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CONDITIONS FOR OPTIMAL SOLUTIONS OF UNBALANCED PROCRUSTES PROBLEM ON STIEFEL MANIFOLD*

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Abstract

We consider the unbalanced Procrustes problem with an orthonormal constraint on solutions: given matrices $A \in \mathcal{R}^{n\times n}$ and $B \in \mathcal{R}^{n\times k}$, $n > k$, minimize the residual $\|AQ - B\|_F$ over the Stiefel manifold of orthonormal matrices. Theoretical analysis on necessary conditions and sufficient conditions for optimal solutions of the unbalanced Procrustes problem is given.

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Key words: Procrustes problem, Stiefel manifold, Necessary condition, Sufficient condition.

1. Introduction

Given two matrices $A \in \mathcal{R}^{m\times n}$ and $B \in \mathcal{R}^{m\times k}$ with $n > k$, we consider the orthonormal Procrustes problem: Find an orthonormal matrix $Q \in \mathcal{R}^{n\times k}$ that solves the following constrained optimization problem:

$$\min_{Q^TQ=I} \|AQ - B\|_F^2, \tag{1.1}$$

where $\|\cdot\|_F$ denote the Frobenius norm. The set of orthonormal matrices in $\mathcal{R}^{n\times k}$ defines the orthonormal Stiefel manifold

$$\mathcal{S} = \{Q \in \mathcal{R}^{n\times k} : Q^TQ = I\}. \tag{1.2}$$

In general, $m \geq n$. If $m \gg n$, the size of the problem can be reduced by QR decomposition with no difficulties. Therefore, without loss of generality, we assume that the matrix A is square with order n, i.e., write (1.1) as

$$\min_{Q^TQ=I} \|AQ - B\|_F^2, \quad A \in \mathcal{R}^{n\times n}, \quad B \in \mathcal{R}^{n\times k}, \quad n \geq k. \tag{1.3}$$

We refer to (1.3) as the *balanced* Procrustes problem if $k = n$, and the *unbalanced* Procrustes problem when $k < n$.

The balanced problem is simple and has been solved analytically [4, 8]; solutions are given by the singular value decomposition (SVD) or pole decomposition of A^TB. However, the unbalanced Procrustes problem seems to be quite difficult. First, if A is rank deficient in column, i.e., $r = \mathrm{rank}(A) < n$, then by SVD $A = U_r\Sigma_rV_r^T$ of A,

$$\|AQ - B\|_F^2 = \|\Sigma_rV_r^TQ - U_r^TB\|_F^2 + \|(U_r^\perp)^TB\|_F^2,$$

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where $U_r^\perp$ denotes the orthogonal complement of U_r. Hence the problem (1.3) is equivalent to $\min_{Q^TQ=I_k} \|\Sigma_r V_r^T Q - U_r^T B\|_F$. Though $\|\Sigma_r V_r^T Q - U_r^T B\|_F = \|\Sigma_r X - U_r^T B\|_F$ with $X = V_r^T Q$ and $\|X\| \leq 1$, the optimization problem mentioned above is not equivalent to the constrained LS problem

$$\min_{\|X\|\leq 1} \|\Sigma_r X - U_r^T B\|_F.$$

Second, necessary and sufficient conditions for a global minimum of the unbalanced problem are still not clear, though some necessary conditions and sufficient conditions for local and/or global optimal solutions have been reported [3]. Third, except the special case when $k = 1$ for which a quadratic convergent method is proposed and careful analysis for its quadratic convergence is also given in [10], no sufficient analysis is reported for the convergence of existing iterative algorithms for solving the unbalanced problem when $k > 1$, partially due to lack of sufficient theoretical analysis for optimal solutions. Indeed, these iterative algorithms may be divergent or/and not efficient when the problem scale is large or A is ill conditioned.

The purpose of this paper is to show a deep understanding to the unbalanced Procrustes problem. We are interested in conditions of optimal solutions for the unbalanced problem. An analysis for local or global optimal solutions is given, which simplifies the discussions given in [3]. Based upon the analysis presented in this paper, a successive projection (SP) method for solving the unbalanced Procrustes problem will be proposed in a separate paper, together with a careful analysis for the convergence of the successive projection method and reports of numerical experiments.

The rest of this paper is arranged as follows. In Section 2, we review the structures of optimal solutions of the balanced problem. A discussion of necessary conditions for global optimization solutions of the unbalanced Procrustes problem is given in Section 3. In Section 4, we present some sufficient conditions of a local and/or global minimum of the unbalanced problem.

Notations. Given an orthonormal matrix $Q \in \mathcal{R}^{n\times k}$, we call $H \in \mathcal{R}^{n\times(n-k)}$ an orthogonal complement of Q if $[Q, H]$ is a (square) orthogonal matrix. The spectral norm of a vector or a matrix is simply denoted as $\|\cdot\|$, while $\|\cdot\|_F$ denotes the Frobenius norm of matrices. As used in general, I denotes an identity matrix with certain matrix size.

2. Structure of Solutions to Balanced Procrustes Problem

The balanced Procrustes problem, i.e., $k = n$, is relatively simple; it can be solved by the SVD of the matrix A^TB. Here we cite a theorem that illustrates the structure of solutions of the balanced Procrustes problem.

Theorem 2.1. [4, p.695] *Let*

$$A^TB = U \begin{bmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{bmatrix} V^T$$

be the singular value decomposition of A^TB, where $\Sigma_1 = \mathrm{diag}(\sigma_1, \cdots, \sigma_r)$, and $r = \mathrm{rank}(A^TB)$. Then all solutions of the balanced Procrustes problem (1.3) *can be formulated as*

$$Q = U \begin{bmatrix} I_r & 0 \\ 0 & T \end{bmatrix} V^T, \tag{2.1}$$

with any orthogonal matrix T.[1)]

It is easy to prove Theorem 2.1. In fact, by the singular value decomposition (SVD) $A^TB = U\mathrm{diag}(\sigma_1, \sigma_2, \cdots, \sigma_p)V^T$ of A^TB with $r = \mathrm{rank}(A^TB)$, one can show that

$$\|AQ - B\|_F^2 = \|A\|_F^2 + \|B\|_F^2 - 2\sum_{i=1}^{r} z_{ii}\sigma_i,$$

where z_{ii} are the first r diagonal elements of the orthogonal matrix $Z = V^TQ^TU$. This equality shows that $\|AQ - B\|_F$ is a minimum if and only if $z_{ii} = 1$ for $i = 1, \cdots, r$, or equivalently, $Z = \mathrm{diag}(I, T)$ with orthogonal matrix of order $n - r$.

The structure (2.1) of an optimal solution Q to the balanced Procrustes problem implies that $Q^TA^TB = V\mathrm{diag}(\sigma_1, \sigma_2, \cdots, \sigma_p)V^T$ is (symmetric) positive semi-definite. In fact, we can prove that it is also true vice versa.

Theorem 2.2. *The orthogonal matrix Q is an optimal solution to the balanced Procrustes problem* (1.3)*, if and only if Q^TA^TB is a positive semi-definite matrix.*

Proof. We only need to show the sufficiency. Let Q be orthogonal and Q^TA^TB positive semi-definite. Also let $A^TB = U_r\Sigma_rV_r^T$ be the SVD of A^TB, where both U_r and V_r are orthonormal and the diagonal matrix $\Sigma_r = \mathrm{diag}(\sigma_1, \sigma_2, \cdots, \sigma_r)$ is nonsingular. By the symmetry of Q^TA^TB, $Q^TU_r\Sigma_rV_r^T = V_r\Sigma_rU_r^TQ$. Denoting by $C = U_r^TQV_r$, we have

$$C^T\Sigma_r = \Sigma_rC, \quad C\Sigma_r = \Sigma_rC^T.$$

It follows that

$$C\Sigma_r^2 = \Sigma_rC^T\Sigma_r = \Sigma_r^2C.$$

Writing $\Sigma_r = \mathrm{diag}(\sigma_{i_1}I, \cdots, \sigma_{i_k}I)$ with different $\sigma_{i_1}, \cdots, \sigma_{i_k}$, we conclude that $C = \mathrm{diag}(C_1, \cdots, C_k)$ with diagonal blocks conforming to those of Σ. Clearly C is symmetric because $C^T\Sigma_r = \Sigma_rC$ implies that $C_1, \cdots, C_k$ are symmetric. Therefore, by $U_r^TQV_r = C$ we have

$$Q^TU_r = V_rC + V_r^{\perp}S, \tag{2.2}$$

where S satisfies $C^TC + S^TS = I$ and $V_r^{\perp}$ is an orthogonal complement of V_r. On the other hand, because

$$Q^TA^TB = V_rC\Sigma_rV_r^T + V_r^{\perp}S\Sigma_rV_r^T$$

is symmetric, $V_r^{\perp}S\Sigma_rV_r^T$ should be symmetric, too, which implies that $S = 0$ and hence C is orthogonal. Thus, C must be the identity matrix since it is orthogonal and symmetric. It follows form (2.2) that $U_r = QV_r$ and that

$$(U_r,\, U_r^{\perp})^TQ(V_r,\, V_r^{\perp}) = \mathrm{diag}(I,\, T),$$

where $U_r^{\perp}$ is an orthogonal complement and T is orthogonal. Therefore we can write

$$Q = (U_r,\, U_r^{\perp})\mathrm{diag}(I,\, T)(V_r,\, V_r^{\perp})^T.$$

1) The formula given in [4] absorbs the orthogonal matrix T into the left or right orthogonal matrices of the SVD implicitly.

By Theorem 2.1, Q is an optimal solution. $\square$

Remark. Theorem 2.2 states that an optimal solution to the balanced problem can be obtained by a polar decomposition of $A^T B$:

$$A^T B = QS,$$

where Q is orthonormal and S is a symmetric and positive semi-definite matrix. However this is not true for the unbalanced problem.

A solution to the unbalanced Procrustes problem is a column part of a solution to a relative balanced Procrustes problem [5, 6]. This property together with Theorem 2.2 helps us to propose conditions for global minimum of the unbalanced Procrustes problem.

3. Necessary Conditions for Unbalanced Procrustes Problems

Let Q be a solution of the unbalanced Procrustes problem (1.3), and H is an orthogonal complement of Q. For any orthogonal matrix $G = [G_1, G_2]$,

$$\|A[Q,\, H] - [B,\, AH]\|_F = \|AQ - B\|_F \le \|AG_1 - B\|_F \le \|AG - [B,\, AH]\|_F.$$

It shows that $[Q,\, H]$ is a solution to the following balanced Procrustes problem:

$$\min_{G^T G = I} \|AG - [B,\, AH]\|_F. \tag{3.1}$$

Conversely, any solution $G = [G_1, G_2]$ to (3.1) gives

$$\|AG_1 - B\|_F = \|AQ - B\|_F, \quad A(G_2 - H) = 0.$$

So we have the following simple result.

Theorem 3.1. *If Q is an optimal solution to the unbalanced Procrustes problem* (1.3)*, and H is an orthogonal complement of Q, then $[Q,\, H]$ is a solution to* (3.1)*, and for any solution $G = [G_1, G_2]$ of* (3.1)*, G_1 is also an optimal solution of* (1.3) *and $A(G_2 - H) = 0$.*

The following two theorems show necessary conditions without involving the orthogonal complement H of a solution Q.

Theorem 3.2. *If Q is an optimal solution to the unbalanced Procrustes problem* (1.3)*, then $Q^T A^T B$ is also positive semidefinite, and there is a symmetric matrix Λ such that*

$$A^T AQ + Q\Lambda = A^T B. \tag{3.2}$$

Proof. By Theorem 3.1, $[Q,\, H]$ is a solution to (3.1). It follows from Theorem 2.2 that $[Q,\, H]^T A^T [B,\, AH]$ is symmetric and positive semi-definite. Hence, its (1,1) block $Q^T A^T B$ is also positive semidefinite. In addition, since $[Q,\, H]^T A^T [B,\, AH]$ is symmetric,

$$H^T (A^T B - A^T AQ) = 0.$$

So, there is a matrix Λ such that $A^T B - A^T AQ = Q\Lambda$. Hence

$$\Lambda = Q^T A^T B - Q^T A^T AQ$$

and is symmetric. $\square$

Theorem 3.3. *Let Q be a solution of the unbalanced Procrustes problem* (1.3)*. Denote $Q_j = [q_1, \cdots, q_{j-1}, q_{j+1}, \cdots, q_k]$. Then*

$$\|Aq_j - b_j\| = \min_{q\perp Q_j, \|q\|=1} \|Aq - b_j\|, \quad j = 1, \cdots, k. \tag{3.3}$$

Proof. The proof is simple. Assume that there is j such that

$$\|Aq_j - b_j\| > \min_{q\perp Q_j, \|q\|=1} \|Aq - b_j\|.$$

Denote $q_j^* = \arg \min_{q\perp Q_j, \|q\|=1} \|Aq - b_j\|$ and $Q^* = [q_1, \cdots, q_{j-1}, q_j^*, q_{j+1}, \cdots, q_k]$. It is easy to verify that

$$\|AQ - B\|_F^2 - \|AQ^* - B\|_F^2 = \|Aq_j - b_j\|^2 - \|Aq_j^* - b_j\|^2 > 0,$$

a contradiction to the assumption that Q is an optimal solution to (1.3). $\square$

The following theorem shows the relations between the conditions (3.3) and (3.2).

Theorem 3.4. *An orthonormal matrix Q satisfies* (3.3) *and that $(AQ)^T B$ is symmetric, if and only if* (3.2) *holds for the symmetric matrix $\Lambda = (AQ)^T(B - AQ)$ and the diagonals λ_{jj} of Λ satisfy*

$$\lambda_{jj} \geq -\sigma_{\min}^2(A[q_j, H]), \quad j = 1, \cdots, k, \tag{3.4}$$

where H is an orthogonal complement matrix of Q.

Proof. First, if Q satisfies (3.3), then for each j, $x = e_1$, the first column of the identity matrix I is an optimal solution to the problem $\min_{\|x\|=1} \|A[q_j, H]x - b_j\|$. By Theorem 2.2 of [10], there exists $\lambda_j \geq -\sigma_{\min}^2(A[q_j, H])$ such that

$$(A[q_j, H])^T A[q_j, H]e_1 - \lambda_j e_1 = (A[q_j, H])^T b_j,$$

i.e.,

$$\begin{bmatrix} q_j^T \\ H^T \end{bmatrix} A^T A q_j + \begin{bmatrix} \lambda_j \\ 0 \end{bmatrix} = \begin{bmatrix} q_j^T \\ H^T \end{bmatrix} A^T b_j. \tag{3.5}$$

It follows that

$$H^T A^T (B - AQ) = 0.$$

We can write $A^T(B - AQ) = Q\Lambda$ with the symmetric matrix $\Lambda = (AQ)^T(B - AQ)$. Obviously, $\lambda_j = q_j^T A^T(b_j - Aq_j) = \lambda_{jj}$.

Conversely, if $A^T AQ + Q\Lambda = A^T B$, we have

$$(A[q_j, H])^T A[q_j, H]e_1 - \lambda_{jj} e_1 = (A[q_j, H])^T b_j.$$

By Theorem 2.2 of [10], if the inequalities in (3.4) hold, then q_j must be the solution of the following problem

$$\min_{q\perp Q_j, \|q\|=1} \|Aq - b_j\|,$$

completing the proof. $\square$

The equality (3.2) is necessary but not sufficient for a global minimum. Theorem 3.4 shows that necessary condition (3.3) for global optimal solutions is stricter than condition (3.2). It is not clear if (3.3) is also sufficient or not. However, it may be much closer to a unknown necessary and sufficient condition. This can be partially verified by comparing the conditions (3.4) and the sufficient conditions (4.1) given later in Theorem 4.1. Besides, the Algorithm SP proposed in [11] is based on solving the problems in (3.3) together with a technique of global correction and always gives a global optimization solution for all the tests we have done. This is also why we should rather consider sufficient conditions by imposing conditions on the necessary condition (3.2) than sufficient conditions based upon (3.3) in the next section.

4. Sufficient Conditions for Unbalanced Procrustes Problems

To show how an orthonormal matrix Q satisfying (3.2) can be a global or local optimal solution, we need following simple and important lemma.

Lemma 4.1. *If an orthonormal matrix Q satisfies $A^TAQ + Q\Lambda = A^TB$ with symmetric Λ, then for any orthonormal matrix $\hat{Q}$,*

$$\|A\hat{Q} - B\|_F^2 = \|AQ - B\|_F^2 + \|A(\hat{Q} - Q)\|_F^2 + \mathrm{tr}(\Lambda(\hat{Q} - Q)^T(\hat{Q} - Q)).$$

Proof. Simply write $A\hat{Q} - B = (AQ - B) + A\Delta$ with $\Delta = \hat{Q} - Q$. Taking norms and using $A^T(AQ - B) = -Q\Lambda$ with symmetric Λ gives

$$\|A\hat{Q} - B\|_F^2 = \|AQ - B\|_F^2 + \|A(\hat{Q} - Q)\|_F^2 - 2\mathrm{tr}((\Delta^TQ + Q^T\Delta)\Lambda).$$

On the other hand, because both $\hat{Q} = Q + \Delta$ and Q are orthonormal, one can verify that

$$\Delta^TQ + Q^T\Delta = -\Delta^T\Delta.$$

Substituting it into the equality above, we obtain the required result. $\square$

By Lemma 4.1, a sufficient condition for a unique global minimum follows immediately: If Λ is positive, the Q is the unique optimal solution to the problem (1.3). However, this condition is too strong to be satisfied generally. The following theorem shows a weaker condition for optimal solutions.

Theorem 4.1. *Let orthonormal matrix Q satisfy $A^TAQ + Q\Lambda = A^TB$ with symmetric Λ. If*

$$\sigma_n^2(A) + \lambda_{\min}(\Lambda) \geq 0, \tag{4.1}$$

then Q is a (global) optimal solution to the unbalanced Procrustes problem (1.3)*. Moreover, if* (4.1) *holds strictly, Q is the unique optimal solution.*

Proof. Let $\hat{Q} = Q + \Delta$ be any orthonormal matrix that differs from Q, and let $\Lambda = U\mathrm{diag}(\lambda_1, \cdots, \lambda_k)U^T$ be the eigenvalue decomposition of Λ. Denote by $W = \Delta \cdot U = [w_1, \cdots, w_k]$. Then

$$\begin{aligned} \|A\Delta\|_F^2 + \mathrm{tr}(\Delta\Lambda(\Delta)^T) &= \|AW\|_F^2 + \mathrm{tr}\big(\mathrm{diag}(\lambda_1, \cdots, \lambda_k)W^TW\big) \\ &= \sum_{j=1}^k \big(\|Aw_j\|^2 + \lambda_j\|w_j\|^2\big) \\ &\geq \sum_{j=1}^k (\sigma_n^2(A) + \lambda_j)\|w_j\|^2 \geq 0. \end{aligned}$$

By Lemma 4.1, we have that $\|A\hat{Q} - B\|_F^2 \geq \|AQ - B\|_F^2$. $\square$

Remark. (4.1) is also a necessary condition if $k = 1$. See [10, Theorem 2.2].

The condition (4.1) is similar in form to a necessary condition given in [3]. Later in this section, we will give an easy-to-follow analysis for local minima.

Theorem 4.2. *Let the orthonormal matrix Q satisfy $A^TAQ + Q\Lambda = A^TB$ with symmetric Λ. If for any nonzero matrix Δ such that $Q^T\Delta$ is skew-symmetric,*

$$\|A\Delta\|_F^2 + \mathrm{tr}(\Delta\Lambda\Delta^T) > 0, \tag{4.2}$$

then Q is a local optimal solution to the unbalanced Procrustes problem.

Proof. If Q is not a local optimal solution to the problem (1.3), then there is a sequence of $\{Q^{(i)}\}$ such that $Q^{(i)} \to Q$ and

$$\|AQ^{(i)} - B\|_F < \|AQ - B\|_F.$$

Denote by

$$\Delta^{(i)} = Q^{(i)} - Q, \quad \alpha^{(i)} = \|\Delta^{(i)}\|, \quad \hat{\Delta}^{(i)} = \Delta^{(i)}/\alpha^{(i)}.$$

Because $\{\hat{\Delta}^{(i)}\}$ is bounded, without loss of generality, we can assume that $\{\hat{\Delta}^{(i)}\}$ is convergent. Let $\Delta = \lim_{i\to\infty} \hat{\Delta}^{(i)}$. Recalling that both Q and $Q^{(i)} = Q + \Delta^{(i)}$ are orthonormal, we have

$$Q^T\Delta^{(i)} + (\Delta^{(i)})^TQ + (\Delta^{(i)})^T\Delta^{(i)} = 0.$$

Dividing the equality above by $\alpha^{(i)}$ and taking $i \to \infty$ yields that Δ^TQ is skew-symmetric. On the other hand, by Lemma 4.1 we have

$$\|A\Delta^{(i)}\|_F^2 + \mathrm{tr}((\Delta^{(i)})^T\Delta^{(i)}\Lambda) < 0.$$

It follows that

$$\|A\Delta\|_F^2 + \mathrm{tr}(\Delta\Lambda(\Delta)^T) \leq 0,$$

contradicting the assumption of the theorem. $\square$

A matrix $\Delta \in \mathcal{R}^{n\times k}$ for which $Q^T\Delta$ is skew-symmetric defines a tangent vector of Q on the Stiefel manifold $\mathcal{S}$ (1.2). The following result shows that (4.2) is essentially necessary for a local minimum in the Stiefel manifold.

Theorem 4.3. *Let the orthonormal matrix Q satisfy $A^TAQ + Q\Lambda = A^TB$ with symmetric Λ. If there is a nonzero matrix Δ such that $Q^T\Delta$ is skew-symmetric and*

$$\|A\Delta\|_F^2 + \mathrm{tr}(\Delta\Lambda\Delta^T) < 0,$$

then Q is not a local optimal solution to the unbalanced Procrustes problem.

Proof. Let $Q(t)$ is a differentiable curve on $\mathcal{S}$ that is defined locally for small t and satisfies $Q(0) = Q$ and $\dot{Q}(0) = \Delta$. Then by Lemma 4.1,

$$\frac{\|AQ(t) - B\|_F^2 - \|AQ - B\|_F^2}{t^2} = \|A\frac{Q(t) - Q}{t}\|_F^2 + \mathrm{tr}(\Lambda\frac{(Q(t) - Q)^T(Q(t) - Q)}{t^2}).$$

Letting $t \to 0$, we have

$$\lim_{t\to 0} \frac{\|AQ(t)-B\|_F^2 - \|AQ-B\|_F^2}{t^2} = \|A\Delta\|_F^2 + \mathrm{tr}(\Lambda\Delta^T\Delta) < 0,$$

which implies that for sufficient $t \neq 0$,

$$\|AQ(t)-B\|_F^2 < \|AQ-B\|_F^2.$$

So Q is not a local minimum. $\square$

Therefore, a weaker sufficient condition for local minimums is that the minimum of $\|A\Delta\|_F^2 + \mathrm{tr}(\Delta\Lambda(\Delta)^T)$ on the tangent space of the Stiefel manifold is positive. Note that a tangent vector Δ can be written in the form $\Delta = QS + HX$ with skew-symmetric S and arbitrary X. For this Δ,

$$\mathrm{tr}(\Delta\Lambda(\Delta)^T) = \mathrm{tr}(\Lambda(S^TS + X^TX)).$$

To drive such a weaker sufficient condition, let us consider the following constrained problem:

$$\begin{array}{l} \min \Big(\|AQS + AHX\|_F^2 + \mathrm{tr}(\Lambda(S^TS + X^TX))\Big) \\ s.t. \quad S^T = -S, \quad \mathrm{tr}(S^TS + X^TX) = 1. \end{array} \tag{4.3}$$

To characterize its minima by Lagrange Multiplier Method, we write

$$\|AQS\|_F^2 + \mathrm{tr}(\Lambda S^TS) = \mathrm{tr}(S^T((AQ)^TAQ + \Lambda)S) = \mathrm{tr}((BS)^TAQS).$$

So the Lagrange multiplier function of (4.3) reads

$$\begin{aligned} L &= \|AQS + AHX\|_F^2 + \mathrm{tr}(\Lambda(S^TS + X^TX)) - \mu(\mathrm{tr}(S^TS + X^TX) - 1) \\ &= \mathrm{tr}\Big((BS)^TAQS + (AHX)^TAHX + \Lambda X^TX + 2(BS)^TAHX\Big) \\ &\quad -\mu\Big(\mathrm{tr}(S^TS + X^TX) - 1\Big). \end{aligned}$$

Taking the derivatives of L on S and X, respectively, and setting them to be zero gives

$$\frac{1}{2}\Big(B^TAQS + SB^TAQ + B^TAHX - (AHX)^TB\Big) = \mu S, \tag{4.4}$$

$$(AH)^TAHX + (AH)^TBS + X\Lambda = \mu X. \tag{4.5}$$

That is, the multiplier μ is an eigenvalue of the linear operator $\mathcal{L}$ defined by

$$\mathcal{L}(S,X) = \left[\begin{array}{c} \frac{1}{2}\Big(B^TA(QS+HX) - \big(B^TA(QS+HX)\big)^T\Big) \\ (AH)^T(AHX + BS) + X\Lambda \end{array}\right].$$

We multiply (4.4) and (4.5) by S^T and X^T on the left-hand sides, respectively. Taking the sum of the traces of the two products yields

$$\begin{aligned} &\|AQS + AHX\|_F^2 + \mathrm{tr}(\Lambda(S^TS + X^TX)) \\ =\ &\mathrm{tr}\Big((BS)^TAQS + (AHX)^TAHX + \Lambda X^TX + 2(BS)^TAHX\Big) = \mu. \end{aligned}$$

Here we have used the condition $\mathrm{tr}(S^TS + X^TX) = 1$ and the symmetry of B^TAQ. Therefore, a minimum of the constrained problem (4.3) is an eigenvalue of $\mathcal{L}$ with respect to $Y = (S, X)$ in the subspace $\mathcal{V} = \mathcal{V}_1 \oplus \mathcal{V}_2$, where

$$\mathcal{V}_1 = \left\{ \begin{pmatrix} S \\ 0 \end{pmatrix} \,\Big|\, S \in \mathcal{R}^{k\times k},\ S^T = -S \right\}, \quad \mathcal{V}_2 = \left\{ \begin{pmatrix} 0 \\ X \end{pmatrix} \,\Big|\, X \in \mathcal{R}^{(n-k)\times k} \right\}.$$

Clearly, $\mathcal{V}_1$ is an invariant subspace of $\mathcal{L}$. $\mathcal{V}_1$ and $\mathcal{V}_2$ are orthogonal to each other with inner product $\mathrm{tr}(Y_1^T Y_2)$. The eigenvalue set of $\mathcal{L}$ consists of the eigenvalues of two linear operators defined in the following lemma.

Lemma 4.2. *Define two linear operators $\mathcal{L}_1$ and $\mathcal{L}_2$ by*

$$\begin{aligned}\mathcal{L}_1(S) &= \frac{1}{2}(B^T AQS - (B^T AQS)^T), \quad S^T = -S \in \mathcal{R}^{k\times k},\\ \mathcal{L}_2(X) &= (AH)^T AHX + X\Lambda, \quad X \in \mathcal{R}^{(n-k)\times k},\end{aligned}$$

respectively. Then the spectrum of $\mathcal{L}$ is given by $\lambda(\mathcal{L}) = \lambda(\mathcal{L}_1) \cup \lambda(\mathcal{L}_2)$.

Proof. Let us denote by $\Phi_1, \cdots, \Phi_{N_1}$ a basis of $\mathcal{V}_1$ and $\Psi_1, \cdots, \Psi_{N_2}$ a basis of $\mathcal{V}_2$. We can write

$$\mathcal{L}(\Phi_j) = \sum_i \Phi_i \alpha_{ij}, \quad \mathcal{L}(\Psi_j) = \sum_i \Phi_i \gamma_{ij} + \sum_i \Psi_i \beta_{ij},$$

or equivalently in matrix form,

$$\mathcal{L}([\Phi_1, \cdots, \Phi_{N_1}, \Psi_1, \cdots, \Psi_{N_2}]) = [\Phi_1, \cdots, \Phi_{N_1}, \Psi_1, \cdots, \Psi_{N_2}] \begin{bmatrix} L_{11} & L_{12} \\ 0 & L_{22} \end{bmatrix},$$

where $L_{11} = (\alpha_{ij})$, $L_{12} = (\gamma_{ij})$, and $L_{22} = (\beta_{ij})$. Therefore the eigenvalues of $\mathcal{L}$ are given by the eigenvalues of L_{11} and L_{22}. Now we show that $\lambda(\mathcal{L}_i) = \lambda(L_{ii})$, $i = 1, 2$. To this end, writing $\Phi_i = [S_i^T,\, 0]^T$ and $\Psi_i = [0, X_i^T]^T$, we have

$$\mathcal{L}_1(S_j) = \sum_i S_i \alpha_{ij}, \quad \mathcal{L}_2(X_j) = [0,\, I]\mathcal{L}(\Psi_j) = \sum_i X_i \beta_{ij}.$$

If μ is an eigenvalue of L_{11}, and $s = (s_1, \cdots, s_{N_1})^T$ is the corresponding eigenvector, we denote $S = \sum_i S_i s_i$, and have

$$\begin{aligned}\mathcal{L}_1(S) &= \sum_j \mathcal{L}_1(S_j)s_j = \sum_j \sum_i S_i \alpha_{ij} s_j\\ &= \sum_i S_i(\sum_j \alpha_{ij} s_j) = \sum_i S_i \mu s_i = \mu S.\end{aligned}$$

One can also verify that eigenvalues of $\mathcal{L}_1$ are eigenvalues of L_{11}. The proof for the equivalence between the eigenvalue sets of $\mathcal{L}_2$ and of L_{22} is similar and is deleted here. □

Now we can show sufficient conditions for local optimal solutions to the unbalanced Procrustes problem.

Theorem 4.4. *Let Q be an orthonormal matrix and H the orthogonal complement of Q. Assume that $A^T AQ + Q\Lambda = A^T B$ holds for symmetric Λ. If $B^T AQ$ is positive definite and*

$$\sigma^2_{\min}(AH) + \lambda_{\min}(\Lambda) > 0, \tag{4.6}$$

then Q is an local optimal solution to (1.3).

Proof. By Lemma 4.2 and the discussions ahead of it, we only need to prove that both $\mathcal{L}_1$ and $\mathcal{L}_2$ are positive definite. First, for nonzero skew-symmetric matrix S,

$$\mathrm{tr}(S^T\mathcal{L}_1(S)) = \mathrm{tr}(S^TB^TAQS).$$

So the first condition that B^TAQ is positive definite implies that $\mathcal{L}_1$ is positive definite. Below we show that the positive definiteness of $\mathcal{L}_2$ follows from the second condition. To this end, let $\Lambda = U\mathrm{diag}(\lambda_1, \cdots, \lambda_k)U^T$ be the eigenvalue decomposition of Λ. Denote $W = XU$. If $X \neq 0$, then $W \neq 0$ and

$$\begin{aligned}
\mathrm{tr}(X^T\mathcal{L}_2(X)) &= \|AHX\|_F^2 + \mathrm{tr}(\Lambda X^TX) \\
&= \|AHW\|_F^2 + \mathrm{tr}(\mathrm{diag}(\lambda_1, \cdots, \lambda_k W^TW) \\
&= \sum_j (\|AHw_j\|^2 + \lambda_j\|w_j\|^2) \\
&\geq \sum_j (\sigma_{\min}^2(AH) + \lambda_j)\|w_j\|^2 > 0,
\end{aligned}$$

completing the proof. $\square$

The conditions (4.1) and (4.6) are quite similar to each other. Since $(AH)^T(AH)$ is a Rayleigh quotient of A^TA,

$$\sigma_{\min}^2(AH) = \lambda_{\min}((AH)^T(AH)) \geq \lambda_{\min}(A^TA) = \sigma_{\min}^2(A).$$

So condition (4.6) is weaker than (4.1). This is why Theorem 4.4 only guarantees a local minimum.

Finally, we propose sufficient conditions for multiple solutions to the problem (1.3).

Theorem 4.5. *Let Q^* be an optimal solution. $Q(t)$ ($t \in [0, 1]$) is the geodesic curve connecting $Q*$ and Q on the orthonormal Stiefel manifold such that $Q(0) = Q^*$ and $Q(1) = Q$. If for each $t \in [0, 1]$, the symmetric matrix $\Lambda(t) = (AQ(t))^T(B - AQ(t))$ satisfies*

$$A^TAQ(t) + Q(t)\Lambda(t) = A^TB, \tag{4.7}$$

then each $Q(t)$ is also an optimal solution.

Proof. For simplicity, we denote by $\dot{Q}(t)$ the component-wise derivative of the matrix $Q(t)$ with respect to t. Note that $Q(t)^TQ(t) = I$. Taking derivatives of the two sides of the equality with respect to t yields that

$$Q^T(t)\dot{Q}(t) + \dot{Q}^T(t)Q(t) = 0.$$

It implies that $Q^T(t)\dot{Q}(t)$ is skew-symmetric. We take the derivative again to the function $\phi(t) = \|AQ(t) - B\|_F^2$, and obtain that

$$\frac{d}{dt}\phi(t) = 2\mathrm{tr}(\dot{Q}(t)^TA^T(AQ(t) - B)) = -2\mathrm{tr}(\dot{Q}(t)^TQ(t)\Lambda(t)) = 0.$$

Therefore,

$$\|AQ(t) - B\|_F = \|AQ^* - B\|_F,$$

i.e., $Q(t)$ is also an optimal solution. $\square$

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