a constant step size \( \lambda, \mu > L_c \) is global-sequence convergence.

**Proof of Theorem 4.2.** Before proving Theorem 4.2, we give out another important definition.

**Definition 4.2 (Kurdyka-Lojasiewicz (KL) property).** [5] We say a proper semi-continuous function \( h(u) \) satisfies Kurdyka-Lojasiewicz (KL) property, if \( u \) is a critical point of \( h(u) \), then there exist \( \delta > 0, \theta \in [0, 1), C_1 > 0 \) such that

\[
|h(u) - h(\overline{u})|^\theta \leq C_1 \text{dist}(0, \partial h(u)), \quad \forall \ u \in B(\overline{u}, \delta)
\]

We mention that the above KL property(also known as KL inequality) states the regularity of \( h(u) \) around its critical point \( u \) and the KL inequality trivially holds at non-critical point. There are a very large set of functions satisfying the KL inequality including any semi-algebraic functions [3]. Clearly, the objective function \( f \) is semi-algebraic as both \( h, \delta_U \) and \( \delta_V \) are semi-algebraic.
Lemma 4.1 (Uniform KL property). There exist \( \delta_0 > 0, \theta_{KL} \in [0, 1), C_{KL} > 0 \) such that for all \( W \) s.t. dist(\( W, \mathbb{C}(W(0)) \)) \( \leq \delta_0 \):

\[
|f(W) - \overline{f}|^{\theta_{KL}} \leq C_{KL} \text{dist}(0, \partial f(W))
\]

with \( \overline{f} \) denoting the limiting function value defined in (P2) of Theorem 4.1.

Proof. First we recognize the union \( \bigcup_i B(W_i^*, \delta_i) \) forms an open cover of \( \mathbb{C}(W(0)) \) with \( W_i^* \) representing all points in \( \mathbb{C}(W(0)) \) and \( \delta_i \) to be chosen so that the the following KL property of \( f \) at \( W_i^* \in \mathbb{C}(W(0)) \) holds:

\[
|f(W) - \overline{f}|^{\theta_{KL}} \leq C_i \text{dist}(0, \partial f(W)) \quad \forall W \in B(W_i^*, \delta_i)
\]

where we have used all \( f(W_i^*) = \overline{f} \) by assertion (P3) of Theorem 4.1. Then due to the compactness of the set \( \mathbb{C}(W(0)) \), it has a finite subcover \( \bigcup_{i=1}^p B(W_{k_i}^*, \delta_{k_i}) \) for some positive integer \( p \). Now combining all, we have for all \( W \in \bigcup_{i=1}^p B(W_{k_i}^*, \delta_{k_i}) \),

\[
|f(W) - \overline{f}|^{\theta_{KL}} \leq C_{KL} \text{dist}(0, \partial f(W))
\]

with \( \theta_{KL} = \max_{i=1}^p \{ \theta_{k_i} \} \) and \( C_{KL} = \max_{i=1}^p \{ C_{k_i} \} \). Finally, since \( \bigcup_{i=1}^p B(W_{k_i}^*, \delta_{k_i}) \) is an open cover of \( \mathbb{C}(W(0)) \), there exists a sufficiently small number \( \delta_0 \) so that

\[
\{ (W) : \text{dist}(W, \mathbb{C}(W(0))) \leq \delta_0 \} \subset \bigcup_{i=1}^p B(W_{k_i}^*, \delta_{k_i}).
\]

Therefore, eq. (33) holds whenever dist(\( W, \mathbb{C}(W(0)) \)) \( \leq \delta_0 \). \( \Box \)

We now turn to prove Theorem 4.2.

According to Definition 4.2, there exists a sufficiently large \( k_0 \) satisfying:

\[
[f(W(k)) - f(W^*)]^{\theta} \leq C_2 \text{dist}(0, \partial f(W(k))), \quad \forall k \geq k_0.
\]

In the subsequent analysis, we restrict to \( k \geq k_0 \). Construct a concave function \( x^{1-\theta} \) for some \( \theta \in [0, 1) \) with domain \( x > 0 \). Obviously, by the concavity, we have

\[
x_2^{1-\theta} - x_1^{1-\theta} \geq (1 - \theta)x_2^{\theta}(x_2 - x_1), \forall x_1 > 0, x_2 > 0
\]

Replacing \( x_1 \) by \( f(W_{k+1}) - f(W^*) \) and \( x_2 \) by \( f(W_k) - f(W^*) \) and using the sufficient decrease property, we have

\[
[f(W(k)) - f(W^*)]^{1-\theta} - [f(W(k+1)) - f(W^*)]^{1-\theta} \\
\geq (1 - \theta)\frac{f(W(k)) - f(W(k+1))}{[f(W(k)) - f(W^*)]^{\theta}} \\
\geq \frac{\lambda(1 - \theta)}{2C_2} \frac{\|W(k) - W(k+1)\|^2_F}{\text{dist}(0, \partial f(W(k)))} \\
\geq \frac{\lambda(1 - \theta)}{2C_2C_3} \frac{\|W(k) - W(k+1)\|^2_F}{\|W(k) - W(k-1)\|^F} \\
= \kappa\left( \frac{\|W(k) - W(k+1)\|^2_F}{\|W(k) - W(k-1)\|^F} + \|W(k) - W(k-1)\|^F - \kappa\|W(k) - W(k-1)\|^F \right) \\
\geq \kappa(2\|W(k) - W(k+1)\|^F - \|W(k) - W(k-1)\|^F)
\]

And accordingly, we have:

\[
2\|W(k) - W(k+1)\|^F - \|W(k) - W(k-1)\|^F \leq \beta \left( [f(W(k)) - f(W^*)]^{1-\theta} - [f(W(k+1)) - f(W^*)]^{1-\theta} \right)
\]

(35)
with $C_3 := 2L_c + \mu + \lambda, \kappa := \frac{\lambda(1 - \theta)}{2C_3}, \beta := \left(\frac{\lambda(1 - \theta)}{2C_3}\right)^{-1}$.

Summing the above inequalities up from some $\tilde{k} > k_0$ to infinity yields

$$\sum_{k=\tilde{k}}^{\infty} \|W(k) - W(k+1)\|_F \leq \|W(\tilde{k}) - W(\tilde{k}-1)\|_F + \beta[f(W(\tilde{k})) - f(W^*)]^{1-\theta}$$

(36)

implying

$$\sum_{k=\tilde{k}}^{\infty} \|W(k) - W(k+1)\|_F < \infty.$$ 

Following some standard arguments one can see that

$$\lim_{t \to \infty, t_1, t_2 \geq t} \|W(t_1) - W(t_2)\|_F = 0$$

which implies that the sequence \{W(k)\} is Cauchy, and hence convergent. Hence, the limit point set $C(W(0))$ is singleton $W^*$.

**Theorem 4.3** (Convergence Rate). The convergence rate is at least sub-linear.

Towards that end, we first know from the above argument that \{W(k)\} converges to some point $W^*$, i.e.,

$$\lim_{k \to \infty} W(k) = W^*.$$ 

Then using Equation (36) and the triangle inequality, we obtain

$$\|W(\tilde{k}) - W^*\|_F \leq \sum_{k=\tilde{k}}^{\infty} \|W(k) - W(k+1)\|_F$$

(37)

$$\leq \|W(\tilde{k}) - W(\tilde{k}-1)\|_F + \beta[f(W(\tilde{k})) - f(W^*)]^{1-\theta}$$

which indicates the convergence rate of $W(\tilde{k}) \to W^*$ is at least as fast as the rate that $\|W(\tilde{k}) - W(\tilde{k}-1)\|_F + \beta[f(W(\tilde{k})) - f(W^*)]^{1-\theta}$ converges to 0. In particular, the second term $\beta[f(W(\tilde{k})) - f(W^*)]^{1-\theta}$ can be controlled:

$$\beta[f(W(\tilde{k})) - f(W^*)]^{\theta} \leq \beta C_2 \text{dist}(0, \partial f(W(\tilde{k})))$$

$$\leq \beta C_2 (2B_0 + \lambda + \|X\|_F) \|W(\tilde{k}) - W(\tilde{k}-1)\|_F$$

(38)

Plugging (38) back to (37), we then have

$$\sum_{k=\tilde{k}}^{\infty} \|W(k) - W(k+1)\|_F \leq \|W(\tilde{k}) - W(\tilde{k}-1)\|_F + \alpha \|W(\tilde{k}) - W(\tilde{k}-1)\|_F^{1-\theta}.$$ 

We divide the following analysis into two cases based on the value of the KL exponent $\theta$.

- **Case 1:** If $\theta = 0$, we set $Q := \{k \in \mathbb{N} : W(k+1) \neq W(k)\}$ and take $k$ in $Q$. When $k$ is sufficiently large, then we have:

$$\|W(k+1) - W(k)\|_F^2 := C_4 > 0$$

(39)

On the other hand,

$$f(W(k+1)) - f(W(k)) \geq \frac{\min(\lambda, \mu) - L_c}{2} \|W(k+1) - W(k)\|_F^2$$

$$= \frac{\min(\lambda, \mu) - L_c}{2} C_4$$

(40)

Since $f(W(k))$ is known to be converging to 0, Eq. (40) implies that $Q$ is finite and sequence $W(k)$ converges in a finite number of steps.
Case II: \( \theta \in (0, \frac{1}{2}] \). This case means \( \frac{1-\theta}{\sigma} \geq 1 \). We define \( P_k = \sum_{i=k}^{\infty} \| W_{i+1} - W_i \|_F \),

\[
P_k \leq P_{k-1} - P_k + \alpha \left[ P_{k-1} - P_k \right]^{\frac{1-\theta}{\sigma}}.
\] (41)

Since \( P_{k-1} - P_k \to 0 \), there exists a positive integer \( k_1 \) such that \( P_{k-1} - P_k < 1 \), \( \forall \bar{k} \geq k_1 \). Thus,

\[
P_k \leq (1 + \alpha) (P_{k-1} - P_k), \quad \forall \bar{k} \geq \max \{ k_0, k_1 \},
\]

which implies that

\[
P_k \leq \rho \cdot P_{k-1}, \quad \forall \bar{k} \geq \max \{ k_0, k_1 \},
\] (42)

where \( \rho = \frac{1+\alpha}{2+\alpha} \in (0, 1) \). This together with (37) gives the linear convergence rate

\[
\| W(k) - W^* \|_F \leq O(\rho^{k-\bar{k}}), \quad \forall k \geq \bar{k}.
\] (43)

where \( \bar{k} = \max \{ k_0, k_1 \} \).

Case III: \( \theta \in (1/2, 1) \). This case means \( \frac{1-\theta}{\sigma} \leq 1 \). Based on the former results, we have

\[
P_k \leq (1 + \alpha) \left[ P_{k-1} - P_k \right]^{\frac{1-\theta}{\sigma}}, \quad \forall \bar{k} \geq \max \{ k_0, k_1 \}.
\]

We now run into the same situation as in [2]. Hence following a similar argument gives

\[
P_{\frac{1-2\theta}{k-1}} - P_{\frac{1-2\theta}{k-1}} \geq \zeta, \quad \forall k \geq \bar{k}
\]

for some \( \zeta > 0 \). Then repeating and summing up the above inequality from \( \bar{k} = \max \{ k_0, k_1 \} \) to any \( k > \bar{k} \), we can conclude

\[
P_k \leq \left[ P_{\frac{1-2\theta}{k-1}} + \zeta (k - \bar{k}) \right]^{-\frac{1-\theta}{2\theta}} = O \left( (k - \bar{k})^{-\frac{1-\theta}{2\theta}} \right).
\]

Finally, the following sublinear convergence holds

\[
\| W(k) - W^* \|_F \leq O \left( (k - \bar{k})^{-\frac{1-\theta}{2\theta}} \right), \quad \forall k > \bar{k}.
\] (44)

We end this proof by commenting that both linear and sublinear convergence rate are closely related to the KL exponent \( \theta \) at the critical point \( W^* \).

5 Experiments

In this section, we are going to apply our proposed spherical PCA to both synthetic data and real-world datasets to test the performance of our proposed method. The experiment on synthetic data will be introduced first followed by experiments on real-world datasets.

5.1 Synthetic Data Experiment

We first generate 200 data, half of which is distributed within the region between \( X = Z \) and \( Z \) axis (denoted as blue dots in the top part of Fig. 2), while another group is generated within the region between \( Y = Z \) and \( Z \) axis (denoted as the red dots). These two clusters of data are generated through different angles. Thus when we do clustering, it should be angle distance rather than Euclidean distance to determine the clustering result. For our method, we learn a projection matrix \( U \in \mathbb{R}^{3 \times 2} \) and plot the component matrix \( V \in \mathbb{R}^{2 \times 200} \) as the bottom part illustrates. We see that, Euclidean distance-based method (such as \( K \)-means) will yield poor clustering result (middle part), while spherical-PCA will obtain good clustering result.

Also, we show the convergence of \( \{ W(k) \}_{k \geq 0} = \{ (U(k), V(k)) \}_{k \geq 0} \) generated by our method. As Fig. 3 shows, after short iterations, the generated sequences will be stable, which is in accordance with the convergence proof. It also illustrates the objective with update. We see that it converges fast with a sublinear rate, which validates our convergence rate analysis.
5.2 Real-world Datasets Experiment

Table 1: Clustering performance of different algorithms on 20-newsgroup dataset

| Methods     | #Groups | Acc | NMI | Acc | NMI | Acc | NMI | Acc | NMI | Acc | NMI | Acc | NMI | Acc | NMI | Acc | NMI |
|-------------|---------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| K-means     | 5       | 0.651 | 0.621 | 0.674 | 0.614 | 0.703 | 0.628 | 0.745 | 0.647 | 0.789 | 0.673 | 0.838 | 0.695 |
|             | 10      | 0.487 | 0.316 | 0.478 | 0.320 | 0.502 | 0.383 | 0.535 | 0.398 | 0.527 | 0.394 | 0.588 | 0.401 |
|             | 15      | 0.398 | 0.307 | 0.387 | 0.301 | 0.412 | 0.319 | 0.423 | 0.320 | 0.461 | 0.377 | 0.486 | 0.385 |
|             | 20      | 0.315 | 0.242 | 0.314 | 0.221 | 0.362 | 0.248 | 0.394 | 0.260 | 0.412 | 0.280 | 0.431 | 0.294 |
| MUA         |         |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| PCA         |         |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| R1-PCA      |         |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| K-SVD       |         |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| Spherical PCA |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |

It is known that in information retrieval, similarities or dissimilarities (proximities) between objects are more critical than Euclidean distance. In this subsection, we will test our proposed method on the widely-used 20-newsgroup dataset for clustering. We have different newsgroups such as: comp.graphics, rec.motorcycles, rec.sport.baseball, sci.space, talk.politics.mideast, etc. 200 documents are randomly sampled from each newsgroup. The word-document matrix X is constructed with 500 words selected according to the mutual information between words and documents. Tf.idf term weighting is used before normalization. Clustering accuracy are computed using the known class labels. Results will be compared including clustering accuracy (Acc.) and Normalized Mutual Information (NMI) [24].

Different clustering algorithms will be compared including:

1. R1-PCA, which proposes a rotational invariant $\ell_1$-norm PCA, where a robust covariance matrix will soften the effects of outliers [7];
Table 2: Clustering performance of different algorithms on four UCI datasets

| Data (#class) | $K$-means | MUA | PCA | R1-PCA | Spherical PCA |
|---------------|-----------|-----|-----|--------|--------------|
| glass (6)     | 0.687     | 0.566 | 0.692 | 0.574 | 0.732 | 0.608 | **0.801** | **0.648** | 0.788 | 0.635 |
| diabetes (2)  | 0.775     | 0.632 | 0.788 | 0.654 | 0.761 | 0.613 | 0.808 | 0.631 | 0.827 | 0.672 | **0.832** | **0.680** |
| mfeat (10)    | 0.365     | 0.223 | 0.358 | 0.211 | 0.371 | 0.225 | **0.431** | **0.342** | 0.412 | 0.328 | 0.425 | 0.330 |
| isole (26)    | 0.267     | 0.198 | 0.253 | 0.181 | 0.262 | 0.182 | 0.324 | 0.201 | 0.357 | 0.246 | **0.373** | **0.250** |

2. **K-SVD**, which is an iterative method that alternates between sparse coding of the examples based on the current dictionary and a process of updating the dictionary atoms to better fit the data [1];

3. **PCA**, i.e. the vanilla PCA method in Eq. (2) without the constraint on $V$, which will be Euclidean distance-based by default;

4. **NMF** Matrix Factorization proposed by [11,13,14,21] where $U$ and $V$ are obtained by Multiplicative Updating Algorithm with nonnegative constraint

5. **$K$-means** [9].

We vary the number of clusters from 5 to 10, 15 and 20. In each newsgroup, 200 documents are randomly sampled, and we repeat for 10 times by taking the average and report the clustering result as Table 1 demonstrates.

We see that our proposed method Spherical PCA can always achieve both higher clustering accuracy and normalized mutual information in text analysis.

We also compare our method with other methods on UCI datasets including: glass, diabetes, mfeat and isole. Table 2 illustrates the results. We see that though our method doesn’t show the absolute advantage as on text, still the result is considerably good.

All the experiments indicate that our method can achieve good performance on both text and non-text datasets, showing its potential for broader application.

6 Conclusion

In this paper, we study spherical PCA where the direction matrix is orthonormal and the component vectors are assumed to lie in the unitary sphere. The benefit is obvious that it can make the angle distance equivalent to Euclidean distance. Due to the nonconvexity of objective function and constraints on the factors which are difficult to tackle, we propose an alternating linearized minimization method to derive the solution, which is proved to be sequence convergent. Moreover, we analyze the convergence rate which is validated by our experiments. The results on real-world datasets and synthetic data illustrate the superiority of our method.

References

[1] Michal Aharon, Michael Elad, Alfred Bruckstein, et al. K-svd: An algorithm for designing overcomplete dictionaries for sparse representation. *IEEE Transactions on signal processing*, 54(11):4311, 2006.

[2] Hedy Attouch and Jérôme Bolte. On the convergence of the proximal algorithm for nonsmooth functions involving analytic features. *Mathematical Programming*, 116(1-2):5–16, 2009.

[3] Hedy Attouch, Jérôme Bolte, and Benar Fux Svaiter. Convergence of descent methods for semi-algebraic and tame problems: proximal algorithms, forward–backward splitting, and regularized gauss–seidel methods. *Mathematical Programming*, 137(1-2):91–129, 2013.
[4] Mikhail Belkin and Partha Niyogi. Laplacian eigenmaps for dimensionality reduction and data representation. *Neural computation*, 15(6):1373–1396, 2003.

[5] Jérôme Bolte, Aris Daniilidis, and Adrian Lewis. The Łojasiewicz inequality for nonsmooth subanalytic functions with applications to subgradient dynamical systems. *SIAM Journal on Optimization*, 17(4):1205–1223, 2007.

[6] Patrick L Combettes and Teemu Pennanen. Proximal methods for cohypomonotone operators. *SIAM journal on control and optimization*, 43(2):731–742, 2004.

[7] Chris Ding, Ding Zhou, Xiaofeng He, and Hongyuan Zha. R 1-pca: rotational invariant l 1-norm principal component analysis for robust subspace factorization. In *Proceedings of the 23rd international conference on Machine learning*, pages 281–288. ACM, 2006.

[8] Hsieh Hou. A fast recursive algorithm for computing the discrete cosine transform. *IEEE Transactions on Acoustics, Speech, and Signal Processing*, 35(10):1455–1461, 1987.

[9] Anil K Jain. Data clustering: 50 years beyond k-means. *Pattern recognition letters*, 31(8):651–666, 2010.

[10] Alexander Kaplan and Rainer Tichatschke. Proximal point methods and nonconvex optimization. *Journal of global Optimization*, 13(4):389–406, 1998.

[11] Daniel D Lee and H Sebastian Seung. Algorithms for non-negative matrix factorization. In *Advances in neural information processing systems*, pages 556–562, 2001.

[12] Qiuwei Li, Zhihui Zhu, and Gongguo Tang. The non-convex geometry of low-rank matrix optimization. *Information and Inference: A Journal of the IMA*, 8(1):51–96, 03 2018.

[13] Kai Liu and Hua Wang. Robust multi-relational clustering via l1-norm symmetric nonnegative matrix factorization. In *Proceedings of the 53rd Annual Meeting of the Association for Computational Linguistics and the 7th International Joint Conference on Natural Language Processing (Volume 2: Short Papers)*, volume 2, pages 397–401, 2015.

[14] Kai Liu and Hua Wang. High-order co-clustering via strictly orthogonal and symmetric l1-norm nonnegative matrix tri-factorization. In *IJCAI*, pages 2454–2460, 2018.

[15] Hieu V Nguyen and Li Bai. Cosine similarity metric learning for face verification. In *Asian conference on computer vision*, pages 709–720. Springer, 2010.

[16] R Tyrrell Rockafellar. Augmented lagrangians and applications of the proximal point algorithm in convex programming. *Mathematics of operations research*, 1(2):97–116, 1976.

[17] Sam T Roweis and Lawrence K Saul. Nonlinear dimensionality reduction by locally linear embedding. *science*, 290(5500):2323–2326, 2000.

[18] Amit Singhal et al. Modern information retrieval: A brief overview. *IEEE Data Eng. Bull.*, 24(4):35–43, 2001.

[19] Dengdi Sun, Chris HQ Ding, Bin Luo, and Jin Tang. Angular decomposition. In *Twenty-Second International Joint Conference on Artificial Intelligence*, 2011.

[20] Joshua B Tenenbaum, Vin De Silva, and John C Langford. A global geometric framework for nonlinear dimensionality reduction. *science*, 290(5500):2319–2323, 2000.

[21] Hua Wang, Heng Huang, and Chris Ding. Simultaneous clustering of multi-type relational data via symmetric nonnegative matrix tri-factorization. In *Proceedings of the 20th ACM international conference on Information and knowledge management*, pages 279–284. ACM, 2011.

[22] Hua Wang, Feiping Nie, and Heng Huang. Multi-view clustering and feature learning via structured sparsity. In *International conference on machine learning*, pages 352–360, 2013.
[23] Hua Wang, Feiping Nie, Heng Huang, and Fillia Makedon. Fast nonnegative matrix tri-factorization for large-scale data co-clustering. In Twenty-Second International Joint Conference on Artificial Intelligence, 2011.

[24] Wei Xu, Xin Liu, and Yihong Gong. Document clustering based on non-negative matrix factorization. In Proceedings of the 26th annual international ACM SIGIR conference on Research and development in information retrieval, pages 267–273. ACM, 2003.

[25] Zhihui Zhu, Qiuwei Li, Gongguo Tang, and Michael B Wakin. Global optimality in low-rank matrix optimization. IEEE Transactions on Signal Processing, 66(13):3614–3628, 2018.