On the rotational invariant $L_1$-norm PCA

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Abstract

Principal component analysis (PCA) is a powerful tool for dimensionality reduction. Unfortunately, it is sensitive to outliers, so that various robust PCA variants were proposed in the literature. Among them the so-called rotational invariant $L_1$-norm PCA is rather popular. In this paper, we reinterpret this robust method as conditional gradient algorithm and show moreover that it coincides with a gradient descent algorithm on Grassmannian manifolds. Based on this point of view, we prove for the first time convergence of the whole series of iterates to a critical point using the Kurdyka-Łojasiewicz property of the energy functional.

Keywords: Principal component analysis, Dimensionality reduction, Robust subspace fitting, Conditional gradient algorithm, Frank-Wolfe algorithm, Optimization on Grassmannian manifolds,

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1. Introduction

In exploratory data analysis, principal component analysis (PCA) [33] still is one of the most popular tools for dimensionality reduction. Given $N \geq d$ data points $x_1, \ldots, x_N \in \mathbb{R}^d$, it finds a $K$-dimensional affine subspace $\{At + b : t \in \mathbb{R}^K\}$, $1 \leq K \leq d$, of $\mathbb{R}^d$ having smallest squared Euclidean distance from the data:

$$(\hat{A}, \hat{b}) \in \arg \min_{A \in \mathbb{R}^{d \times K}, b \in \mathbb{R}^d} \sum_{i=1}^{N} \min_{t \in \mathbb{R}^K} \|At + b - x_i\|_2^2, \quad (1)$$

where $\| \cdot \|$ denotes the Euclidean norm. While $\hat{b}$ in the above minimization problem is not unique, every minimizing affine subspace goes through the offset(bias) $\hat{b} := \frac{1}{N}(x_1 + \ldots + x_N)$. Therefore, we restrict our attention to data points $y_i := x_i - \hat{b}$, $i = 1, \ldots, N$, and subspaces

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through the origin minimizing the squared Euclidean distances to the $y_i$, $i = 1, \ldots, N$. Setting further the gradient with respect to $t \in \mathbb{R}^K$ to zero and allowing only orthonormal columns in $A$, the PCA problem becomes

$$
\hat{A} \in \arg \min_{A \in \mathbb{R}^{d,K}, A^T A = I_K} \sum_{i=1}^{N} \|P_A y_i\|^2,
$$

where $$P_A := I_d - AA^T$$ denotes the orthogonal projection onto $\mathcal{R}(A)^\perp = \mathcal{N}(A^T)$ and $I_d$ the $d \times d$ identity matrix. Here $\mathcal{R}(A)$ denotes the range and $\mathcal{N}(A)$ the kernel of $A$. One convenient property of PCA is the nestedness of the PCA subspaces, i.e., for $K < \tilde{K} \leq d$, the optimal $K$-dimensional PCA subspace is contained in the $\tilde{K}$-dimensional one.

Unfortunately, PCA is sensitive to outliers appearing quite often in real-world data sets. A lot of different methods in robust statistics \[14, 27, 22\] and optimization were proposed to make the dimensionality reduction more robust. One possibility consists of removing outliers before computing the principal components which has the serious drawback that outliers are difficult to identify and other data points are often falsely labeled as outliers. Another approach assigns different weights to data points based on their estimated relevancy, to get a weighted PCA, see, e.g. \[18\]. The RANSAC algorithm \[10\] repeatedly estimates the model parameters from a random subset of the data points until a satisfactory result is obtained as indicated by the number of data points within a certain error threshold. In a similar vein, least trimmed squares PCA models \[36, 34\] aim to exclude outliers from the squared error function, but in a deterministic way. The variational model in \[6\] decomposes the data matrix $Y = (y_1 \ldots y_N)$ into a low rank and a sparse part. Related approaches such as \[25, 38\] separate the low rank component from the column sparse one using different norms in the variational model. However, such a decomposition is not always realistic. Another group of robust PCA approaches replaces the squared $L_2$ norm in the PCA by the $L_1$ norm. Then, the minimization of the energy functional can be addressed by linear programming, see, e.g., Ke and Kanade \[16\]. Unfortunately, this norm is not rotationally invariant.

In this paper, the focus lies on the model

$$
(\hat{A}, \hat{b}) \in \arg \min_{A \in \mathbb{R}^{d,K}, b \in \mathbb{R}^d} \sum_{i=1}^{N} \min_{t \in \mathbb{R}^K} \|At + b - x_i\| \tag{2}
$$

where in contrast to (1) we do not square the Euclidean norm. First of all, let us mention that the determination of the offset $b \in \mathbb{R}^d$ becomes a serious problem now. In general $\hat{b} \in \mathbb{R}^d$ is not the frequently used geometric median of the data. However, in this paper it is assumed that $b \in \mathbb{R}^d$ is fixed and already subtracted from the data. Then (2) reduces to

$$
\hat{A} \in \arg \min_{A \in \mathbb{R}^{d,K}, A^T A = I_K} \sum_{i=1}^{N} \|P_A y_i\|. \tag{3}
$$

A slightly different form of this model became popular under the name rotational invariant $L_1$-norm PCA by a paper of Ding et al. \[8\]. These authors also suggest a constrained minimization scheme without convergence proof.
Figure 1: Global minimizing line/plane corresponding to $K = 1, 2$ in (3) demonstrating the loss of the nestedness property of the PCA. The data $y_i \in \mathbb{R}^3$ (black dots) are given by the points $\{(0.005l, 0, 0.005l) : l \in \{0, \ldots, 30\}\}$ on a line along with points $(1, 0, 0)^T$, $(-1, 0, 0)^T$, $(1/\sqrt{2}, 1/\sqrt{2}, 0)^T$, $(-1/\sqrt{2}, 1/\sqrt{2}, 0)^T$, $(1/\sqrt{2}, -1/\sqrt{2}, 0)^T$, $(-1/\sqrt{2}, -1/\sqrt{2}, 0)^T$ on an ellipse. The direction $\hat{a}_1 = (1/\sqrt{2}, 0, 1/\sqrt{2})^T$ (red line) does not lie on the blue plane generated by $\hat{A}$ which has the columns $(1, 0, 0)^T$ and $(0, 1, 0)^T$.

It is important to note that in contrast to the classical PCA the hierarchical structure of the approach is lost. This is exemplified in Fig. 1. We mention that several models applying the deflation technique of standard PCA in a robust setting were also provided in the literature. These models are not of interest in this paper, but we refer to the book [13, p. 203] and the collection of papers [12, 17, 20, 21, 23, 28, 31] which is clearly not complete.

Recall that we are not interested in the columns of the minimizer $\hat{A}$ in (3) itself, but just in the subspace spanned by the columns. Such $K$-dimensional subspaces of $\mathbb{R}^d$ are described by Grassmannian manifolds. In this paper, the iterative algorithm of Ding et al. [8] is interpreted as a conditional gradient algorithm, also known as Frank-Wolfe algorithm, which implies a certain convergence behavior of subsequences of the iterates. Further, the algorithm can also be interpreted as a gradient descent algorithm on the Grassmannian manifold, which enables us to prove convergence of the whole sequence of iterates provided that no point is reached where the functional in (3) is not differentiable.

The paper is organized as follows: In Section 2 we recall preliminaries on Stiefel and Grassmannian manifolds. We discuss important properties of the robust PCA model in Section 3. Section 4 shows the equivalence of the algorithm of Ding et al. [8], the conditional gradient algorithm and a gradient descent algorithm on Grassmannians. The convergence proof is given in Section 5. So far we have to assume that the algorithm avoids points where the functional is not differentiable. Fortunately, this is the case in most applications. However, Section 6 addresses the topic of these so-called anchor points. The paper ends with conclusions and future directions of research in Section 7.
2. Preliminaries on Stiefel and Grassmannian Manifolds

In this section, we briefly provide the basic notation on Stiefel and Grassmannian manifolds which is required in our approach. Good references on the topic, in particular for optimization on these manifolds, are \[1, 9\].

Let \( K \leq d \). The (compact) Stiefel manifold is defined by

\[
S_{d,K} := \left\{ A \in \mathbb{R}^{d,K} : A^T A = I_K \right\}.
\]

For \( K = 1 \), it coincides with the unit sphere \( S_{d,1} = S^{d-1} \) in \( \mathbb{R}^d \) and for \( K = d \) with the orthogonal matrices \( S_{d,d} = O(d) \). The tangent space at \( A \in S_{d,K} \) is given by

\[
T_A S_{d,K} := \left\{ V \in \mathbb{R}^{d,K} : V^T A + A^T V = 0 \right\} = \left\{ V \in \mathbb{R}^{d,K} : V = AX + A_\perp Z, \quad X \in \mathbb{R}^{K,K} \text{ skew symmetric}, \quad Z \in \mathbb{R}^{d-K,K} \right\},
\]

where \( A_\perp \) denotes a matrix with orthonormal columns which are in addition orthogonal to the columns of \( A \). There are two common ways to define inner products on the tangent space such that \( S_{d,K} \) becomes a Riemannian manifold, namely i) the Frobenius inner product \( \langle V, W \rangle_F := \text{tr}(V^T W) \), or ii) the canonical inner product \( \langle V, W \rangle_A := \text{tr}(V^T (I_d - \frac{1}{2} A A^T) W) \).

The first one appears when considering \( S_{d,K} \) as submanifold of the Euclidean space \( \mathbb{R}^{d,K} \), while the second one relies the quotient structure \( S_{d,K} = O(d)/O(d - K) \). We are mainly interested in the \( K \)-dimensional subspace spanned by the columns of \( A \in S_{d,K} \), which does not change if we multiply \( A \) from the right with an orthogonal matrix \( Q \in O(K) \). This is pictured by the Grassmannian manifold or just Grassmannian which can be defined as quotient manifold of the Stiefel manifold \( G_{d,K} := S_{d,K}/O(K) \). The equivalence classes \( [A] := \{ AQ : Q \in O(K) \} \) belonging to \( G_{d,K} \) can be represented by elements \( A \) of the Stiefel manifold. The tangent space of \( G_{d,K} \) at \( [A] \) can be identified with its horizontal lift at \( A \),

\[
T_{[A]} G_{d,K} := \left\{ A_\perp Z : Z \in \mathbb{R}^{d-K,K} \right\}.
\]

Further, the Grassmannian becomes a Riemannian manifold by reducing the Riemannian metrics in i) or equivalently ii) to \( T_{[A]} G_{d,K} \), i.e., for any representative \( A \in S_{d,K} \) and \( V, W \in T_{[A]} G_{d,K} \),

\[
\langle V, W \rangle_{[A]} := \langle V, W \rangle_A = \text{tr} \left( V^T (I_K - \frac{1}{2} A A^T) W \right) = \text{tr} (V^T W) = \langle V, W \rangle_F.
\]

A possible choice for a metric on the Grassmannian is given by

\[
d_{G_{d,K}} ([A_1], [A_2]) := \| A_1 A_1^T - A_2 A_2^T \|_2,
\]

where \( A_1, A_2 \in S_{d,K} \) and \( \| \cdot \|_2 \) is the spectral norm.

In PCA we aim to find an optimal subspace, which means that we are interested in elements of Grassmannians. In practice, working with equivalence classes is difficult and hence calculations are performed with representatives on the Stiefel manifold.

The proposed optimization algorithms make use of the orthogonal projection \( \Pi_{S_{d,K}} : \mathbb{R}^{d,K} \rightarrow S_{d,K} \), i.e.,

\[
\Pi_{S_{d,K}} (M) = \arg \min_{O \in S_{d,K}} \| M - O \|^2 = \arg \max_{O \in S_{d,K}} \langle O, M \rangle.
\]
To this end, recall that the polar decomposition of a matrix $M \in \mathbb{R}^{d,K}$ is given by $M = QS$, where $Q \in S_{d,K}$ and $S \in \mathbb{R}^{K,K}$ is symmetric and positive semi-definite. Starting with the (economy-size) singular value decomposition $M = U \Sigma V^T$, where $U \in S_{d,K}$, $\Sigma \in \mathbb{R}^{K,K}$ is a diagonal matrix and and $V \in S_{K,K}$, the polar decomposition is determined by $Q := \text{Polar}(M) := UV^T$ and $S := V \Sigma V^T$. The following lemma can be found e.g. in \cite{15, 34}.

**Lemma 2.1.** The orthogonal projection $\Pi_{S_{d,K}} : \mathbb{R}^{d,K} \to S_{d,K}$ is given by

$$\Pi_{S_{d,K}}(M) = \text{Polar}(M).$$

If $M$ has full rank, then $\text{Polar}(M) = M(M^TM)^{-\frac{1}{2}}$.

### 3. Model Analysis

In this section, the main focus lies on investigating our rotational invariant $L_1$-norm model

$$\hat{A} \in \arg \min_{A \in S_{d,K}} \sum_{i=1}^N \|PAy_i\|.$$ 

To be precise, we are actually only interested in minimizing over equivalence classes $[\hat{A}] := \{\hat{A}Q : Q \in O(K)\}$. Besides the objective function

$$E(A) = \sum_{i=1}^N E_i(A) := \sum_{i=1}^N \|PAy_i\| = \sum_{i=1}^N \|(I_d - AA^T)y_i\|,$$  \hfill (4)

we also deal with the function

$$F(A) = \sum_{i=1}^N F_i(A) := \sum_{i=1}^N \sqrt{y_i^T P Ay_i} = \sum_{i=1}^N \sqrt{\|y_i\|^2 - \|A^Ty_i\|^2}. \hfill (5)$$

Clearly, these two functions take the same values on the Stiefel manifold $S_{d,K}$. However, they have quite different properties as functions on $\mathbb{R}^{d,K}$. While $E$ is well-defined on the whole $\mathbb{R}^{d,K}$, the function $F$ is only well defined on the closed domain

$$\mathcal{D} := \bigcap_{i=1}^N \mathcal{D}_i, \quad \mathcal{D}_i := \{A \in \mathbb{R}^{K,d} : \|y_i\|^2 - \|A^Ty_i\|^2 \geq 0\}$$

and therefore it is extended to the whole $\mathbb{R}^{d,K}$ by

$$F(A) := -\infty \text{ if } A \notin \mathcal{D}. \hfill (6)$$

For $A \in S_{d,K}$ and all $y \in \mathbb{R}^d$, it holds $\|ATy\| \leq \|y\|$ so that $S_{d,K} \subseteq \mathcal{D}$. Further, $A \in S_{d,K} \cap \partial \mathcal{D}$ if and only if $\|PAy_i\| = 0$ for some $i \in \{1, \ldots, N\}$. The set

$$\mathcal{A} := \{A \in S_{d,K} : \|PAy_i\| = 0 \text{ for some } i \in \{1, \ldots, N\}\}$$

is called **anchor set** and a compact subset of $\mathbb{R}^{d,K}$.

In the simple case $N = d = K = 1$ and $y_1 = 1$, the above functions read $E(A) = |1 - A^2|$ and $F(A) = \sqrt{1 - A^2}$ with $A \in \mathbb{R}$. While the first function is locally Lipschitz continuous on $[-1, 1]$, the second one does not have this property at $A = \pm 1$. The following two lemmata state properties of $E$ and $F$. 

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Lemma 3.1. The function $E$ defined by (4) is locally Lipschitz continuous on $\mathbb{R}^{d,K}$.

Proof. It suffices to show the property for the summands $E_i$. For an arbitrary fixed $A \in \mathbb{S}_{d,K}$, let $\|A - A_i\| \leq \varepsilon$, $i = 1, 2$. Then, we obtain

\[
\|E_i(A_1) - E_i(A_2)\| = \|P_{A_1}y_i - P_{A_2}y_i\| \leq \|P_{A_1}y_i - P_{A_2}y_i\| \\
\leq \|A_1A_1^T - A_2A_2^T\| \|y_i\| \\
= \frac{1}{2}(\|A_1 - A_2\| + \|A_1^T A_2 + A_2^T A_1\| + \|A_1 + A_2\|) \|y_i\| \\
\leq 2(\|A\| + \varepsilon) \|y_i\| \|A_1 - A_2\|.
\]

In general, the function $E$ is neither convex nor concave on $\mathcal{D}$, see Fig. 2. In contrast, $F$ is concave as the following lemma shows.

Lemma 3.2. The function $F$ defined by (5) and (6) fulfills the following relations:

1. $\text{dom}(-F) := \{A \in \mathbb{R}^{d,K} : -F(A) < +\infty\} = \mathcal{D}$ is convex.

2. $-F$ is convex.

3. The subdifferential of $-F$ is empty at the boundary of $\mathcal{D}$, i.e. at $A \in \mathbb{R}^{d,K}$ with $\|y_i\|^2 - \|A^T y_i\|^2 = 0$ for some $i \in \{1, \ldots, N\}$.

Proof. 1. It holds $A \in \text{dom}(-F)$ if and only if

\[
\|y_i\|^2 - \|A^T y_i\|^2 \geq 0
\]

for all $i = 1, \ldots, N$. Since the intersection of convex sets is convex, it suffices to show convexity of $\text{dom}(-F_i)$ separately. Let $A_1, A_2 \in \text{dom}(-F_i)$. Then, using (7), we obtain

Figure 2: Plot of $E(A)$ on $\mathcal{D}$ for $d = 2$ with data points $y_1 = (1, 0)^T$ and $y_2 = (0, 1)^T$. 
for \( \lambda \in [0, 1] \) that
\[
\|y_i\|^2 - (\lambda A_1 + (1 - \lambda) A_2)^T y_i^2 \\
= \|y_i\|^2 - (\lambda^2\|A_1^T y_i\|^2 + 2\lambda(1 - \lambda)\langle A_1^T y_i, A_2^T y_i \rangle + (1 - \lambda)^2\|A_2^T y_i\|^2) \\
\geq \|y_i\|^2 - (\lambda^2\|A_1^T y_i\|^2 + 2\lambda(1 - \lambda)\|A_1^T y_i\|\|A_2^T y_i\| + (1 - \lambda)^2\|A_2^T y_i\|^2) \\
\geq \|y_i\|^2 - (\lambda^2\|y_i\|^2 + 2\lambda(1 - \lambda)\|y_i\|^2 + (1 - \lambda)^2\|y_i\|^2) = 0.
\]
Thus, \( \lambda A_1 + (1 - \lambda) A_2 \in \text{dom}(-F_i) \) and the claim follows.

2. Since the sum of concave functions is concave again, it suffices to consider the individual summands \( F_i \) again. For \( \varepsilon > 0 \), we define
\[
F_\varepsilon(A) := \sqrt{\|y_i\|^2 - \|A^T y_i\|^2 + \varepsilon},
\]
which is differentiable on an open set containing \( D_i \). By the chain rule and since
\[
\frac{\partial}{\partial y_i} \text{tr}(y_i^T A A^T y_i) = 2y_i y_i^T A,
\]
the gradient of \( F_\varepsilon \) is
\[
\nabla F_\varepsilon(A) = -\frac{1}{F_\varepsilon(A)} y_i y_i^T A.
\]
Using the product rule and the chain rule, the Hessian is given by
\[
\nabla^2 F_\varepsilon(A)[H] = -\frac{1}{F_\varepsilon(A)^2} \left( y_i y_i^T H F_\varepsilon(A) + \frac{1}{F_\varepsilon(A)} \langle y_i y_i^T A, H \rangle y_i y_i^T A \right),
\]
for all \( H \in \mathbb{R}^{d,K} \) so that
\[
\langle \nabla^2 F_\varepsilon(A)[H], H \rangle = -\frac{1}{F_\varepsilon(A)^2} \left( F_\varepsilon(A) \langle y_i y_i^T H, H \rangle + \frac{1}{F_\varepsilon(A)} \langle y_i y_i^T A, H \rangle^2 \right) \\
= -\frac{1}{F_\varepsilon(A)^2} \left( F_\varepsilon(A) \|H^T y_i\|^2 + \frac{1}{F_\varepsilon(A)} \langle y_i y_i^T A, H \rangle^2 \right) \leq 0.
\]
Consequently, the Hessian is negative semidefinite and \( F_\varepsilon \) concave in \( D_i \) for all \( \varepsilon > 0 \).
Finally,
\[
F_i = \inf \{ F_\varepsilon : \varepsilon > 0 \}
\]
is concave as the pointwise infimum of a family of concave functions.

3. For an arbitrary fixed \( i \in \{1, \ldots, N\} \), let \( A_0 \in \mathbb{R}^{d,K} \) with \( \|y_i\|^2 - \|A_0^T y_i\|^2 = 0 \). We consider the subdifferential of \( F_i \) at \( A_0 \) given by
\[
\partial F_i(A_0) = \left\{ P \in \mathbb{R}^{d,K} : -F_i(A) \geq -F_i(A_0) + \langle P, A - A_0 \rangle, \quad \forall A \in \mathbb{R}^{d,K} \right\} \\
= \left\{ P \in \mathbb{R}^{d,K} : -\sqrt{\|A_0^T y_i\|^2 - \|A^T y_i\|^2} \geq \langle P, A - A_0 \rangle, \quad \forall A \in \mathbb{R}^{d,K} \right\}.
\]
Choosing \( A := \alpha A_0 \) with \( \alpha \in [0, 1] \), a subgradient \( P \) must fulfill
\[
-\|A^T y_i\|\sqrt{1 - \alpha^2} \geq (\alpha - 1)\langle P, A_0 \rangle, \\
\|A^T y_i\|\sqrt{1 + \alpha} \leq \sqrt{1 - \alpha} \langle P, A_0 \rangle,
\]
which leads to a contradiction if \( \alpha \to 1 \). Hence, the subdifferential is empty. \( \square \)
For the algorithms the gradient and the Riemannian gradient on the Grassmannian of the functions $E$ and $F$ are required.

**Lemma 3.3.** Let $E$ and $F$ be defined by (4) and (5), respectively. Then, the gradient $\nabla$ and the Riemannian gradient $\nabla_A$ on $S_{d,K}$ at $A \in S_{d,K} \setminus \mathcal{A}$ are given by

$$
\nabla F(A) = -C_A A, \quad \nabla E(A) = \nabla_A E(A) = \nabla_A F(A) = -P_A C_A A,
$$

where

$$
C_A := \sum_{i=1}^{N} \frac{y_i y_i^T}{\|P_A y_i\|}.
$$

Note that $-P_A C_A A$ is also the horizontal lift of the gradient $\nabla_{[A]} \tilde{E}([A])$ on the Grassmannian at $A$, where $E = \tilde{E} \circ \pi$ and $\pi$ is the projection from $S_{K,d}$ onto $G_{K,d}$.

**Proof.** By straightforward computation we obtain for $A \in \mathbb{R}^{d,K}$ that

$$
\nabla E_i(A) = -\frac{1}{\|P_A y_i\|} \left( P_A y_i y_i^T A + y_i y_i^T P_A A \right) \quad \text{if} \quad P_A y_i \neq 0,
$$

$$
\nabla F_i(A) = -\frac{1}{\left(\|y_i\|^2 - \|A^T y_i\|^2\right)^{\frac{1}{2}}} y_i y_i^T A \quad \text{if} \quad A \in \text{int}(\text{dom}(-F_i)) = \text{int}(D_i).
$$

For $A \in S_{d,K}$ the gradient of $E_i$ coincides with the Riemannian gradient of $E_i$ on $S_{d,K}$, i.e.,

$$
\nabla_A E_i(A) = -\frac{1}{\|P_A y_i\|} P_A y_i y_i^T A \quad \text{for} \quad A \in S_{d,K}.
$$

This implies the assertion. □

We call $A \in S_{d,K} \setminus \mathcal{A}$ a critical point of $F$, resp. $E$ if

$$
\nabla_A E(A) = \nabla_A F(A) = -P_A C_A A = 0.
$$

\section{Minimization Algorithms}

In this section, we show that the constrained minimization algorithm of Ding et al. \cite{8} can be interpreted as a conditional gradient algorithm. The conditional gradient algorithm, also known as Frank-Wolfe algorithm, was originally proposed 1956 in \cite{11} for solving linearly constrained quadratic programs and was later adapted to other problems. For a good overview, we refer to \cite{25} and the references therein. At the end of the section, a gradient descent algorithm on Grassmannians which turns out to be equivalent to the conditional gradient algorithm is provided.
**Constrained Minimization Algorithm.** Ding et al. [8] consider the constrained optimization problem

$$\arg\min_{A \in \mathbb{R}^{d, K}} F(A) \quad \text{subject to} \quad A^T A = I_K.$$  \hspace{1cm} (9)

The authors claimed without proof that the function $F$ is convex in $AA^T$ and has a unique global minimizer. Both statements are not correct: for $N = K = d = 1$ and $y_1 = 1$ it is easy to check that $F(A) = \sqrt{1 - A^2}$ is concave in $A^2 \in [0, 1]$; for $N = 2$, $K = 1$, $d = 2$ with centered data points $y_1 = (-1/2, \sqrt{3}/2)^T$ and $y_2 = (1/2, \sqrt{3}/2)^T$ the minimizers of $F(A)$ are given by $A = (-1/2, \sqrt{3}/2)^T$ and $A = (1/2, \sqrt{3}/2)^T$, which span different subspaces.

Penalizing the constraint in [9] via a symmetric Lagrange multiplier $\Lambda \in \mathbb{R}^{K, K}$, setting the gradient of the resulting Lagrangian $L(A, \Lambda) := F(A) + \langle \Lambda, A^T A - I_K \rangle$ with respect to $A$ to zero and applying an orthogonalization procedure, see Lemma 2.1, the authors arrive at the following iteration scheme: if $A^{(r)} \notin \mathcal{A}$,

$$A^{(r+1)} := \Pi_{S_{d, K}} \left( C_{A^{(r)}} A^{(r)} \right) = C_{A^{(r)}} A^{(r)} \left( (A^{(r)})^T C_{A^{(r)}} (A^{(r)}) \right)^{-\frac{1}{2}}.$$  \hspace{1cm} (10)

**Conditional Gradient Algorithm.** The conditional gradient algorithm is commonly used to minimize a convex function over a compact set. However, as in [26], we apply it for maximizing the convex function $-F$.

In general, for a proper convex function $f : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ and a nonempty, compact set $\mathcal{K} \subset \text{int}(\text{dom } f)$, the conditional gradient algorithm is the update scheme

$$u^{(r+1)} \in \arg\max_{u \in \mathcal{K}} \left\{ u - u^{(r)}, p^{(r)} \right\}, \quad p^{(r)} \in \partial f(u^{(r)}).$$  \hspace{1cm} (11)

Note that according to [35] Corollary 32.4.1], the value $\hat{u} \in \mathcal{K}$ is a local maximizer of $f$ over $\mathcal{K}$ if for all $v \in \mathcal{K}$,

$$\langle v - \hat{u}, \hat{p} \rangle \leq 0 \quad \text{for all} \quad \hat{p} \in \partial f(\hat{u}).$$  \hspace{1cm} (12)

By definition of the subdifferential we have

$$f(u^{(r+1)}) - f(u^{(r)}) \geq \left\langle u^{(r+1)} - u^{(r)}, p^{(r)} \right\rangle = \max_{v \in \mathcal{K}} \left\langle v - u^{(r)}, p^{(r)} \right\rangle \geq 0,$$

where the last equation follows by choosing $v = u^{(r)} \in \mathcal{K}$.

For finite convex functions $f : \mathbb{R}^n \to \mathbb{R}$ the following convergence result was proved in [26] based on [25]. The proof can be modified for $f$ with values in the extended real numbers and $\mathcal{K} \subset \text{int}(\text{dom } f)$ in a straightforward way.

**Theorem 4.1.** Let $f : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ a proper convex function and $\mathcal{K} \subset \text{int}(\text{dom } f)$ a nonempty, compact set. Then the sequence $\{f(u^{(r)})\}_r$ generated by (11) is strictly increasing except when $\max_{u \in \mathcal{K}} \langle u - u^{(r)}, p^{(r)} \rangle = 0$, in which case it terminates at $u^{(r)}$ satisfying (12).

If $f$ is continuously differentiable on $\text{int}(\text{dom } f)$, then every accumulation point $\hat{u}$ of the sequence $\{u^{(r)}\}_r$ fulfills (12).

We want to apply the scheme (11) for $f := -F$ and $\mathcal{K} = \mathcal{K}_\varepsilon := S_{d, K} \setminus \mathcal{A}_\varepsilon \subset \text{int}(\text{dom}(-F))$, where $\mathcal{A}_\varepsilon := \{A \in S_{d, K} : \text{dist}(A, \mathcal{A}) < \varepsilon\}$ denotes the set of matrices in $S_{d, K}$ having a distance
smaller than some \( \varepsilon > 0 \) from the anchor set. To this end, the maximization problem \((11)\) has to be solved, but first we have to find a suitable \( \varepsilon \). For this purpose define the iteration

\[
A^{(r+1)} = \arg \max_{U \in S_{d,K}} \left\langle U, \nabla (-F) (A^{(r)}) \right\rangle = \arg \max_{U \in S_{d,K}} \left\langle U, C_{A^{(r)}} A^{(r)} \right\rangle
\]

for \( A^{(r)} \notin \mathcal{A} \), where we plugged in \( \nabla F \) as in Lemma 3.3. Now, assume that we can find \( \varepsilon > 0 \) such that \( A^{(r)} \in \mathcal{K}_{\varepsilon} \) for all \( r \geq 0 \). In this case

\[
A^{(r+1)} = \arg \max_{U \in \mathcal{K}_{\varepsilon}} \left\langle U, C_{A^{(r)}} A^{(r)} \right\rangle.
\]

Note that we can always find such an \( \varepsilon \) for \( r \) large enough if all accumulation points of \( A^{(r)} \) as in \((13)\) are non-anchor points. Using Lemma 2.1 we obtain

\[
A^{(r+1)} = \Pi_{S_{d,K}} (C_{A^{(r)}} A^{(r)}) = C_{A^{(r)}} A^{(r)} \left( (A^{(r)})^T C^2_{A^{(r)}} A^{(r)} \right)^{-\frac{1}{2}},
\]

which is exactly the iteration scheme \((10)\) proposed by Ding et al. Based on Theorem 4.1 we have the following corollary for our special setting.

**Corollary 4.2.** Let \( F \) be defined by \((5)\)–\((6)\). Assume that the sequence \( \{A^{(r)}\}_r \) generated by \((14)\) has no element in \( \mathcal{A} \) and that the set of accumulation points has a positive distance from \( \mathcal{A} \). Then the sequence \( \{F (A^{(r)})\}_r \) is strictly decreasing except for iterates where

\[
\left\langle C_{A^{(r)}} A^{(r)} \left( (A^{(r)})^T C^2_{A^{(r)}} A^{(r)} \right)^{-\frac{1}{2}} - A^{(r)}, C_{A^{(r)}} A^{(r)} \right\rangle = 0,
\]

in which case the iteration terminates at \( A^{(r)} \) which is a critical point. Condition \((15)\) is equivalent to \( A^{(r+1)} = A^{(r)} \), resp. to \( \nabla_{A^{(r)}} F (A^{(r)}) = 0 \). If the iteration does not terminate after a finite number of steps, every accumulation point of \( \{A^{(r)}\}_r \) is a critical point.

**Proof.** We show that the three stopping criteria are equivalent. Let \( A := A^{(r)} \notin \mathcal{A} \) and recall that \( \nabla A F (A) = -P_A C_A A \).

1. If \( A^{(r+1)} = A \), then \( C_A A = A (A^T C^2_A A)^{\frac{1}{2}} \) and thus \( P_A C_A A = 0 \).
2. If \( P_A C_A A = 0 \), then \( C_A A = A (A^T C_A A) \) and thus

\[
A^{(r+1)} = C_A A (A^T C^2_A A)^{-\frac{1}{2}} = A (A^T C_A A) (A^T C_A A) (A^T C_A A)^{-\frac{1}{2}} = A.
\]

Further, this implies \((15)\).

3. Assume now that \((15)\) is fulfilled. Then, we have

\[
0 = \left\langle C_A A (A^T C^2_A A)^{-\frac{1}{2}} - A, C_A A \right\rangle = \left\langle (A^T C^2_A A)^{\frac{1}{2}} - A^T C_A A, I_K \right\rangle
\]

\[
= \text{tr} \left( (A^T C^2_A A)^{\frac{1}{2}} - A^T C_A A \right).
\]

On the other hand, we have with \( \text{tr}(AB) = \text{tr}(BA) \) that

\[
\|P_A C_A A\|^2 = \langle P_A C_A A, P_A C_A A \rangle = \text{tr} \left( A^T C^2_A A - (A^T C_A A)^2 \right)
\]

\[
= \text{tr} \left( ((A^T C^2_A A)^{\frac{1}{2}} - A^T C_A A) \left( (A^T C^2_A A)^{\frac{1}{2}} + A^T C_A A \right) \right)
\]

\[
\leq \lambda_{\text{max}} \text{tr} \left( (A^T C^2_A A)^{\frac{1}{2}} - A^T C_A A \right) = 0,
\]

10
where \( \lambda_{\text{max}} \) denotes the largest eigenvalue of the matrix \((A^T C_A^2 A)^{\frac{1}{2}} + A^T C_A A\). Hence, \( P_A C_A A = 0 \).

It remains to show that all accumulation points of infinite sequences are critical points. Let \( A \notin \mathcal{A} \) be an accumulation point of such a sequence. As the set of accumulation points has positive distance from \( \mathcal{A} \), we can choose \( \epsilon \) small enough that all iterates are in \( \text{int}(\mathcal{K}_\epsilon) \) for \( r \) large enough. Then by Theorem 4.1, \( \tilde{A} \) fulfills (12) and as \( E \) is differentiable in \( \tilde{A} \), this implies that \( \tilde{A} \) is a critical point.

Proof. Note the strong connection of this iterative scheme to the Weiszfeld algorithm [4, 37] and majorize-minimize strategies [7].

Remark 4.3. Unfortunately, the function \( -F \) has no subdifferential at the boundary of its domain and \( S_{d,K} \) touches this boundary in the anchor set. A remedy would be to use instead of \( F \) the function
\[
F_\varepsilon(A) := \sum_{i=1}^N \sqrt{\|y_i\|^2 - \|A^T y_i\|^2 + \varepsilon}, \quad \varepsilon > 0.
\]

By the proof of Lemma 3.2, we conclude that \( -F_\varepsilon \) is convex on an open set which contains \( D \) and therefore also \( S_{d,K} \). Thus, accumulation points of the sequence produced by the conditional gradient algorithm are critical points by Theorem 4.1. Another idea consists of switching to a function with summands \( \varphi(\sqrt{\|y_i\|^2 - \|A^T y_i\|^2}) \), where \( \varphi \) is e.g. the Huber function as proposed in [8]. This approach is not pursued any further, since we are more interested in finding an algorithm for the original function without an additional parameter.

**Gradient Descent Algorithm on** \( G_{d,K} \). By [8], a matrix \( A \in S_{d,K} \setminus \mathcal{A} \) is a critical point of \( E \), resp. \( F \) on \( S_{d,K} \) if and only if \( P_A C_A A = 0 \). This can be rewritten as

\[
A(A^T C_A A) = C_A A, \\
A = C_A A S_A^{-1} \quad \text{with} \quad S_A := A^T C_A A, \\
A = A + P_A C_A A S_A^{-1},
\]

where \( S_A \in \mathbb{R}^{K,K} \) is assumed to be invertible which is the case under the reasonable assumption that \( \text{span}(A) \subset \text{span}(Y) \) and \( \text{dim}(\text{span}(Y)) \geq K \). Note that \( -\nabla A E(A) S_A^{-1} = P_A C_A A S_A^{-1} \in T_A G_{d,K} \subset T A S_{d,K} \).

Remark 4.4. The Grassmannian \( G_{d,K} \) can be also obtained as quotient manifold of the non-compact Stiefel manifold \( S_{K,d} := \{ W \in \mathbb{R}^{d,K} : \text{rank}(W) = K \} \) with equivalence classes \([W] := \{ WS : S \in \text{GL}(K) \}\). Then \( -P_A C_A A S_A^{-1} \) can be seen as horizontal lift of \( \nabla_{[A]} \tilde{E}([A]) \) at \( W = AS_A^{-1} \), where \( E = \tilde{E} \circ \pi \) and \( \pi \) is the natural projection from \( S_{K,d}^* \) onto \( G_{d,K} \). In other words, \( P_A C_A A S_A^{-1} = -\nabla W E(\text{Polar}(W)) \).

Together with Lemma 2.1, this gives rise to the following descent scheme on \( S_{d,K} \), resp. \( G_{d,K} \):

\[
A^{(r+1)} := \Pi_{S_{d,K}} \left( C_A^{(r)} A^{(r)} S_A^{-1} \right) = C_A^{(r)} A^{(r)} S_A^{-1} \left( S_A^{-1} \left( A^{(r)} \right)^T C_A^{(r)} A^{(r)} S_A^{-1} \right)^{-\frac{1}{2}} . (16)
\]

Note the strong connection of this iterative scheme to the Weiszfeld algorithm [11, 37] and majorize-minimize strategies [7].

By the following lemma, the gradient descent iteration (16) coincides with those of the conditional gradient algorithm (14) on the Grassmannian \( G_{d,K} \).
Lemma 4.5. For the same input matrix $A^{(0)}$, the iterates generated by the schemes \cite{16} and \cite{14} coincide on $G_{d,K}$, i.e., they span the same subspace.

Proof. Since $C_{AQ} = CA$ for $Q \in O(K)$, we observe that the matrices produced by the update schemes \cite{16} and \cite{14} span the same subspace as they differ only by a multiplication with an invertible matrix from the right. Since both iterates are in the Stiefel manifold, they can only differ by orthogonal matrix, i.e., $\Pi_{S_{d,K}}(CA^{(r)}A^{(r)}S_{A^{(r)}}^{-1}) = \Pi_{S_{d,K}}(CA^{(r)}A^{(r)})Q$ for some $Q \in O(K)$.

The following lemma quantizes the relation from Corollary \cite{4.2} that $\{E(A^{(r)})\}_r$ is decreasing.

Lemma 4.6. If $A^{(r)} \notin A$ for all $r \geq 0$ generated by \cite{16}, then

$$E(A^{(r+1)}) - E(A^{(r)}) \leq - \sum_{i=1}^{N} \frac{\|A^{(r+1)}(A^{(r+1)})^T y_i - A^{(r)}(A^{(r)})^T y_i\|^2}{2\|P_{A^{(r)}} y_i\|^2}.$$ 

Proof. For $x \geq 0, y > 0$ it holds $x - y \leq \frac{x^2 - y^2}{2y}$ so that

$$E(A^{(r+1)}) - E(A^{(r)}) = \sum_{i=1}^{N} \|P_{A^{(r+1)}} y_i\| - \|P_{A^{(r)}} y_i\|$$

$$\leq \sum_{i=1}^{N} \frac{\|P_{A^{(r+1)}} y_i\|^2 - \|P_{A^{(r)}} y_i\|^2}{2\|P_{A^{(r)}} y_i\|^2}$$

$$= \sum_{i=1}^{N} \frac{\|A^{(r+1)}(A^{(r+1)})^T y_i - y_i\|^2 - \|A^{(r)}(A^{(r)})^T y_i - y_i\|^2}{2\|P_{A^{(r)}} y_i\|^2}.$$ 

Using $\|u - v\|^2 - \|w - v\|^2 = 2\langle u - w, u - v \rangle - \|u - w\|^2$, this can be rewritten as

$$\sum_{i=1}^{N} \frac{1}{\|P_{A^{(r)}} y_i\|^2} \langle A^{(r+1)}(A^{(r+1)})^T y_i - A^{(r)}(A^{(r)})^T y_i, A^{(r+1)}(A^{(r+1)})^T y_i - y_i \rangle$$

$$- \sum_{i=1}^{N} \frac{\|A^{(r+1)}(A^{(r+1)})^T y_i - A^{(r)}(A^{(r)})^T y_i\|^2}{2\|P_{A^{(r)}} y_i\|^2}$$

$$= \sum_{i=1}^{N} \frac{\langle A^{(r)}(A^{(r)})^T y_i, P_{A^{(r+1)}} y_i \rangle}{\|P_{A^{(r)}} y_i\|^2} \quad - \sum_{i=1}^{N} \frac{\|A^{(r+1)}(A^{(r+1)})^T y_i - A^{(r)}(A^{(r)})^T y_i\|^2}{2\|P_{A^{(r)}} y_i\|^2}. $$
Then the whole sequence \( \{ A^{(r)}(A^{(r)})^T y_i, P_{A^{(r+1)}} y_i \} \) can be simplified as

\[
\sum_{i=1}^{N} \frac{A^{(r)}(A^{(r)})^T y_i}{\|P_{A^{(r+1)}} y_i\|} = \text{tr} \left( \sum_{i=1}^{N} \frac{y_i y_i^T}{\|P_{A^{(r+1)}} y_i\|} A^{(r)}(A^{(r)})^T P_{A^{(r+1)}} \right)
\]

\[
= \text{tr} \left( C_{A^{(r)}} A^{(r)}(A^{(r)})^T (I - A^{(r+1)}(A^{(r+1)})^T) \right)
\]

\[
= \text{tr} \left( C_{A^{(r)}} A^{(r)}(A^{(r)})^T \left( I - C_{A^{(r)}} A^{(r)} ((A^{(r)})^T C_{A^{(r)}} A^{(r)})^{-1} (A^{(r)})^T C_{A^{(r)}} \right) \right)
\]

\[
= \text{tr} \left( (A^{(r)})^T \left( C_{A^{(r)}} - C_{A^{(r)}} A^{(r)} ((A^{(r)})^T C_{A^{(r)}} A^{(r)})^{-1} (A^{(r)})^T C_{A^{(r)}} \right) \right)
\]

\[
= 0,
\]

so that

\[
E(A^{(r+1)}) - E(A^{(r)}) \leq - \sum_{i=1}^{N} \frac{\|A^{(r+1)}(A^{(r+1)})^T y_i - A^{(r)}(A^{(r)})^T y_i\|^2}{2\|P_{A^{(r+1)}} y_i\|}.
\]

\[\square\]

5. Convergence Analysis

In this section, we give a convergence proof for algorithm \([16]\). By Corollary \([4, 2]\) only convergence of a subsequence to a critical point is ensured. To this end, note that both \(E\) and \(F\) are semi-algebraic functions. Such functions are typical examples of so-called Kurdyka–Lojasiewicz (KL) functions \([2, 19, 24]\) and for convenience, the definition can be found in Appendix \(A\). For such functions, the following theorem \([3, \text{Theorem 2.9}]\) holds.

**Theorem 5.1.** Let \(f: \mathbb{R}^d \to \mathbb{R} \cup \{\infty\}\) be a KL function. Let \(\{u^{(r)}\}_{r \in \mathbb{N}}\) be a sequence which fulfills the following conditions:

C1) There exists \(K_1 > 0\) such that \(f(u^{(r+1)}) - f(u^{(r)}) \leq -K_1\|u^{(r+1)} - u^{(r)}\|^2\) for every \(r \in \mathbb{N}\).

C2) There exists \(K_2 > 0\) such that for every \(r \in \mathbb{N}\) there exists \(w_{r+1} \in \partial f(u^{(r+1)})\) with \(\|w_{r+1}\| \leq K_2\|u^{(r+1)} - u^{(r)}\|\), where \(\partial f\) denotes the Fréchet limiting subdifferential of \(f\) \([29]\).

C3) There exists a convergent subsequence \(\{u^{(r)}\}_{j \in \mathbb{N}}\) with limit \(\hat{u}\) and \(f(u^{(r)}) \to f(\hat{u})\).

Then the whole sequence \(\{u^{(r)}\}_{r \in \mathbb{N}}\) converges to \(\hat{u}\) and \(\hat{u}\) is a critical point of \(f\) in the sense that \(0 \in \partial f(u)\). Moreover the sequence has finite length, i.e.,

\[
\sum_{r=0}^{\infty} \|u^{(r+1)} - u^{(r)}\| < \infty.
\]

We start by showing property C1) for the sequence of iterates in \([16]\).
Lemma 5.2. Assume that $A^{(r)} \notin \mathcal{A}$ for all $r \geq 1$ generated by \cite{16}. Then, there exists $K_1 > 0$ such that

$$E(A^{(r+1)}) - E(A^{(r)}) \leq -K_1 \|A^{(r+1)} - A^{(r)}\|^2.$$  \hfill (17)

Proof. By Lemma \ref{Lemma:4.6} and since $\|P_{A^{(r)}}y_i\| \leq \|y_i\| \leq \max_{i=1,...,N} \|y_i\| =: 1/2C$, we estimate

$$E(A^{(r+1)}) - E(A^{(r)}) \leq -C \sum_{i=1}^N \|A^{(r+1)}(A^{(r+1)})^T y_i - A^{(r)}(A^{(r)})^T y_i\|^2.$$ \hfill (18)

Next, we want to estimate the sum on the right. To this end, note that

$$\|A^{(r+1)}(A^{(r+1)})^T - A^{(r)}(A^{(r)})^T\|_2 = \max_{\|y\|=1} \|(A^{(r+1)}(A^{(r+1)})^T - A^{(r)}(A^{(r)})^T)y\|$$

$$= \|(A^{(r+1)}(A^{(r+1)})^T - A^{(r)}(A^{(r)})^T)\|_2$$

with some unit vector $y^{(r)} \in \mathcal{R}(Y)$ as $\mathcal{R}(A^{(r)}) \subseteq \mathcal{R}(Y)$ for all $r \geq 1$. The latter follows directly from the fact that the columns of $C_{A^{(r)}}$ are in $\mathcal{R}(Y)$. We can choose a basis of $\mathcal{R}(Y)$ from the data points and w.l.o.g., $y^{(r)} = \sum_{i=1}^{N_1} \alpha_i^{(r)} y_i$, where $N_1 = \dim(\mathcal{R}(Y))$. Then, setting $Y_{N_1} := (y_1 \ldots y_{N_1})$, the coefficients can be estimated by $|\alpha_i^{(r)}| \leq \alpha^* := \|[Y_{N_1}^TY_{N_1}]^{-1}Y_{N_1}^T\|_\infty$ for $i = 1, \ldots, N_1$ and $r \geq 1$. Setting $\alpha_i^{(r)} = 0$ for all $i > N_1$, we obtain

$$\|A^{(r+1)}(A^{(r+1)})^T - A^{(r)}(A^{(r)})^T\|_2^2 = \left\|(A^{(r+1)}(A^{(r+1)})^T - A^{(r)}(A^{(r)})^T) \sum_{i=1}^N \alpha_i^{(r)} y_i\right\|^2$$

$$\leq \left(\sum_{i=1}^N \|(A^{(r+1)}(A^{(r+1)})^T - A^{(r)}(A^{(r)})^T)\alpha_i^{(r)}\|^2\right)^2$$

$$\leq N(\alpha^*)^2 \sum_{i=1}^N \|A^{(r+1)}(A^{(r+1)})^T y_i - A^{(r)}(A^{(r)})^T y_i\|^2.$$\hfill (18)

Using the equivalence of Frobenius and spectral norm, \cite{18} now results in the estimate

$$E(A^{(r+1)}) - E(A^{(r)}) \leq -\frac{C}{2N(\alpha^*)^2} \|A^{(r+1)}(A^{(r+1)})^T - A^{(r)}(A^{(r)})^T\|_2^2$$

$$\leq -C \|A^{(r+1)}(A^{(r+1)})^T - A^{(r)}(A^{(r)})^T\|_2^2.$$\hfill (18)

It remains to show that $\|A^{(r+1)}(A^{(r+1)})^T - A^{(r)}(A^{(r)})^T\|^2 \geq \|A^{(r+1)} - A^{(r)}\|^2$. Since $A^{(r)} \in S_{d,K}$, we get

$$\|A^{(r+1)}(A^{(r+1)})^T - A^{(r)}(A^{(r)})^T\|^2 = \text{tr}(I_K) - 2 \text{tr}\left((A^{(r)})^TA^{(r+1)}(A^{r+1})^TA^{(r)}\right) + \text{tr}(I_K)$$

$$= 2 \text{tr}\left(I_K - (B^{(r)})^{-1}\right),$$

where

$$B^{(r)} := (A^{(r)})^TA^{(r+1)}(A^{(r+1)})^TA^{(r)} = S_{A^{(r)}}^{-1}(A^{(r)})^TC_{A^{(r)}}^2A^{(r)}S_{A^{(r)}}^{-1}$$

$$= I_K + S_{A^{(r)}}^{-1}(A^{(r)})^TC_{A^{(r)}}P_{A^{(r)}}C_{A^{(r)}}A^{(r)}S_{A^{(r)}}^{-1}. $$
All eigenvalues of $B^{(r)}$ are larger than 1, so that all eigenvalues of $(B^{(r)})^{-1}$ are smaller than 1 and larger than 0. On the other hand, it holds

$$
\|A^{(r+1)} - A^{(r)}\|^2 = \text{tr}(I_K) - 2 \text{tr}((A^{(r)})^T A^{(r+1)}) + \text{tr}(I_K) = 2 \text{tr} (I_K - (B^{(r)})^{-\frac{1}{2}}) \quad (19)
$$

This finally implies

$$
\|A^{(r+1)}(A^{(r+1)})^T - A^{(r)}(A^{(r)})^T\|^2 = 2 \text{tr} (I_K - (B^{(r)})^{-1})
$$

$$
= 2 \text{tr} ((I_K + (B^{(r)})^{-\frac{1}{2}})(I_K - (B^{(r)})^{-\frac{1}{2}}))
$$

$$
\geq 2 \lambda_{\min} \text{tr} (I_K - (B^{(r)})^{-\frac{1}{2}})
$$

$$
\geq 2 \text{tr} (I_K - (B^{(r)})^{-\frac{1}{2}})
$$

$$
= \|A^{(r+1)} - A^{(r)}\|^2,
$$

where $\lambda_{\min}$ refers to the smallest eigenvalue of the matrix $I_K + (B^{(r)})^{-\frac{1}{2}}$.

\[ \square \]

**Corollary 5.3.** Assume that $A^{(r)} \notin \mathcal{A}$ for all $r \geq 1$ generated by (16). Then, it holds

$$
\lim_{r \to \infty} \|A^{(r+1)} - A^{(r)}\| = 0.
$$

Further, there exists a convergent subsequence $\{A^{(r_j)}\}_j$ with limit $\hat{A}$ and $E(A^{(r_j)}) \to E(\hat{A})$. The set of accumulation points of $\{A^{(r)}\}_r$ is compact and connected in $S_{d,K}$. Every accumulation point $\hat{A}$ which is not an anchor point is a critical point of $E$, i.e. $\nabla_{\hat{A}} E(\hat{A}) = 0$. The same statements hold true for the corresponding equivalence classes in $G_{d,K}$.

**Proof.** 1. Since $\{E(A^{(r)})\}_r$ is decreasing and bounded below by zero, we know that $
\lim_{r \to \infty} E(A^{(r)}) = \hat{E}$ for some $\hat{E} \geq 0$. Multiplying (17) by $-1$, summing and taking the limit yields

$$
E(A^{(0)}) - \hat{E} \geq K_1 \sum_{r=0}^{\infty} \|A^{(r+1)} - A^{(r)}\|^2.
$$

Consequently, the series on the right-hand side converges and $\lim_{r \to \infty} \|A^{(r+1)} - A^{(r)}\| = 0$. Using the estimate

$$
\|A^{(r+1)}(A^{(r+1)})^T - A^{(r)}(A^{(r)})^T\|_2 = \frac{1}{2} \|((A^{(r+1)} - A^{(r)})(A^{(r+1)})^T + (A^{(r)})^T\|_2
$$

$$
+ \|((A^{(r+1)} - A^{(r)})(A^{(r+1)})^T - (A^{(r)})^T\|_2
$$

$$
\leq C \|A^{(r+1)} - A^{(r)}\| \quad C > 0,
$$

the statement also holds on $G_{d,K}$.

2. By the theorem of Ostrowski [32, p. 173], it follows that the set of accumulation points of $\{A^{(r)}\}_r$ is compact and connected both in $S_{d,K}$ and $G_{d,K}$.

3. Since the sequence $\{A^{(r)}\}_r$ is bounded, it has a convergent subsequence. Let $A^{(r)}$ be a subsequence converging to a non-anchor point $\hat{A}$ and $T$ be the update operator in (16), i.e., $T(A^{(r)}) = A^{(r+1)}$. Then, using the continuity of $T$ outside $\mathcal{A}$, we have $\lim_{j \to \infty} A^{(r_j+1)} = \lim_{j \to \infty} T(A^{(r_j)}) = T(\hat{A})$. By continuity of $E$, this implies

$$
E(\hat{A}) = \lim_{j \to \infty} E(A^{(r_j)}) = \hat{E} = \lim_{j \to \infty} E(A^{(r_j+1)}) = E(T(\hat{A})).
$$

By Corollary 4.2, $E$ is strictly decreasing except for $\hat{A} = T(\hat{A})$ in which case $\nabla_{\hat{A}} E(\hat{A}) = 0$. \[ \square \]
Lemma 5.4. Assume that the elements of the sequence \( \{A^{(r)}\}_r \) are generated by (16) and the accumulation points do not belong to the anchor set \( \mathcal{A} \). Then the sequence fulfills C2) in Theorem 5.1, i.e., there exists \( K_2 > 0 \) such that

\[
\| \nabla E(A^{(r+1)}) \| \leq K_2 \| A^{(r+1)} - A^{(r)} \|.
\]

Proof. By the assumptions and Corollary 5.3 the set of accumulation points has a positive distance \( \varepsilon \) from \( \mathcal{A} \). Since \( \lim_{r \to \infty} \| A^{(r+1)} - A^{(r)} \| = 0 \), we have for \( r \) large enough that \( A^{(r)}A^{(r+1)} \subseteq \Omega := \overline{B(0, R)} \setminus \mathcal{A} \) for some \( R > 0 \). Further, \( E \) is smooth on an open set containing \( \Omega \) so that the mean value theorem implies

\[
\| \nabla E(A^{(r+1)}) - \nabla E(A^{(r)}) \| \leq C \| A^{(r+1)} - A^{(r)} \|.
\]

Hence, we can estimate

\[
\| \nabla E(A^{(r+1)}) \| \leq \| \nabla E(A^{(r)}) \| + \| \nabla E(A^{(r+1)}) - \nabla E(A^{(r)}) \|
\leq \left( \frac{\| \nabla E(A^{(r)}) \|}{\| A^{(r+1)} - A^{(r)} \|} + C \right) \| A^{(r+1)} - A^{(r)} \|.
\]

Now, (19) implies that

\[
\| A^{(r+1)} - A^{(r)} \|^2 = 2 \operatorname{tr}(I_K) - 2 \operatorname{tr}\left((I_K + S^{-1}_{A^{(r)}} A^{(r)} T C A^{(r)} P A^{(r)} C A^{(r)} A^{(r)} S^{-1}_{A^{(r)}})^{-\frac{1}{2}}\right).
\]

Using Corollary 5.3, we conclude \( \lim_{r \to \infty} \| \nabla E(A^{(r)}) S^{-1}_{A^{(r)}} \| = 0 \), so that the series expansion of the square root implies

\[
\operatorname{tr}\left((I_K + S^{-1}_{A^{(r)}} \nabla E(A^{(r)})^T \nabla E(A^{(r)}) S^{-1}_{A^{(r)}})^{-\frac{1}{2}}\right) = \operatorname{tr}(I_K) - \frac{1}{2} \| \nabla E(A^{(r)}) S^{-1}_{A^{(r)}} \|^2 + O\left(\| \nabla E(A^{(r)}) S^{-1}_{A^{(r)}} \|^4\right).
\]

Plugging this in yields

\[
\frac{\| A^{(r+1)} - A^{(r)} \|^2}{\| \nabla E(A^{(r)}) \|^2} = \frac{\| \nabla E(A^{(r)}) S^{-1}_{A^{(r)}} \|^2 - O\left(\| \nabla E(A^{(r)}) S^{-1}_{A^{(r)}} \|^4\right)}{\| \nabla E(A^{(r)}) \|^2}
\geq \frac{\| \nabla E(A^{(r)}) \|^2 \lambda_{\min}(S^{-1}_{A^{(r)}})^2 - O\left(\| \nabla E(A^{(r)}) \|^4 \lambda_{\max}(S^{-1}_{A^{(r)}})^4\right)}{\| \nabla E(A^{(r)}) \|^2}
= \lambda_{\min}(S^{-1}_{A^{(r)}})^2 - O\left(\| \nabla E(A^{(r)}) \|^2 \lambda_{\max}(S^{-1}_{A^{(r)}})^4\right)
\geq C,
\]

where the last inequality follows since the continuous functions \( \lambda_{\min/\max}(S^{-1})^2 \) have positive minima/maxima on \( \Omega \).

Theorem 5.5. Assume that the set of iterates \( \{A^{(r)} : r \in \mathbb{N}\} \) generated by (16) is infinite and fulfills \( A^{(r)} \notin \mathcal{A} \) for all \( r \geq 0 \). Suppose that there is an accumulation point which is not in \( \mathcal{A} \). Then the whole sequence \( \{A^{(r)}\}_r \) converges a critical point.
Proof. We distinguish two cases.

1. If all accumulation points are non-anchor points, then the assertion follows by Theorem 5.1 together with Lemma 5.2, Corollary 5.3, and Lemma 5.4.

2. If the set accumulation points consists of both anchor and non-anchor points we will show convergence to a non-anchor point by applying Corollary A.1. Let \( \tilde{A} \) be an accumulation point which is not in the anchor set \( A \), i.e., \( E_i(\tilde{A}) = P_{\tilde{A}}y_i \neq 0 \) for all \( i = 1, \ldots, N \). Due to the continuity of \( E \) and \( \phi \), see also the proof of [3, Theorem 2.9], we can choose a ball \( B(\tilde{A}, \delta) \) around \( \tilde{A} \) which has positive distance to all anchor points. Next, for all the iterates \( A^{(r)} \in B(\tilde{A}, R/2) \) and \( r \) large enough, C1) and C2) are fulfilled by Lemma 5.2 and Lemma 5.4. By the continuity of \( E \) and \( \phi \), see also the proof of [3, Theorem 2.9], we can choose a ball \( B(\tilde{A}, \delta) \) such that for all \( r \geq r_0 \) such that

\[
A^{(r)} \in B(\tilde{A}, \rho) \implies A^{(r+1)} \in B(\tilde{A}, \delta), \quad E(A^{(r+1)}) \geq E(\tilde{A})
\]

for all \( r \geq r_0 \). Either all iterates after \( A^{(r_0)} \) are in \( B(\tilde{A}, \rho) \) or there is a finite sequence \( A^{(r_0)}, A^{(r_0+1)}, \ldots, A^{(r_n)} \) such that \( A^{(r_n+1)} \) is the first element outside \( B(\tilde{A}, \rho) \). But then, by Corollary A.1, also the iterate \( A^{(r_n+1)} \) is inside \( B(\tilde{A}, \rho) \) and hence all iterates stay in \( B(\tilde{A}, \rho) \), which is a contradiction. As \( \rho \) can be chosen arbitrarily small, the whole sequence converges to the anchor point \( \tilde{A} \).

\[ \square \]

6. A Glimpse at Anchor Points

While a local minimizer of \( F \) (and \( E \)) on \( S_{d,K} \cap \text{int}(D) \) can be described by setting the Riemannian gradient to zero, this is not possible for minimizers lying in the anchor set \( A \), since \( E \) is not differentiable and the subdifferential of \( -F \) is empty there. This is usually not an issue in applications, but we still want to present some results for this case.

To formulate optimality conditions for matrices in the anchor set, we use the definition of one-sided directional derivatives. The one-sided directional derivative of a function \( f: \mathbb{R}^n \to \mathbb{R} \), \( n \in \mathbb{N} \), at a point \( x \in \mathbb{R}^n \) in direction \( h \in \mathbb{R}^n \) is defined by

\[
Df(x; h) := \lim_{\alpha \downarrow 0} \frac{f(x + \alpha h) - f(x)}{\alpha}.
\]

The following theorem gives a general necessary and sufficient condition for local minimizers of Lipschitz continuous functions on embedded manifolds using the notion of one-sided derivatives. For the Euclidean setting \( M = \mathbb{R}^n \), the first relation of the theorem is trivially fulfilled for any function \( f: \mathbb{R}^n \to \mathbb{R} \), while a proof of the sufficient minimality condition in the second part was given in [5]. Moreover, the authors of [5] gave an example that Lipschitz continuity in the second part cannot be weakened to just continuity. For the manifold setting, the Lipschitz continuity of \( f \) is also necessary in the first part of the theorem, as Example B.2 shows.
Theorem 6.1. Let $\mathcal{M} \subset \mathbb{R}^n$ be an $m$-dimensional submanifold of $\mathbb{R}^n$ and $f: \mathbb{R}^n \rightarrow \mathbb{R}$ a locally Lipschitz continuous function. Then the following holds true:

1. If $\hat{x} \in \mathcal{M}$ is a local minimizer of $f$ on $\mathcal{M}$, then $Df(\hat{x}; h) \geq 0$ for all $h \in T_{\hat{x}}\mathcal{M}$.

2. If $Df(\hat{x}; h) > 0$ for all $h \in T_{\hat{x}}\mathcal{M} \setminus \{0\}$, then $\hat{x}$ is a strict local minimizer of $f$ on $\mathcal{M}$.

For convenience the proof is given in the Appendix B. Note that $Df(\hat{x}; h) \geq 0$ for all $h \in T_{\hat{x}}\mathcal{M} \setminus \{0\}$ does not imply that $\hat{x}$ is a local minimizer of $f$ on $\mathcal{M}$.

We want to apply Theorem 6.1 for the Lipschitz continuous energy function $E$. To this end, the norm on $\mathbb{R}^{n,m}$ is defined by 

$$\|B\|_{2,1} := \sum_{i=1}^{m} \|b_i\|, \quad B := (b_1 \ldots b_m).$$

Then, it is easy to check that the dual norm is given by

$$\|B\|_{2,1}^* = \sup_{\|Z\|_{2,1} = 1} \langle Z, B \rangle_F = \max_{i=1,\ldots,m} \|b_i\| =: \|B\|_{2,\infty}. \quad (20)$$

First, the one-sided derivative of $E$ at $A \in S_{d,K}$ in direction $H \in T_A S_{d,K}$ is computed.

Lemma 6.2. The one-sided derivative of $E$ defined in (4) on $S_{d,K}$ reads for $A \in S_{d,K}$ and $H = AX + A_\perp Z \in T_A S_{d,K}$ as follows

$$DE(A; H) = -\langle Z, A^T C_{A,J} A \rangle_F + \|ZA^T Y_J\|_{2,1}, \quad (21)$$

where $J := \{j \in \{1,\ldots,N\} : \|P_A y_j\| = 0\}$, $Y_J := (y_j)_{j \in J}$ and

$$C_{A,J} := \sum_{i=1}^{N} \frac{1}{\|P_A y_i\|} y_i y_i^T.$$ 

Clearly, if $J$ is empty, then (21) simplifies to $DE(A; H) = \langle \nabla E, H \rangle$.

Proof. First, we consider $j \in J$, i.e. $P_A y_j = 0$ and $y_j = A A^T y_j$. Then, we obtain for $A \in S_{d,K}$ and $H \in T_A S_{d,K}$ that

$$DE_j(A; H) = \lim_{\alpha \downarrow 0} \frac{E_j(A + \alpha H) - E_j(A)}{\alpha} = \lim_{\alpha \downarrow 0} \frac{\| (I - (A + \alpha H)(A + \alpha H)^T ) y_j \|}{\alpha}$$

$$= \lim_{\alpha \downarrow 0} \frac{\| \alpha A H^T y_j + \alpha H A^T y_j + \alpha^2 H H^T y_j \|}{\alpha}$$

$$= \| (A H^T + H A^T ) y_j \|$$

and with $H = AX + A_\perp Z$, $X^T = -X$ and since $y_j \in \mathcal{R}(A)$ further

$$DE_j(A; H) = \| A_\perp Z A^T y_j \| = \| Z A^T y_j \|.$$ 

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For $j \notin \mathcal{J}$, the one-sided derivative in direction $H$ is just the inner product of $\nabla E_j$ and $H$ so that

$$DE(A;H) = -\langle P_A C_{A,\mathcal{J}} A, H \rangle + \sum_{j \in \mathcal{J}} \|ZA^T y_j\|_2$$

and using the structure of $H$ again,

$$DE(A;H) = -\langle Z, A^T_\perp C_{A,\mathcal{J}} A \rangle + \|ZA^T Y_{\mathcal{J}}\|_{2,1}.$$ 

Under certain conditions, it is possible to formulate a minimality condition also for matrices in the anchor set.

**Theorem 6.3.** Let $y_j \in \mathbb{R}^d$, $j = 1, \ldots, N$ and $A \in \mathbb{S}_{d,K}$, where $K \leq d$. Let $\mathcal{J} := \{k \in \{1, \ldots, N\} : \|P_A y_j\| = 0\}$ have cardinality $\kappa \geq 1$. Assume that the matrix $Y_{\mathcal{J}} := (y_j)_{j \in \mathcal{J}} \in \mathbb{R}^{d,\kappa}$ has range $m \leq K$, where the columns are ordered so that the first $m$ are linearly independent and denoted by $Y_m$ and the other ones are their multiples, i.e., $Y_{\mathcal{J}} = (Y_m, Y_m D)$, where $D \in \mathbb{R}^{m,K-m}$ is a matrix whose columns contain exactly one nonzero entry. Then $A \in \mathbb{S}_{d,K}$ is a strict local minimizer of $E$ on $\mathbb{S}_{d,K}$ if and only if the following two conditions are fulfilled

$$\|P_A C_{A,\mathcal{J}} (Y_m^T Y_m)^{-1} \text{diag}(1 + |D|)_{1 \times (m-1)}\|_{2,\infty} < 1 \quad \text{and} \quad P_A C_{A,\mathcal{J}} A (A^T Y_m)_{\perp} = 0_{d-K,m}, \quad (22)$$

where the absolute value of $D$ has to be understood componentwise, $1_{1 \times (m-1)}$ denotes the vector with $m-1$ entries one, and $(A^T Y_m)_{\perp} \in \mathbb{R}^{K,m}$ is any matrix of rank $K-m$ which columns are orthogonal to those of $A^T Y_m \in \mathbb{R}^{K,m}$.

If $Y_{\mathcal{J}}$ contains only vectors which are multiples of $y_1 \in \mathbb{R}^d$, then $A \in \mathbb{S}_{d,K}$ is a strict local minimizer of $E$ on $\mathbb{S}_{d,K}$ if and only if the following conditions are fulfilled

$$\|P_A C_{A,\mathcal{J}} \frac{y_1}{\|y_1\|}\| < \|Y_{\mathcal{J}}\|_{2,1} \quad \text{and} \quad P_A C_{A,\mathcal{J}} A = P_A C_{A,\mathcal{J}} \frac{y_1 y_1^T}{\|y_1\|^2} A. \quad (23)$$

**Proof.** By Theorem 6.1 and [21], $A$ is a strict local minimizer of $E$ on $\mathbb{S}_{d,K}$ if and only if

$$\langle Z, A^T_\perp C_{A,\mathcal{J}} A \rangle < \sum_{k=1}^\kappa \|ZA^T y_j\|_2 = \|ZA^T Y_{\mathcal{J}}\|_{2,1}$$

for all $Z \in \mathbb{R}^{d-K,K}$. Replacing $Z$ by $Z \left(\frac{Y_m^T A}{(Y_m^T A)_{\perp}}\right)$, where $(Y_m^T A)_{\perp} = (A^T Y_m)_{\perp}^T$, this is equivalent to

$$\left\langle Z \left(\frac{Y_m^T A}{(Y_m^T A)_{\perp}}\right), A^T_\perp C_{A,\mathcal{J}} A \right\rangle = \left\langle Z, A^T_\perp C_{A,\mathcal{J}} A (A^T Y_m | (A^T Y_m)_{\perp}) \right\rangle < \left\|Z \left(\frac{Y_m^T A A^T Y_{\mathcal{J}}}{0_{r \times (m,\kappa)}}\right)\right\|_{2,1}$$

for all $Z \in \mathbb{R}^{d-K,K}$. Clearly, the condition is fulfilled if and only if

$$\langle Z_m, A^T_\perp C_{A,\mathcal{J}} A (A^T Y_m)_{\perp} \rangle < \|Z_m Y_m^T A A^T Y_{\mathcal{J}}\|_{2,1} \quad \text{and} \quad A^T_\perp C_{A,\mathcal{J}} A (A^T Y_m)_{\perp} = 0_{d-K,m}$$

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for all $Z_m \in \mathbb{R}^{d-K,m}$. The second part implies that the columns of $C_{A,J}A(A^TY_m)_{\perp}$ are in the range of $A$ which gives the second condition in (22).

Now, $\|P_Ay_j\| = 0$ implies $AA^Ty_j = y_j$, $j \in J$ so that the first condition becomes

$$\langle Z_m, A^TY_m \rangle < \|Z_mY_m^TY_J\|_{2,1}.$$ Using $Y_J = (Y_m | Y_mD)$ and the definition of $\| \cdot \|_{2,1}$, the right-hand side can be rewritten as

$$\|Z_mY_m^TY_J\|_{2,1} = \|Z_m(Y_m^TY_m)(I_m + \text{diag}(D_{1\kappa,m}))\|_{2,1}$$ so that the condition can be rewritten as

$$\langle Z_m, A^TY_m \rangle \leq \|Z_m(Y_m^TY_m)(I_m + \text{diag}(D_{1\kappa,m}))\|_{2,1}$$ for all $Z_m \in \mathbb{R}^{d-K,m}$. By (20) this is fulfilled if and only if

$$\|A^TY_m(\text{diag}(1 + |D|_{1\kappa,m})^{-1})\|_{2,\infty} < 1.$$ Using $\|P_Ay\| = \|A^Ty\|$ for all $y \in \mathbb{R}^d$, this gives the assertion (22).

Assume that the columns of $Y_J$ are multiples of $y_1$. Then the first condition of the simplification (23) follows immediately from

$$(Y_m^TY_m)\text{diag}(1 + |D|_{1\kappa-m}) = \sum_{k\in J} \|y_j\| = \|Y_J\|_{2,1}.$$ Since for every $x \in \mathbb{R}^K$, $x \neq 0$ the columns of $I_K - xx^T/\|x\|^2$ span the linear space orthogonal to $x$, the second condition can be deduced using $P_A C_{A,J}A(I_K - A^Ty_1y_1^T/\|y_1\|^2) = 0_{d,K}$ and $AA^Ty_1 = y_1$. \hfill \Box

7. Conclusions

We proved that the iterates (on the Grassmannian) of the popular rotational invariant $L_1$-norm PCA converge to a critical point if they do not reach anchor points. Interestingly, the rotational invariant $L_1$-norm PCA minimization algorithm proposed by Ding et al. [8] can be considered as conditional gradient algorithm or as gradient descent algorithm on the Grassmannian manifold. It would be interesting to consider the relation between these algorithms in the more general setting of embedded compact Riemannian manifolds. We gave criteria to decide if special anchor points are local minimizers of the functional. A challenging aspect is the full treatment of anchor points including a general procedure to decide if an anchor point is a local minimizer. For one-dimensional subspaces, i.e., $K = 1$, this was done in [30]. Finally, the incorporation of an offset term would be interesting.

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A. KL Functions

The function \( f: \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\} \) with Fréchet limiting subdifferential \( \partial f \), see \([29]\), is said to have the Kurdyka–Lojasiewicz (KL) property at \( u^* \in \text{dom} \partial f \) if there exist \( \eta \in (0, +\infty) \), a neighborhood \( U \) of \( u^* \) and a continuous concave function \( \phi: [0, \eta) \to \mathbb{R} \geq 0 \) such that

1. \( \phi(0) = 0 \),
2. \( \phi \) is \( C^1 \) on \( (0, \eta) \),
3. for all \( s \in (0, \eta) \) it holds \( \phi'(s) > 0 \),
4. for all \( x \in U \cup [f(u^*) < f < f(u^*) + \eta] \), the Kurdyka–Lojasiewicz inequality \( \phi'(f(u) - f(u^*))d(0, \partial f(u)) \geq 1 \) holds true.

A proper, lower semi-continuous (lsc) function which satisfies the KL property at each point of \( \text{dom} \partial f \) is called KL-function.

Similar arguments as used in the proof of Theorem (5.1) lead to the next corollary, see \([3, \text{Corollary 2.7}]\).

**Corollary A.1.** Let \( f: \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\} \) be a KL function. Denote by \( U \), \( \eta \) and \( \phi \) the objects appearing in the definition of the KL function. Let \( \delta, \rho > 0 \) be such that \( B(u^*, \delta) \subset U \) with \( \rho \in (0, \delta) \). Consider a finite sequence \( u^{(r)}, r = 0, \ldots, n \), which satisfies the Conditions C1 and C2 of Theorem 5.1 and additionally

\( C4) \ f(u^*) \leq f(u^{(0)}) < f(u^*) + \eta, \)
\( C5) \ ||u^* - u^{(0)}|| + 2\sqrt{\frac{f(u^{(0)}) - f(u^*)}{K_1}} + \frac{K_2}{K_1} \phi(f(u^{(0)}) - f(u^*)) \leq \rho. \)

If for all \( r = 0, \ldots, n \) it holds

\( u^{(r)} \in B(u^*, \rho) \implies u^{(r+1)} \in B(u^*, \delta) \) and \( f(u^{(r+1)}) \geq f(u^*) \),

then \( u^{(r)} \in B(u^*, \rho) \) for all \( r = 0, \ldots, n + 1 \).

B. Minimizers on Embedded Manifolds

Recall that \( \mathcal{M} \subseteq \mathbb{R}^n \) is an \( m \)-dimensional submanifold of \( \mathbb{R}^n \) if for each point \( x \in \mathcal{M} \) there exists an open neighborhood \( U \subseteq \mathbb{R}^n \) as well as an open set \( \Omega \subseteq \mathbb{R}^n \) and a so-called parameterization \( \varphi \in C^1(\Omega, \mathbb{R}^n) \) of \( \mathcal{M} \) with the properties

i) \( \varphi(\Omega) = \mathcal{M} \cap U \),

ii) \( \varphi^{-1}: \mathcal{M} \cap U \to \Omega \) is surjective and continuous, and

iii) \( D\varphi(x) \) has full rank \( m \) for all \( x \in \Omega \).

To prove Theorem B.1 we need the following lemma which proof we have not found in the literature.
Lemma B.1. Let $\mathcal{M} \subset \mathbb{R}^n$ be an $m$-dimensional manifold of $\mathbb{R}^n$. Then the tangent space $T_x\mathcal{M}$ and the tangent cone

$$T_x\mathcal{M} := \left\{ u \in \mathbb{R}^n : \exists \text{ sequence } (x_k)_k \subset \mathcal{M} \setminus \{x\} \text{ with } x_k \to x \text{ s.t. } \frac{x_k - x}{\|x_k - x\|} \to \frac{u}{\|u\|} \right\} \cup \{0\}$$

coincide.

Proof. 1. Let $\xi \in T_x\mathcal{M}$. Then there exists a curve $\gamma : (0, \epsilon) \to \mathcal{M}$ with $\gamma(0) = x$ and $\gamma(\epsilon) = \xi$. Choose $x_k = \gamma(\frac{1}{k})$, then

$$\lim_{k \to \infty} \frac{x_k - x}{\frac{1}{k}} = \lim_{k \to \infty} \frac{\gamma(\frac{1}{k}) - \gamma(0)}{\frac{1}{k}} = \dot{\gamma}(0) = \xi$$

and consequently

$$\lim_{k \to \infty} \frac{x_k - x}{\|x_k - x\|} = \lim_{k \to \infty} \frac{k(x_k - x)}{\|k(x_k - x)\|} = \frac{\xi}{\|\xi\|},$$

so that $\xi \in T_x\mathcal{M}$.

2. Conversely, let $u \in T_x\mathcal{M}$ along with a sequence of points $x_k \in \mathcal{M}$ fulfilling $\lim_{k \to \infty} x_k = x$ and $\lim_{k \to \infty} \frac{x_k - x}{\|x_k - x\|} = \frac{u}{\|u\|}$. Let $\Omega \subseteq \mathbb{R}^n$ be an open neighborhood of 0 and $U \subseteq \mathbb{R}^d$ an open neighborhood of $x$, and $\varphi : \Omega \to \mathcal{M}$ a parameterization of $\mathcal{M}$ with $\varphi(0) = x$. Then there is some $K$, such that for all $k \geq K$ we have $x_k \in U \cap \mathcal{M}$ and we can find $y_k \in \Omega$ with $\varphi(y_k) = x_k$ Since $\varphi$ is a homeomorphism, it holds $y_k \to 0$ as $k \to \infty$. By the mean value theorem we have

$$x_k - x = \varphi(y_k) - \varphi(0) = \int_0^1 D\varphi(ty_k) dt y_k$$

and further

$$\left\| \int_0^1 D\varphi(ty_k) dt - D\varphi(0) \right\| = \left\| \int_0^1 D\varphi(ty_k) - D\varphi(0) dt \right\| \leq \int_0^1 \|D\varphi(ty_k) - D\varphi(0)\| dt$$

which tends to zero as $k \to \infty$ due to continuity of $D\varphi$. Thus,

$$\lim_{k \to \infty} \int_0^1 D\varphi(ty_k) dt = D\varphi(0).$$

Then

$$\frac{x_k - x}{\|x_k - x\|} = \frac{\varphi(y_k) - \varphi(0)}{\|\varphi(y_k) - \varphi(0)\|} = \int_0^1 D\varphi(ty_k) dt \frac{y_k}{\|\varphi(y_k) - \varphi(0)\|}$$

and the quotient on the right hand side is bounded since the left hand side is bounded and there exists $\epsilon > 0$ with

$$\min_{\|x\| = 1} \left\| \int_0^1 D\varphi(ty) dt \right\| \geq \min_{\|x\| = 1} \left\| D\varphi(0) x - \int_0^1 D\varphi(ty) dt \right\| > \epsilon$$

for $k$ large enough as $D\varphi(0)$ has full rank. Switching to a convergent subsequence if necessary, we call its limit $y^*$ and obtain

$$\frac{u}{\|u\|} = \lim_{k \to \infty} \frac{x_k - x}{\|x_k - x\|} = D\varphi(0)y^*$$

which is in $T_x\mathcal{M}$. \qed
Proof of Theorem 6.1

1. Let \( \hat{x} \in \mathcal{M} \) be a local minimizer of \( f \). Assume for the sake of contradiction that 
\[
Df(\hat{x}; h) < 0 \quad \text{for some } h \in T_{\hat{x}}\mathcal{M}.
\]
Then there exists \( \beta, \delta > 0 \) such that for all \( \alpha \in (0, \delta) \),
\[
\begin{align*}
\frac{f(\hat{x} + ah) - f(\hat{x})}{\alpha} &< -\beta, \\
f(\hat{x} + ah) - f(\hat{x}) &< -\alpha \beta.
\end{align*}
\]
Let \( \varphi : \Omega \to \mathbb{R}^n \) be a parametrization of \( \mathcal{M} \) with \( \varphi(0) = \hat{x} \) and \( A := D\varphi(0) \). Then we have \( T_{\hat{x}}\mathcal{M} = \{ Aw : w \in \mathbb{R}^m \} \). By \( A^\dagger := (A^T A)^{-1} A^T \) we denote the Moore-Penrose inverse of \( A \). For \( U_1 := \{ \xi \in \mathbb{R}^n : A^\dagger \xi \in \Omega \} \), we define
\[
\psi := \varphi \circ A^\dagger : \mathbb{R}^n \supseteq U_1 \to \mathbb{R}^n.
\]
Then, for \( \alpha \) small enough, \( \psi(\alpha h) \in \mathcal{M} \). By the the local Lipschitz continuity of \( f \) with Lipschitz constant \( L > 0 \) we obtain for \( \alpha \) small enough
\[
\begin{align*}
f(\psi(\alpha h)) - f(\hat{x}) &= f(\psi(\alpha h)) - f(\hat{x} + ah) + f(\hat{x} + ah) - f(\hat{x}) \\
&< f(\psi(\alpha h)) - f(\hat{x} + ah) - \alpha \beta \\
&\leq L \| \psi(\alpha h) - (\hat{x} + ah) \| - \alpha \beta \\
&= L \| \psi(\alpha h) - \psi(0) - \alpha h \| - \alpha \beta.
\end{align*}
\]
By the mean value theorem
\[
\psi(\alpha h) - \psi(0) = \alpha \int_0^1 D\psi(t\alpha h) dt h
\]
so that
\[
f(\psi(\alpha h)) - f(\hat{x}) < \alpha \left( L \| \int_0^1 D\psi(t\alpha h) dt h - h \| - \beta \right).
\]
By the chain rule and since \( h \in T_{\hat{x}}\mathcal{M} \) we have
\[
\lim_{\alpha \downarrow 0} \| \int_0^1 D\psi(t\alpha h) dt h - h \| = \| \lim_{\alpha \downarrow 0} \int_0^1 D\varphi(t\alpha h) dt A^\dagger h - h \| = \| AA^\dagger h - h \| = 0
\]
Thus, for \( \alpha > 0 \) small enough so that \( \| \int_0^1 D\psi(t\alpha h) dt h - h \| < \beta / L \) we get \( f(\psi(\alpha h)) - f(\hat{x}) < 0 \) which is a contradiction to \( \hat{x} \) being a local minimizer.

2. Let \( Df(\hat{x}; h) > 0 \) for all \( h \in T_{\hat{x}}\mathcal{M} \setminus \{ 0 \} \). Suppose for the sake of contradiction that \( \hat{x} \) is not a strict local minimizer of \( f \) on \( \mathcal{M} \). Then there exists a sequence \( \{ x_k \} \subseteq \mathcal{M} \) with \( x_k \neq \hat{x} \) and \( f(x_k) \leq f(\hat{x}) \) for all \( k \in \mathbb{N} \), and \( \lim_{k \to \infty} x_k = \hat{x} \). Let \( \lambda_k := \| x_k - \hat{x} \| \). Since \( \frac{x_k - \hat{x}}{\lambda_k} \) is bounded, it has a convergent subsequence which we denote again by \( \{ \frac{x_k - \hat{x}}{\lambda_k} \} \). Then
\[
\lim_{k \to \infty} \frac{x_k - \hat{x}}{\lambda_k} = h \in T_{\hat{x}}\mathcal{M} \setminus \{ 0 \}.
\]
Indeed, \( h \in T_{\hat{x}}\mathcal{M} \setminus \{ 0 \} \), since the tangent space at \( \hat{x} \) coincides with the tangent cone of \( \mathcal{M} \) at \( \hat{x} \), see appendix. By assumption we know
\[
0 \geq f(x_k) - f(\hat{x}) = f(x_k) - f(\hat{x} + \lambda_k h) + f(\hat{x} + \lambda_k h) - f(\hat{x}).
\]

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Dividing by \( \lambda_k \) we obtain by the Lipschitz continuity of \( f \) that

\[
\frac{|f(x_k) - f(\hat{x} + \lambda_k h)|}{\lambda_k} \leq L \frac{\|x_k - \hat{x} - \lambda_k h\|}{\lambda_k} = L \frac{\|x_k - \hat{x}\|}{\lambda_k} - h,
\]

which tends to zero as \( k \to \infty \). Hence we get

\[
0 \geq \lim_{k \to \infty} \frac{f(x_k) - f(\hat{x} + \lambda_k h)}{\lambda_k} + \frac{f(\hat{x} + \lambda_k h) - f(\hat{x})}{\lambda_k} = Df(\hat{x}, h),
\]

which contradicts the positivity of the one-sided directional derivatives. \( \square \)

For the manifold setting, the following example demonstrates that we need the Lipschitz continuity also in the first part of the proposition.

**Example B.2.** Consider \( \mathcal{M} := \{ (x, -x^2)^T : x \in \mathbb{R} \} \) and the function

\[
f(x_1, x_2) = \begin{cases} 
-\frac{1}{2}|x_1| & \text{if } |x_2| < \frac{1}{2}x_1^2, \\
\sqrt{|x_2| - \frac{1}{2}x_1^2} - \frac{1}{2}|x_1| & \text{if } |x_2| \geq \frac{1}{2}x_1^2.
\end{cases}
\]

Then \( f \) is continuous, but not Lipschitz continuous as \( f(0, x_2) = \sqrt{|x_2|} \). We observe that \( (0, 0)^T \) is the global minimizer on \( \mathcal{M} \) as \( f(x, -x^2) = (\frac{1}{\sqrt{2}} - \frac{1}{2})|x| > 0 \) for \( x \neq 0 \). But for the directional derivative along the first axis we get \( Df((0, 0), (1, 0)^T) = -\frac{1}{2} < 0 \).

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