

DUAL ALGORITHMS FOR ORTHOGONAL PROCRUSTES ROTATIONS*

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Abstract. This paper considers a problem of rotating m matrices toward a best least-squares fit. The problem is known as the orthogonal Procrustes problem. For $m = 2$ the solution of this problem is known and can be given in a closed form using the singular value decomposition. It appears that the general case of $m > 2$ cannot be solved explicitly and an iterative procedure is required. The authors discuss a dual approach to the Procrustes problem where the maximal value of the objective function is approximated from above. This involves minimization of the sum of k largest eigenvalues of a symmetric matrix. It will be shown that under certain conditions ensuring differentiability of the obtained function at the minimum, this method gives the global solution of the Procrustes problem.

Key words. orthogonal rotation, best least-squares fit, singular value decomposition, least upper bound, eigenvalues, nonsmooth optimization

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1. Introduction. In this paper we consider the problem of rotating m matrices towards a best least-squares fit. Let $A_i, i = 1, \dots, m$, be a family of $n \times k$ matrices. Then it is necessary to find orthogonal $k \times k$ matrices $Y_i, i = 1, \dots, m$, for which the function

$$f(Y_1, \dots, Y_m) = \sum_{i < j} \text{tr} (A_i Y_i - A_j Y_j)^T (A_i Y_i - A_j Y_j)$$

is minimized, or equivalently, for which the function

$$g(Y_1, \dots, Y_m) = \sum_{i < j} \text{tr} Y_i^T A_i^T A_j Y_j$$

is maximized. The problem has been discussed extensively in the psychometric literature and is known as the orthogonal Procrustes problem (see [2], [4], [8]–[10], and references therein). For $m = 2$ the solution is known and can be given in a closed form using the singular value decomposition of the matrix $A_1^T A_2$ (von Neumann [11]). That is, let $A_1^T A_2 = PDQ^T$, where P and Q are orthogonal matrices and D is a nonnegative definite diagonal matrix. Then $Y_1 = P$ and $Y_2 = Q$ solves the problem. It appears that the general case of $m > 2$ cannot be solved explicitly and an iterative procedure is required. A numerical algorithm employing singular value decompositions successively was proposed in Ten Berge [9]. It can be shown that this algorithm converges, but there is no guarantee that the calculated stationary point corresponds to the global optimum. Therefore various upper bounds for the maximum of the objective function g have been introduced [9].

We consider a dual approach to the Procrustes problem where the maximal value of the function g is approximated from above. The corresponding algorithm involves minimization of the sum of k largest eigenvalues of a symmetric matrix considered as a function of some elements of this matrix. The objective function is then convex, but is not necessarily differentiable. It will be shown that under conditions ensuring differentiability of the objective function at the minimum, this algorithm gives the global solution of the Procrustes problem.

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2. Upper bounds. In this section we discuss some upper bounds for the maximal value of the function g . Consider the $k \times k$ matrices $S_{ij} = A_i^T A_j$ and let $S_{ij} = P_{ij} D_{ij} Q_{ij}^T$ be their singular value decompositions. Then

$$(1) \quad d^* = \sum_{i < j} \text{tr } D_{ij}$$

gives an upper bound for the maximum of $g(Y_1, \dots, Y_m)$ with respect to orthogonal matrices Y_1, \dots, Y_m [9, p. 273]. We consider another upper bound for the maximum of g . Let

$$S(X) = \begin{bmatrix} X_1 & S_{12} & \cdots & S_{1m} \\ S_{21} & X_2 & \cdots & S_{2m} \\ \dots & \dots & \dots & \dots \\ S_{m1} & S_{m2} & \cdots & X_m \end{bmatrix}$$

be the $mk \times mk$ symmetric matrix considered as a function of the symmetric block diagonal matrix $X = \text{diag}(X_1, \dots, X_m)$. Denote by $\lambda_1(X) \geq \dots \geq \lambda_{mk}(X)$ the eigenvalues of $S(X)$. Then the following result holds.

THEOREM 1. *For every X the number*

$$(2) \quad l(X) = \frac{1}{2} \left[m \sum_{i=1}^k \lambda_i(X) - \text{tr } S(X) \right]$$

gives an upper bound for the maximum of g .

Proof. The sum of k largest eigenvalues of the symmetric matrix $S(X)$ can be represented in the form (Ky Fan [5])

$$(3) \quad \lambda_1(X) + \dots + \lambda_k(X) = \max_Z \text{tr } Z^T S(X) Z,$$

where the maximum in the right-hand side of (3) is taken over all $mk \times k$ matrices Z such that $Z^T Z = I_k$. (I_k denotes the $k \times k$ identity matrix.) Now let Y_1, \dots, Y_m be a set of orthogonal matrices and consider the corresponding $mk \times k$ matrix $Y = (Y_1^T, \dots, Y_m^T)^T$. Then $Y^T Y = m I_k$, and hence it follows from (3) that

$$m \sum_{i=1}^k \lambda_i(X) \geq \text{tr } Y^T S(X) Y.$$

Moreover,

$$\text{tr } Y^T S(X) Y = 2 \sum_{i < j} \text{tr } Y_i^T S_{ij} Y_j + \sum_{i=1}^m \text{tr } X_i,$$

and hence

$$g(Y_1, \dots, Y_m) \leq l(X).$$

Since the orthogonal matrices Y_1, \dots, Y_m are arbitrary, this completes the proof. \square

It is natural now to minimize the function $l(X)$. We show in the next theorem that the obtained upper bound is always better than the upper bound given in (1).

THEOREM 2. *Let d^* be the upper bound given by the right-hand side of (1). Then*

$$(4) \quad d^* \geq \inf l(X).$$

Proof. Let $P_{ij}D_{ij}Q_{ij}^T$ be singular value decompositions of the matrices S_{ij} . Consider the symmetric matrices

$$(5) \quad X_i^* = - \sum_{\substack{j=1 \\ j \neq i}}^m P_{ij}D_{ij}P_{ij}^T,$$

$i = 1, \dots, m$. We show that

$$(6) \quad d^* \geq l(X^*).$$

First we observe that

$$\text{tr } S(X^*) = - \sum_{i \neq j} \text{tr } D_{ij}.$$

Therefore in order to prove (6) it will be sufficient to show that the matrix $S(X^*)$ is nonpositive definite, i.e., $\lambda_1(X^*) \leq 0$, and hence $\lambda_1(X^*) + \dots + \lambda_k(X^*) \leq 0$. Consider vectors $y_1, \dots, y_m \in \mathbb{R}^k$. For any two vectors $a, b \in \mathbb{R}^k$ we have that

$$2a^Tb \leq a^T a + b^T b,$$

and hence, by taking $a = D_{ij}^{1/2} P_{ij}^T y_i$ and $b = D_{ij}^{1/2} Q_{ij}^T y_j$, we obtain

$$y_i^T P_{ij} D_{ij} Q_{ij}^T y_j \leq \frac{1}{2} (y_i^T P_{ij} D_{ij} P_{ij}^T y_i + y_j^T Q_{ij} D_{ij} Q_{ij}^T y_j).$$

Now form the $mk \times 1$ vector $y = (y_1^T, \dots, y_m^T)^T$. It then follows that

$$\begin{aligned} y^T S(X^*) y &= \sum_{i \neq j} y_i^T S_{ij} y_j + \sum_{i=1}^m y_i^T X_i^* y_i \\ &\leq \frac{1}{2} \sum_{i \neq j} y_i^T P_{ij} D_{ij} P_{ij}^T y_i + \frac{1}{2} \sum_{i \neq j} y_j^T Q_{ij} D_{ij} Q_{ij}^T y_j + \sum_{i=1}^m y_i^T X_i^* y_i. \end{aligned}$$

Moreover, since $S_{ij}^T = S_{ji}$ we have that $Q_{ij} D_{ij} P_{ij}^T = P_{ji} D_{ji} Q_{ji}^T$, and hence we can choose $Q_{ij} = P_{ji}$. Therefore

$$\begin{aligned} y^T S(X^*) y &\leq \sum_{i \neq j} y_i^T P_{ij} D_{ij} P_{ij}^T y_i + \sum_i y_i^T X_i^* y_i \\ &= \sum_{i \neq j} y_i^T P_{ij} D_{ij} P_{ij}^T y_i - \sum_i y_i^T \left(\sum_{j \neq i} P_{ij} D_{ij} P_{ij}^T \right) y_i = 0. \end{aligned}$$

Since vector y is arbitrary this proves that the matrix $S(X^*)$ is nonpositive definite, and hence the inequality (6) follows. Clearly (6) implies (4) and the proof is complete. \square

Notice that the proof of Theorem 2 is constructive. Inequality (6) suggests X^* as a good starting point in minimization of the function $l(X)$. It was found in extensive numerical experimentations that this choice of the starting point is indeed a very good one.

Now we discuss some properties of the function $l(X)$. First we observe that it follows from the max-representation (3) that the sum $\sum_{i=1}^k \lambda_i(X)$, and hence the function $l(X)$, are convex. Using this max-representation it is also possible to calculate the subdifferential of $l(X)$ (cf. [1, Lemma 4.4]). For our purposes the following result will be particularly useful. Consider a block diagonal matrix X_0 and let $E = [e_1, \dots, e_k]$ be an $mk \times k$ matrix whose columns e_1, \dots, e_k form a set of orthonormal eigenvectors of $S(X_0)$ corresponding to the eigenvalues $\lambda_1(X_0), \dots, \lambda_k(X_0)$, respectively. We denote $\text{diag}_X(EE^T)$

the block diagonal submatrix of EE^T corresponding to the block diagonal elements of X .

THEOREM 3. *The function $l(X)$ is the differentiable at X_0 if and only if $\lambda_k(X_0)$ is strictly greater than $\lambda_{k+1}(X_0)$. In the last case the gradient of l at X_0 is given by*

$$(7) \quad \nabla l(X_0) = \frac{1}{2} \{m \operatorname{diag}_X (EE^T) - I_{mk}\}.$$

Proof. Consider the max-representation (3). The function $\operatorname{tr} Z^T S(X) Z$ is linear in X and its gradient is given by $\operatorname{diag}_X (ZZ^T)$. Then it follows from a theorem of Danskin [3] that the subdifferential $\partial h(X)$ of the (convex) function $h(X) = \lambda_1(X) + \dots + \lambda_k(X)$ is the convex hull of block diagonal matrices $\operatorname{diag}_X (ZZ^T)$ taken over all maximizers in the right-hand side of (3) (see Rockafellar [7, § 23] for the definition and basic properties of subdifferentials). Notice that a matrix Z is such a maximizer if and only if its columns form a set of orthonormal eigenvectors of $S(X)$ corresponding to k largest eigenvalues. It follows that the subdifferential $\partial h(X_0)$ is a singleton if and only if

$$(8) \quad \lambda_k(X_0) > \lambda_{k+1}(X_0).$$

Therefore the function $h(X)$ and then $l(X)$ are differentiable at X_0 if and only if (8) holds. In the last case (7) follows. \square

Now let X_0 be a minimizer of $l(X)$ and consider the partition

$$E = [E_1^T, \dots, E_m^T]^T,$$

E_i are $k \times k$, of the associated matrix E . Suppose that (8) holds. Then the gradient $\nabla l(X_0)$ is zero, and hence it follows from (7) that

$$m \operatorname{diag}_X (EE^T) = I_{mk}.$$

This implies that $mE_i E_i^T = I_k$, and hence

$$(9) \quad Y_i = m^{1/2} E_i, \quad i = 1, \dots, m$$

are orthogonal matrices. Moreover, the proof of Theorem 1 shows that in this case the orthogonal matrices Y_i given in (9) maximize the function g . We obtain that the dual problem of minimization of the function $l(X)$ not only provides an upper bound but actually solves the primary Procrustes problem if the corresponding minimizer X_0 satisfies (8).

3. Numerical experimentations. The main difficulty in numerical minimization of the function $l(X)$ is that it is not everywhere differentiable. Although considerable attention has been attracted to minimization of nondifferentiable convex functions, the developed algorithms are quite complicated and, what is more important, are slow to converge (cf. Cullum, Donath, and Wolfe [1]). In any case we are really interested in situations where the objective function $l(X)$ is differentiable at the minimum and consequently the dual problem provides a solution for the primary problem. Therefore some standard “differentiable” approaches have been applied. The point X^* , given in (5), proved to be a very good starting point. In fact, in many cases the gradient $\nabla l(X^*)$ was closed to zero so that the eigenvectors of $S(X^*)$, via formula (9), gave numerically acceptable solutions for the Procrustes problem.

A number of experiments were performed for various choices of m , n , and k . We briefly discuss two, namely $(m, n, k) = (8, 3, 3)$ and $(5, 4, 4)$. Denote by g_0 the maximal value of the function g as obtained by the Ten Berge algorithm proposed in [9] and by l_0 the minimal value of l as obtained by a slightly modified Newton method we will discuss later.

For each choice of (m, n, k) we generated ten sets, each containing m matrices A_1, \dots, A_m . The entries of each A_i consisted of uniformly and independently distributed random numbers between -1 and 1 . We first tried to minimize l by using the conjugate gradient algorithm. This turned out to be rather unsatisfactory since the convergence was slow, and in some cases it was not even achieved after 100 iterations.

Then the Newton method was tried. Notice that for computational purposes, the symmetry of X should be kept in mind. Therefore the function $l(X)$ was considered as a function of the $mk(k + 1)/2 \times 1$ vector $x = (\text{vecs}^T X_1, \dots, \text{vecs}^T X_m)^T$, where $\text{vecs} X_i$ stands for the $k(k + 1)/2 \times 1$ symmetric mode vector representation of X_i . We denote by x_{ij} the entry of x corresponding to the (i, j) element of X . It follows that $\partial l / \partial x_{ii} = [\nabla l(X)]_{ii}$ and $\partial l / \partial x_{ij} = 2[\nabla l(X)]_{ij}$ when $i \neq j$. Here $\nabla l(X)$ is the gradient of l as it is given in (7). Now let $\{e_1, \dots, e_{km}\}$ be a set of orthonormal eigenvectors of $S(X)$ corresponding to the eigenvalues $\lambda_1(X), \dots, \lambda_{km}(X)$. Denote e_{ij} the i th entry of e_j . Then if we assume $\lambda_k(X) \neq \lambda_{k+1}(X)$ and let

$$a_{st,uv} = m \sum_{i=1}^k \sum_{j=k+1}^{km} (\lambda_i(X) - \lambda_j(X))^{-1} e_{si} e_{tj} e_{ui} e_{vj},$$

the elements of the $mk(k + 1)/2 \times mk(k + 1)/2$ Hessian matrix $H(X)$ of l at X can be shown to be

$$\frac{\partial^2 l}{\partial x_{st} \partial x_{uv}} = \begin{cases} a_{st,uv}, & s = t, \quad u = v, \\ a_{st,uv} + a_{ts,uv}, & s \neq t, \quad u = v, \\ a_{st,uv} + a_{st,vu}, & s = t, \quad u \neq v, \\ a_{st,uv} + a_{st,vu} + a_{ts,uv} + a_{ts,vu}, & s \neq t, \quad u \neq v \end{cases}$$

(cf. Lancaster [6]).

For each set of matrices A_1, \dots, A_m the value g_0 was calculated. Then the Newton algorithm for minimization of $l(X)$ was implemented with X^* , defined in Theorem 2, taken as the starting point. Notice that the Hessian matrix $H(X)$ is always *singular*. Therefore it was stabilized at each iteration by adding $\epsilon = 0.1$ along its diagonal. After each iteration the new value of l was verified in order to see if it was less than the previous one. If not, a line search was performed along the direction $-H^{-1}(X)\nabla l(X)$. This became especially necessary after a number of iterations, when in some cases the k th and $(k + 1)$ th eigenvalues tend to converge to a common value. Convergence of the first algorithm was assumed when the difference between consecutive values of g was less than 0.0001. The difference value 0.01 was taken for the second. A point to which the Newton algorithm converged is denoted by X_0 , i.e., $l_0 = l(X_0)$.

Tables 1 and 2 sum up the results obtained.

From these results the following observations are made:

(1) The point X^* seems to be a good starting point and $l(X^*)$ is a good approximation for l_0 and g_0 .

(2) Whenever the difference $\lambda_k(X_0) - \lambda_{k+1}(X_0)$ is greater than about 0.1, the Newton algorithm converges in a few iterations and the corresponding value of $l_0 - g_0$ is very small. This suggests that the Ten Berge algorithm also converges in each such case to the global maximum of g .

(3) The k th and $(k + 1)$ th eigenvalues frequently converge to a common value, in which case the function l is not differentiable at the corresponding point X_0 . Despite this the obtained upper bound l_0 is still a very good one.

(4) For all the data we generated the Ten Berge algorithm seemed to converge to the global maximum of g . This is rather surprising, since the corresponding problem is not a convex one and only certain stationarity of the calculated point is ensured by the

TABLE 1
Case $(m, n, k) = (8, 3, 3)$.

g_0	l_0	$l(X^*)$	$l_0 - g_0$	$l(X^*) - l_0$	$\lambda_k(X_0) - \lambda_{k+1}(X_0)$
83.074	83.072	83.095	-0.002	0.023	0.526136
71.997	71.996	72.126	-0.001	0.130	1.098260
63.835	63.864	64.079	0.029	0.215	0.000105
64.790	64.845	65.078	0.055	0.233	0.000706
64.102	64.102	64.837	0.000	0.735	0.000021
66.012	66.013	66.140	0.001	0.126	1.046920
65.310	65.317	65.670	0.007	0.353	0.000066
61.931	62.186	62.911	0.255	0.724	0.000061
73.106	73.346	73.829	0.240	0.483	0.000116
58.036	58.035	58.341	0.001	0.306	0.336850

TABLE 2
Case $(m, n, k) = (5, 4, 4)$.

g_0	l_0	$l(X^*)$	$l_0 - g_0$	$l(X^*) - l_0$	$\lambda_k(X_0) - \lambda_{k+1}(X_0)$
51.020	51.020	51.069	0.000	0.049	0.238905
46.016	46.078	46.199	0.061	0.121	0.000088
37.538	37.565	38.098	0.027	0.533	0.000109
44.478	44.524	44.708	0.047	0.183	0.000085
40.082	40.195	40.413	0.114	0.217	0.000115
36.503	36.546	36.880	0.044	0.333	0.000014
40.044	40.082	40.217	0.038	0.134	0.000964
45.232	45.428	45.942	0.196	0.514	0.000342
36.439	36.456	36.616	0.017	0.159	0.000986
45.284	45.436	46.623	0.152	1.187	0.002255

general theory. Whenever the difference $l_0 - g_0$ became reasonably significant, the difference $\lambda_k(X_0) - \lambda_{k+1}(X_0)$ was invariably very small and the Newton method did not converge.

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