NASA CR-
151235

DEPARTMENT OF MATHEMATICS
UNIVERSITY OF HOUSTON HOUSTON, TEXAS

(NASA-CR-151235) THE ROLE OF EIGENVALUES IN LINEAR FEATURE SELECTION THEORY (Houston Univ.) 19 p HC A02/MF A01 CSCL 12A

N77-19808

Unclas
G3/64 20571

THE ROLE OF EIGENVALUES IN
LINEAR FEATURE SELECTION THEORY
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REPORT #61 DECEMBER 1976

PREPARED FOR
EARTH OBSERVATION DIVISION, JSC
UNDER
CONTRACT NAS-9-15000

HOUSTON, TEXAS 77004

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December, 1976
Report 61
NAS-9-15000

The Role of Eigenvalues in Linear Feature Selection Theory

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Introduction. Recent statistical work in feature selection for the multivariate normal pattern recognition problem has concentrated on linearly transforming pattern classes so that the transformed pattern classes are equivalently distinguishable. Since, in general, this is not possible, techniques have been developed to preserve the distinction of the transformed pattern classes using various measures of distinction. These measures of pattern class distinction are most often treated as eigenvalue problems ([1], [2], [5], [6], [7], [9], [13], [14], [15]). In this paper we consider a particular measure of pattern class distinction called the average interclass divergence, or more simply, divergence, ([1], [2], [4], [6], [7], [8], [9], [10], [11]), where divergence will be the pairwise average of the expected interclass divergence derived from Hajek's two-class divergence as defined, for example, in [9].

This work was supported in part by NASA under Contract JSC-NAS-15000.

It has been shown in [4] that there always exists a $k \times n$ real matrix B such that the transformation determined by B maximizes divergence in k-dimensional space, and, in fact, that B can be written in the form $(I_k | Z)U$, where U is an orthogonal $n \times n$ matrix. We will investigate the role of the eigenvalues of U in such problems, and give an example demonstrating that the divergence measure of pattern class distinction does not depend on these eigenvalues (Theorem 7).

Our example is derived from the family of examples constructed in [3]. This special class of examples permits analytical calculation of divergence, a task ordinarily eschewed as unrealistic, and yields a precise expression for divergence. The reader is cautioned, however, not to confuse the numerical simplicity of this example with impracticality, since, mathematically, the failure of the eigenvalues of U to affect divergence in the restricted case erases any hope that they might be meaningful in an arbitrary case, however applied.

1. Special divergence formulas. Let $\Omega_1, \ldots, \Omega_m$ and $\mu_1, \ldots, \mu_m$ be the covariance matrices and means for m classes, where for each $i = 1, \ldots, m$, Ω_i is an $n \times n$ positive definite matrix and μ_i is a column n vector. Let

$$S_i = \Sigma_{\substack{j=1 \\ j \neq i}}^{m} (\Omega_j + \delta_{ij}\delta_{ij}^T), \text{ where } \delta_{ij} = \mu_i - \mu_j .$$

Then, assuming equal a priori probabilities, the average interclass divergence for these m classes is given by

$$D = \tfrac{1}{2}\,\mathrm{tr}\left(\sum_{i=1}^{m} \Omega_i^{-1} S_i\right) - \tfrac{1}{2}\, m(m-1)n \tag{1}$$

while, if B is a $k \times n$ matrix, the B-average interclass divergence is

$$D_B = \tfrac{1}{2}\,\mathrm{tr}\left(\sum_{i=1}^{m} (B\Omega_i B^T)^{-1}(BS_i B^T)\right) - \tfrac{1}{2}\, m(m-1)k \tag{2}$$

where tr represents the trace function.

Moreover, as observed in [3], if

$$\mathcal{G} = \{B \in M_{kn}\colon BB^T = I_k \text{ and } (B^TB)\Omega_i = \Omega_i(B^TB),\ i = 1,\ldots,m\}\ ,$$

where I_k is the $k \times k$ identity matrix and M_{kn} is the set of all $k \times n$ real matrices, then, for any $B \in \mathcal{G}$, (2) may be rewritten as

$$D_B = \tfrac{1}{2}\,\mathrm{tr}\left(B\left(\sum_{i=1}^{m} \Omega_i^{-1} S_i\right)B^T\right) - \tfrac{1}{2}\, m(m-1)k \tag{3}$$

For the remainder of the paper we assume that each Ω_i is a diagonal matrix of the form: $\begin{pmatrix} x_i & \\ & I_{n-1} \end{pmatrix}$, where x_i is a positive real number, and $\mu_i = \mu_j$ for all i,j. Under these restrictions, $\sum_{i=1}^{m} \Omega_i^{-1} S_i$ is a diagonal matrix of the form $\begin{pmatrix} x & \\ & pI_{n-1} \end{pmatrix}$, where

$x = \sum_{i=1}^{m} \frac{1}{x_i}\left(\sum_{\substack{j=1 \\ j\neq i}}^{m} x_j\right)$ and $p = m(m-1)$. It follows from (1) that the average interclass divergence for the m classes is given by

$$D = \tfrac{1}{2}(x - p) \tag{4}$$

As observed in the introduction, in seeking to maximize the B-average interclass divergence D_B, it suffices to consider those $k \times n$ matrices of the form $(I_k|Z)U$, where U is an $n \times n$ orthogonal matrix. In the sequel, when considering D_B, we shall always assume that B is of this form. For any such $k \times n$ matrix B, it is obvious that $BB^T = I_k$, and hence $B \in \mathcal{C}$ if and only if $(B^TB)\Omega_i = \Omega_i(B^TB)$ for $i = 1,\ldots,m$. We will derive necessary and sufficient conditions in order that $B \in \mathcal{C}$ (Theorem 2), but first we calculate D_B in the case that formula (3) is valid. Recall that all means are hereafter considered equal and all covariance matrices diagonal of the form stated above.

Theorem 1. Let $B = (I_k|Z)U$, where $U = (u_{ij})$ is an $n \times n$ orthogonal matrix, and suppose D_B is given as in (3) above. Then

$$D_B = (\sum_{i=1}^{k} u_{i1}^2)D \tag{5}$$

Proof: Since $tr(XY) = tr(YX)$ whenever both products are defined, we have in this case $D_B = \frac{1}{2}\, tr(B^TB(\sum_{i=1}^{m} \Omega_i^{-1} S_i)) - \frac{1}{2}\, pk$. If U is written in block form, $U = \begin{pmatrix} A & C \\ E & F \end{pmatrix}$, where A is $k \times k$, then

$B^TB = U^T(I_k|Z)^T(I_k|Z)U = \begin{pmatrix} A^TA & A^TC \\ C^TA & C^TC \end{pmatrix}$. Since $\sum_{i=1}^{m} \Omega_i^{-1} S_i = \begin{pmatrix} x & \\ & pI_{n-1} \end{pmatrix}$ = $p\cdot\begin{pmatrix} \frac{x}{p} & \\ & I_{n-1} \end{pmatrix} = p\begin{pmatrix} M & \\ & I_{n-k} \end{pmatrix}$, where M is the $k \times k$ matrix $\begin{pmatrix} \frac{x}{p} & \\ & I_{k-1} \end{pmatrix}$,

then $B^TB(\sum_{i=1}^{m} \Omega_i^{-1} S_i) = p\cdot\begin{pmatrix} A^TAM & A^TC \\ C^TAM & C^TC \end{pmatrix}$. Therefore, $tr(B^TB(\sum_{i=1}^{m} \Omega_i^{-1} S_i)) =$ $p(tr(A^TAM) + tr(C^TC)) = p((\sum_{j=1}^{k} u_{j1}^2)\frac{x}{p} + \sum_{q=2}^{k} (\sum_{j=1}^{k} u_{jq}^2) + \sum_{q=k+1}^{n} (\sum_{j=1}^{k} u_{jq}^2)) =$ $(\sum_{j=1}^{k} u_{j1}^2)x + p(\sum_{q=2}^{n} (\sum_{j=1}^{k} u_{jq}^2))$. Since U is orthogonal, $\sum_{q=2}^{n} (\sum_{j=1}^{k} u_{jq}^2) =$

$\sum_{j=1}^{k} (1 - u_{j1}^2) = k - \sum_{j=1}^{k} u_{j1}^2$, so that $D_B = \frac{1}{2}((\sum_{j=1}^{k} u_{j1}^2)x + p(k - \sum_{j=1}^{k} u_{j1}^2)) - \frac{1}{2} pk =$

$(\sum_{j=1}^{k} u_{j1}^2)(\frac{x-p}{2}) = (\sum_{j=1}^{k} u_{j1}^2)D$.

Our next result gives necessary and sufficient conditions in order that $B = (I_k|Z)U \in \mathcal{C}$. While the proof is rather tedious, these conditions are particularly easy to apply and hence useful in seeking examples.

<u>Theorem 2</u>. Let $B = (I_k|Z)U$, where $U = (u_{ij})$ is an $n \times n$ orthogonal matrix. If, for each $i = 1,\ldots,m$, $\Omega_i = \begin{pmatrix} x_i & \\ & I_{n-1} \end{pmatrix}$, then:

(1) if $x_i = 1$ for all i, then $B \in \mathcal{C}$;

(2) if $x_i \neq 1$ for at least one i, then $B \in \mathcal{C}$ if and only if $\sum_{j=1}^{k} u_{j1}^2 = 1$ or $\sum_{j=1}^{k} u_{j1}^2 = 0$.

<u>Proof</u>: If $x_i = 1$, then $\Omega_i = I_n$ and $(B^TB)\Omega_i = \Omega_i(B^TB)$ for any $k \times n$ matrix B. Thus, if $x_i = 1$ for all i, then $B \in \mathcal{C}$ for any $k \times n$ matrix of the form $(I_k|Z)U$. We suppose that $x_i \neq 1$ for at least one i. As in the proof of Theorem 1, we decompose U into the block form $\begin{pmatrix} A & C \\ E & F \end{pmatrix}$, so that $B^TB = \begin{pmatrix} A^TA & A^TC \\ C^TA & C^TC \end{pmatrix}$, where A is again $k \times k$. For a fixed i such that $x_i \neq 1$, write Ω_i in block form $\begin{pmatrix} G_i & \\ & I_{n-k} \end{pmatrix}$, where G_i is the $k \times k$ matrix $\begin{pmatrix} x_i & \\ & I_{k-1} \end{pmatrix}$. Then $(B^TB)\Omega_i = \begin{pmatrix} A^TAG_i & A^TC \\ C^TAG_i & C^TC \end{pmatrix}$, while $\Omega_i(B^TB) = \begin{pmatrix} G_iA^TA & G_iA^TC \\ C^TA & C^TC \end{pmatrix}$. Thus, B^TB commutes with Ω_i if and only if

(1) $A^TAG_i = G_iA^TA$ and (2) $C^TAG_i = C^TA$. We write A^TA and C^TA in block form: $A^TA = \begin{pmatrix} L & M \\ N & W \end{pmatrix}$, $C^TA = \begin{pmatrix} P & Q \\ R & S \end{pmatrix}$, where L and P are 1×1. Since A^TA is symmetric, $N = M^T$. Therefore, $A^TAG_i = \begin{pmatrix} Lx_i & M \\ M^Tx_i & W \end{pmatrix}$,

and $G_iA^TA = \begin{pmatrix} x_iL & x_iM \\ M^T & W \end{pmatrix}$. Thus $A^TAG_i = G_iA^TA$ if and only if $M = x_iM$ and similarly, $C^TAG_i = C^TA$ if and only if $Px_i = P$ and $Rx_i = R$. Since

$M = (\sum_{j=1}^{k} u_{j1}u_{j2}, \ldots, \sum_{j=1}^{k} u_{j1}u_{jk})$ and $\begin{pmatrix} P \\ R \end{pmatrix} = \begin{pmatrix} \sum_{j=1}^{k} u_{jk+1}u_{j1} \\ \vdots \\ \sum_{j=1}^{k} u_{jn}u_{j1} \end{pmatrix}$, it

follows that $Mx_i = M$, $Px_i = P$, and $Rx_i = R$ if and only if $x_i(\sum_{j=1}^{k} u_{j1}u_{jq} = \sum_{j=1}^{k} u_{j1}u_{jq}$ for $q = 2,\ldots,n$. Thus, since $x_i \neq 1$, we have that $(B^TB)\Omega_i = \Omega_i(B^TB)$ if and only if $\sum_{j=1}^{k} u_{j1}u_{jq} = 0$ for $q = 2,\ldots,n$. Since the above argument is valid for any Ω_i for which $x_i \neq 1$, and since B^TB commutes with Ω_i for any i for which $x_i = 1$, it follows that $B \in \mathcal{G}$ if and only if $\sum_{j=1}^{k} u_{j1}u_{jq} = 0$ for $q = 2,\ldots,n$. We next show that $\sum_{j=1}^{k} u_{j1}u_{jq} = 0$ for $q = 2,\ldots,n$ if and only if $\sum_{j=1}^{k} u_{j1}^2 = 1$ or $\sum_{j=1}^{k} u_{j1}^2 = 0$. Since U is orthogonal, $\sum_{j=1}^{n} u_{j1}u_{jq} = \sum_{j=1}^{k} u_{j1}u_{jq} + \sum_{j=k+1}^{n} u_{j1}u_{jq} = 0$ for $q = 2,\ldots,n$, while $1 = \sum_{j=1}^{n} u_{j1}^2 = \sum_{j=1}^{k} u_{j1}^2 + \sum_{j=k+1}^{n} u_{j1}^2$. Thus, if $\sum_{j=1}^{k} u_{j1}^2 = 1$, then $u_{j1} = 0$ for $j = k+1,\ldots,n$, and $\sum_{j=1}^{n} u_{j1}u_{jq} = \sum_{j=1}^{k} u_{j1}u_{jq} = 0$ for $q = 2,\ldots,n$. If $\sum_{j=1}^{k} u_{j1}^2 = 0$, then $u_{j1} = 0$ for $j = 1,\ldots,k$ and, obviously $\sum_{j=1}^{k} u_{j1}u_{jq} = 0$ for $q = 2,\ldots,n$.

Conversely, suppose that $\sum_{j=1}^{k} u_{j1}u_{jq} = 0$ for $q = 2,\dots,n$. If $u_{11} = \dots = u_{k1} = 0$, then $\sum_{j=1}^{k} u_{j1}^2 = 0$ and the proof is complete. Otherwise, let u_{r1} be the first non-zero element in the first column of U, where $r \le k$. Then $0 = \sum_{j=1}^{k} u_{j1}u_{jq} = u_{r1}u_{rq} + \sum_{j=r+1}^{k} u_{j1}u_{jq}$, so that $u_{rq} = \frac{-1}{u_{r1}} \left(\sum_{j=r+1}^{k} u_{j1}u_{jq}\right)$ for $q = 2,\dots,n$. Thus, if $u_{r+1\,1},\dots,u_{k1} = 0$, then $u_{rq} = 0$ for $q = 2,\dots,n$ and it follows that $1 = u_{r1}^2 = \sum_{j=1}^{k} u_{j1}^2$. Suppose $u_{w1} \neq 0$ where $r < w \le k$. Since $u_{r1}u_{w1} + \sum_{q=2}^{n} u_{wq}u_{rq} = 0$, then substituting for u_{rq}, $q \ge 2$, we have

$$u_{r1}u_{w1} + \sum_{q=2}^{n} u_{wq}\left(\frac{-1}{u_{r1}} \sum_{j=r+1}^{k} u_{j1}u_{jq}\right) = u_{r1}u_{w1} + \left(\frac{-1}{u_{r1}}\right) \sum_{j=r+1}^{k} u_{j1}\left(\sum_{q=2}^{n} u_{wq}u_{jq}\right) = 0 \quad (6)$$

Since U is orthogonal, then for $j \neq w$, $\sum_{q=2}^{n} u_{wq}u_{jq} = -u_{w1}u_{j1}$ and for $j = w$, $\sum_{q=2}^{n} u_{wq}u_{jq} = \sum_{q=2}^{n} u_{wq}^2 = 1 - u_{w1}^2$. It follows that $\sum_{j=r+1}^{k} u_{j1}\left(\sum_{q=2}^{n} u_{wq}u_{jq}\right) = u_{w1}\left(\sum_{j=r+1}^{k} (-u_{j1}^2)\right) + u_{w1}$, and, substituting in (6), we have $u_{w1}\left(u_{r1} + \left(\frac{-1}{u_{r1}}\right)\left(\sum_{j=r+1}^{k}(-u_{j1}^2)\right) + \left(\frac{-1}{u_{r1}}\right)\right) = 0$. Multiplying by u_{r1}, we have $u_{w1}\left(u_{r1}^2 + \sum_{j=r+1}^{k} u_{j1}^2 - 1\right) = u_{w1}\left(\sum_{j=r}^{k} u_{j1}^2 - 1\right) = 0$. Since $u_{w1} \neq 0$, it now follows that $1 = \sum_{j=r}^{k} u_{j1}^2 = \sum_{j=1}^{k} u_{j1}^2$.

We note that, if there exists at least one Ω_j which is not the identity matrix I_n, then the proof of Theorem 2 shows that B^TB commutes with all Ω_i's if and only if B^TB commutes with Ω_j. Moreover, in this case, the elements of $\mathcal{G}$ are precisely those $B = (I_k|Z)U$ for which the first column of

U is of the form $\begin{pmatrix} u_{11} \\ \vdots \\ u_{k1} \\ 0 \\ \vdots \\ 0 \end{pmatrix}$ or $\begin{pmatrix} 0 \\ \vdots \\ u_{k+11} \\ \vdots \\ u_{n1} \end{pmatrix}$.

Hence, by Theorem 1, if $B \in \mathcal{G}$, then $D_B = D$ or $D_B = 0$. (Note that if $\Omega_i = I_n$ for all i, then $D = 0$.)

We close this section with a definition. If V denotes the set of all $n \times n$ orthogonal matrices, let $\mathcal{S} = \{U = (u_{ij}) \in V : \sum_{j=1}^{k} u_{j1}^2 = 1 \text{ or } 0\}$. Thus, if there exists $\Omega_j \neq I_n$, then $B = (I_k|Z)U \in \mathcal{G}$ if and only if $U \in \mathcal{S}$.

2. Eigenvalues of U . Let $U = (u_{ij})$ be an $n \times n$ orthogonal matrix. As is well known, [12] , the eigenvalues of U lie on the unit circle in the complex plane and non-real eigenvalues occur in conjugate pairs. Thus, if U has a real eigenvalue λ, then $\lambda = \pm 1$, and, if $\mu = a + bi$, $b \neq 0$ is an eigenvalue of U, then $\overline{\mu} = a - bi$ is also an eigenvalue of U . Clearly, $\det U = \pm 1$. Moreover, if 1 has multiplicity p as an eigenvalue of U, -1 multiplicity m, and $\{a_j + b_j i, a_j - b_j i\}_{j=1}^{q}$ $(b_j \neq 0)$ are the remaining eigenvalues of U, then U is similar to a block diagonal orthogonal matrix PUP^{-1} of the form:

$$PUP^{-1} = \begin{pmatrix} \Lambda_1 & & & & & & \\ & \ddots & & & & & \\ & & \Lambda_q & & & & \\ & & & 1 & & & \\ & & & & \ddots & & \\ & & & & & 1 & \\ & & & & & & -1 \\ & & & & & & & \ddots \\ & & & & & & & & -1 \end{pmatrix} \qquad (7)$$

where 1 appears on the diagonal p times, -1 appears m times, and each $A_j = \begin{pmatrix} a_j & b_j \\ -b_j & a_j \end{pmatrix}$ is a 2×2 orthogonal matrix with eigenvalues $a_j + b_j i$, $a_j - b_j i$. Furthermore, the order in which the A_j's, 1's, and -1's appear on the diagonal can be changed to any desired order by a similarity transformation. Thus, any two orthogonal $n \times n$ matrices with the same set of eigenvalues are similar. Finally, we observe that if U is a 2×2 orthogonal matrix, then $U = \begin{pmatrix} c & d \\ d & -c \end{pmatrix}$ or $U = \begin{pmatrix} c & d \\ -d & c \end{pmatrix}$ where $c^2 + d^2 = 1$.

Let $B = (I_k|Z)U \in \mathcal{C}$. For the remainder of the paper we will be concerned with determining what role, if any, the eigenvalues of U play in determining D_B. If $\{\lambda_1, \ldots, \lambda_n\}$ is a set of n not necessarily distinct complex numbers for which there exists an $n \times n$ orthogonal matrix U with eigenvalues $\lambda_1, \ldots, \lambda_n$, then we will say that $\{\lambda_1, \ldots, \lambda_n\}$ is a (*) <u>set</u>. We note that if $T = \{\lambda_1, \ldots, \lambda_n\}$ is a set of n not necessarily distinct complex numbers such that T is closed under conjugation and every element of T has modulus 1, then T is a (*) <u>set</u>. Throughout the following, we assume that $1 \le k < n$, where k and n are positive integers, and we assume that at least one covariance matrix $\Omega_i \neq I_n$.

<u>Proposition 3</u>. Let $\{\lambda_1, \ldots, \lambda_n\}$ be a (*) set. Then there exists an orthogonal matrix U with eigenvalues $\lambda_1, \ldots, \lambda_n$ such that $B = (I_k|Z)U \in \mathcal{C}$ and $D_B = D$ if and only if one of the following conditions holds:

(i) λ_i is real for some i.

(ii) $k \ge 2$ and no λ_i is real.

Proof: Observe that if at least one λ_j is real, say λ_1, then by (7) there exists a block diagonal orthogonal matrix U of the form $U = \begin{pmatrix} \lambda_1 & \\ & C \end{pmatrix}$, where C is an $(n-1) \times (n-1)$ block diagonal orthogonal matrix with eigenvalues $\lambda_2,\ldots,\lambda_n$. Thus, if $U = (u_{ij})$, then $\sum_{j=1}^{k} u_{j1}^2 = u_{j1}^2 = \lambda_1^2 = 1$, so that $B = (I_k|Z)U \in \mathcal{C}$ and $D_B = D$ (Theorem 2). If no λ_j is real, then n is even, and by (7) there exists a block diagonal orthogonal matrix U with eigenvalues $\lambda_1,\ldots,\lambda_n$ such that $U = \begin{pmatrix} A_1 & & \\ & \ddots & \\ & & A_{\frac{n}{2}} \end{pmatrix}$, where each A_j is a 2×2 matrix of the form $\begin{pmatrix} a_j & b_j \\ -b_j & a_j \end{pmatrix}$, $b_j \neq 0$. Thus, the first column of U is $\begin{pmatrix} a_1 \\ -b_1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$, and hence, if $k \geq 2$, then $B = (I_k|Z)U \in \mathcal{C}$ and $D_B = D$.

Conversely, suppose that $k = 1$. If there exists an orthogonal matrix U with eigenvalues $\lambda_1,\ldots,\lambda_n$ such that $B = (I_k|Z)U \in \mathcal{C}$, then $U \in \mathcal{L}$. Thus, if $D_B = D$, then U is of the form $\begin{pmatrix} a & 0 & \cdots & 0 \\ 0 & & & \\ 0 & & C & \\ \vdots & & & \\ 0 & & & \end{pmatrix}$, where $a = \pm 1$ and C is an $(n-1) \times (n-1)$ orthogonal matrix. Therefore, a is an eigenvalue of U and $\lambda_i = a$ is real for some i.

It is natural to consider the analogous condition $D_B = 0$. That is, given a (*) set $\{\lambda_1, \ldots, \lambda_n\}$, does there exist an orthogonal matrix U with these eigenvalues such that $B = (I_k|Z)U \in \wp$ and $D_B = 0$? The answer, as in the preceding case, is no in general, but it is true in some important cases.

<u>Proposition 4</u>. Let $T = \{\lambda_1, \ldots, \lambda_n\}$ be a (*) set. If either

(i) 1 and $-1 \in T$, or;

(ii) i and $-i \in T$,

then there exists an orthogonal matrix U with eigenvalues $\{\lambda_1, \ldots, \lambda_n\}$ such that $B = (I_k|Z)U \in \wp$ and $D_B = 0$.

<u>Proof</u>. Let λ_1 and λ_2 denote the pair $1, -1$ or $i, -i$, let H be any $(n - 2) \times (n - 2)$ orthogonal matrix with eigenvalues $\lambda_3, \ldots, \lambda_n$, and let

$$U = \begin{pmatrix} 0 & Z & b_1 \\ Z & H & Z \\ b_2 & Z & 0 \end{pmatrix}$$

, where Z denotes an $(n - 2)$ row or column vector of zeros, and if $\{\lambda_1, \lambda_2\} = \{1, -1\}$, then $b_1 = b_2 = 1$, and if $\{\lambda_1, \lambda_2\} = \{i, -i\}$, then $b_1 = 1$, $b_2 = -1$.

Clearly, U is an orthogonal matrix. Moreover, the eigenvalues of U are $\{\lambda_1, \ldots, \lambda_n\}$, since $\det(xI_n - U) = (x^2 - b_1b_2) \det(xI_{n-2} - H)$ and hence the roots of $\det(xI_n - U) = 0$ are the roots of $\det(xI_{n-2} - H) = 0$, together with the roots of $x^2 - b_1b_2 = 0$. Since the roots of the former equation are the eigenvalues of H, its suffices to show that λ_1 and λ_2 are the roots of $x^2 - b_1b_2 = 0$. This follows immediately from the relationship defined between the values of λ_1 and λ_2 and the choices of b_1 and b_2. Thus, since we assume $k < n$, then Theorem 2 implies that $U \varepsilon \mathcal{S}$, so that $B = (I_k|Z)U \varepsilon \mathcal{C}$, and, by Theorem 1, $D_B = 0$.

Our next result shows that, if $n = 3$, then Proposition 4 does not characterize those (*) sets T for which there exists an orthogonal matrix U with set of eigenvalues T such that $B = (I_k|Z)U \varepsilon \mathcal{C}$ and $D_B = 0$. We will obtain a partial extension of this result to arbitrary n and we will make strong use of the extension in our main result, Theorem 7.

<u>Lemma 5</u>. Let $n = 3$, $k = 2$, and suppose that $\{\lambda_1, \lambda_2, \lambda_3\}$ is a (*) set, where $\lambda_1 = a + bi$, $\lambda_2 = a - bi$.

(1) If $\lambda_3 = 1$, then there exists a 3×3 orthogonal matrix U with eigenvalues $\lambda_1, \lambda_2, \lambda_3$ such that $U \varepsilon \mathcal{S}$ and $D_B = 0$, $B = (I_k|Z)U$, if and only if a, the real part of λ_1 and λ_2, is less than or equal to zero;

(2) if $\lambda_3 = -1$, then there exists a 3×3 orthogonal matrix U with eigenvalues $\lambda_1, \lambda_2, \lambda_3$ such that $U \varepsilon \mathcal{S}$ and $D_B = 0$, $B = (I_k|Z)U$, if and only if a, the real part of λ_1 and λ_2, is greater than or equal to zero.

<u>Proof</u>. Observe that if $U \varepsilon \mathcal{S}$ is such that $D_B = 0$, where $B = (I_k|Z)U$, then by Theorems 1 and 2, U is of the form $\begin{pmatrix} 0 & A \\ 0 & \\ v & 0\ 0 \end{pmatrix}$, where $v = \pm 1$ and A is a 2×2 orthogonal matrix. Moreover, if U has eigenvalues

$\lambda_1, \lambda_2, \lambda_3$, then $\det(U) = \lambda_1\lambda_2\lambda_3$. Thus, if $\lambda_3 = 1$, then $\det(U) = 1$, and if $\lambda_3 = -1$, then $\det(U) = -1$. We consider the case $\lambda_3 = 1$, the case $\lambda_3 = -1$ being similar.

If $v = 1$, then A is of the form $\begin{pmatrix} c & d \\ -d & c \end{pmatrix}$. Then $\det(xI_3 - U) = x^3 + dx^2 - dx - 1$, so that the eigenvalues of U are 1, $\frac{-(1+d) \pm i\sqrt{3-2d-d^2}}{2}$. Thus, there exists U with eigenvalues $\lambda_1, \lambda_2, 1$ if and only if there exists a real number d, $|d| \le 1$, such that

$$a = \frac{-(1+d)}{2} \quad , \quad b = \frac{\sqrt{3-2d-d^2}}{2} \quad . \tag{8}$$

Since $|d| \le 1$, then $\frac{-(1+d)}{2} \le 0$, and thus, if U exists, then $a \le 0$. Conversely, if $a \le 0$, then $d = -(1+2a)$ satisfies both equations in (8) and $|d| \le 1$. If $v = -1$, then $A = \begin{pmatrix} c & d \\ d & -c \end{pmatrix}$, and the eigenvalues of U are 1, $\frac{(d-1) \pm i\sqrt{3+2d-d^2}}{2}$. An argument similar to the preceding one shows that there exists U with eigenvalues $\lambda_1, \lambda_2, 1$ if and only if $a \le 0$.

<u>Corollary 6</u>. Let n and k be positive integers, $1 \le k < n$, and suppose that $T = \{\lambda_1, \ldots, \lambda_n\}$ is a (*) set.

(1) If $1 \in T$ and if there exists $a + bi \in T$, with $a \le 0$, then there exists an $n \times n$ orthogonal matrix U with eigenvalues T such that $U \in \mathcal{J}$ and $D_B = 0$, where $B = (I_k|Z)U$.

(2) If $-1 \in T$ and if there exists $a + bi \in T$, with $a \ge 0$, then there exists an $n \times n$ orthogonal matrix U with eigenvalues T such that $U \in \mathcal{J}$ and $D_B = 0$, where $B = (I_k|Z)U$.

Proof. By Lemma 5 and its proof, if $a \leq 0$, then $A = \begin{pmatrix} 0 & c & d \\ 0 & -d & c \\ 1 & 0 & 0 \end{pmatrix}$,
where $d = -(1 + 2a)$, is an orthogonal matrix with eigenvalues 1, $a \pm bi$. Thus, if $\overline{U}$ is the $n \times n$ block diagonal matrix $\begin{pmatrix} A & Z \\ Z & H \end{pmatrix}$, where H is an $(n - 3) \times (n - 3)$ orthogonal matrix with eigenvalues $T\backslash\{1, a \pm bi\}$, then $\overline{U}$ is an orthogonal matrix with eigenvalues the elements of T. Therefore, if U is the $n \times n$ matrix obtained from $\overline{U}$ by interchanging the third and n^{th} rows and columns of $\overline{U}$, then U is orthogonal, and, since U is similar to $\overline{U}$, the eigenvalues of U are also the elements of T. Finally, since the first column of U is $\begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}$, we have $U \in \mathcal{J}$, and, by Theorems 1 and 2, $D_B = 0$, where $B = (I_k|Z)U$ and $k < n$. The proof of (2) is similar.

We make a few additional observations before stating our main result. Let U be an $n \times n$ orthogonal matrix with eigenvalues λ_1, $\{a_j + b_j i\}_{j=2}^{n}$, where b_j may be zero. Since $tr(U)$ is the sum of the eigenvalues of U, it follows that if $\lambda_1 = 1$ and $a_j > 0$ for $j = 2,\ldots,n$, then $tr(U) = 1 + \sum_{j=2}^{n} a_j > +1$, while if $\lambda_1 = -1$ and $a_j < 0$ for $j = 2,\ldots,n$ then $tr(U) = -1 + \sum_{j=2}^{n} a_j < -1$. Also, if A is orthogonal and $\det(A) = -1$, then -1 is an eigenvalue of A. This follows immediately from the fact that $\det(A)$ is the product of the eigenvalues of A, repeated to their respective multiplicities. Finally, if A is orthogonal, $n \times n$, and n is even, then $\det(A) = -1$ implies that both -1 and 1 are eigenvalues of A.

<u>Theorem 7</u>. Let n and k be positive integers, $1 \leq k < n$, let U be an $n \times n$ orthogonal matrix, and let $B = (I_k|Z)U$ be such that $D_B = D$. If $\overline{U} = \begin{pmatrix} I_{n-1} & Z \\ Z & -1 \end{pmatrix} U$ and if $\overline{B} = (I_k|Z)\overline{U}$, then $B = \overline{B}$, so that $D_{\overline{B}} = D_B = D$. Either U or $\overline{U}$ is similar to an $n \times n$ orthogonal matrix $U_1 \in \mathcal{J}$ such that $D_{B_1} = 0$, where $B_1 = (I_k|Z)U_1$.

<u>Proof</u>. Note that the matrix $\overline{U}$ differs from U only in that the last row of $\overline{U}$ is the negative of the last row of U. Clearly, since $k < n$, we have $\overline{B} = B$.

Now suppose that n is even. If $\det(U) = -1$, then 1 and -1 are eigenvalues of U and thus, by Proposition 4, there exists an orthogonal matrix U_1 similar to U such that $B_1 = (I_k|Z)U_1 \in \mathcal{C}$ and $D_{B_1} = 0$. If $\det(U) = 1$, then $\det(\overline{U}) = -1$, and the above argument applied to $\overline{U}$ yields the same conclusion.

Suppose that n is odd. Then U must have at least one real eigenvalue, λ. If $\lambda = 1$ and if U has another eigenvalue $a + bi$, $a \leq 0$, then the conclusion follows from (1) of Corollary 6. Similarly, if $\lambda = -1$ and if U has another eigenvalue $a + bi$, $a \geq 0$, then the conclusion follows from (2) of Corollary 6. Suppose now that $\lambda = 1$ is an eigenvalue of U and that $a > 0$ for all other eigenvalues $a + bi$ of U. Then $\det(U) = 1$ and $tr(U) > 1$. Since $\det(\overline{U}) = -1$, it follows that -1 is an eigenvalue of $\overline{U}$, and, since $tr(\overline{U})$ can differ from $tr(U)$ by at most 2, we have that $tr(\overline{U}) > -1$. Thus, $\overline{U}$ must have an eigenvalue of the form $c + di$, where $c > 0$, and hence, by (2) of Corollary 6, there exists an orthogonal matrix

U_1, similar to $\bar{U}$, such that $B_1 = (I_k|Z)U_1 \in \zeta$ and $D_{B_1} = 0$. The case in which $\lambda = -1$ is an eigenvalue of U and that $a < 0$ for all other eigenvalues $a + bi$ of U is handled in a similar manner, and we omit the proof.

3. Conclusion. This paper provides an example to show that, even under extremely strong conditions, the eigenvalues of U do not affect the value of divergence $D_{(I_k|Z)U}$ in the space of reduced dimension.

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