

GENERALIZED EIGENVALUE PROBLEMS WITH POSITIVE SEMI-DEFINITE MATRICES

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In a recent paper in this journal McDonald, Torii, and Nishisato show that generalized eigenvalue problems in which both matrices are singular can sometimes be solved by reducing them to similar problems of smaller order. In this paper a more extensive analysis of such problems is used to sharpen and clarify the results of McDonald, Torii, and Nishisato. Possible extensions are also indicated. The relevant mathematical literature is reviewed briefly.

Key words: eigenvalues, eigenvectors, optimal scaling, simultaneous diagonalization.

Introduction, Motivation

Many of the problems of multivariate analysis and scaling can be reduced to finding the maximum, minimum, or other critical values of a ratio of quadratic forms. Principal component analysis, classical multidimensional scaling, correspondence analysis, multiple group discriminant analysis, canonical analysis, multivariate analysis of variance, and "dual" or "optimal" scaling of categorical variables are all of this type. It is usually assumed in the literature that at least one of the matrices of the quadratic forms is positive definite, which makes it possible to transform the problem to an ordinary eigenvalue-eigenvector problem.

In this paper we want to study what happens if both matrices are singular, although we continue to assume that they are positive semi-definite. We have been inspired by a recent paper of McDonald, Torii, and Nishisato [1979], who study a more general problem. Their basic Theorem 1 can be sharpened if we assume positive semi-definiteness of both matrices.

Notation, Definitions, Problems

Suppose A and B are real symmetric matrices of order n . For all $x \in \mathbb{R}^n$ we set

$$\alpha(x) \triangleq x'Ax, \quad (1a)$$

$$\beta(x) \triangleq x'Bx, \quad (1b)$$

where the symbol \triangleq is used for definitions. We also define

$$S_B^0 \triangleq \{x \in \mathbb{R}^n \mid \beta(x) = 0\}, \quad (2a)$$

$$S_B^+ \triangleq \{x \in \mathbb{R}^n \mid \beta(x) > 0\}, \quad (2b)$$

$$S_B^1 \triangleq \{x \in \mathbb{R}^n \mid \beta(x) = 1\}. \quad (2c)$$

The basic *assumption*, used throughout this paper, except in the section on generalizations, is that both $\alpha(x) \geq 0$ and $\beta(x) \geq 0$ for all $x \in \mathbb{R}^n$. In words: both A and B are *positive semi-definite*, often abbreviated to psd. As indicated in the definitions of $\alpha(x)$ and $\beta(x)$ all vectors are column vectors. Row vectors are indicated by transposition, transposition of vectors and matrices is indicated by using a prime.

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We now describe the *problems* we want to solve in this paper.

Problem I: Find the *maximum, minimum, critical values, maximizer, minimizer, critical points* of $\lambda(x) \triangleq \alpha(x)/\beta(x)$ on S_B^+ if they exist.

Problem II: The same for $\alpha(x)$ on S_B^1 .

Problem III: Find all pairs (λ, x) , with λ a real nonnegative number and with $x \in \mathbb{R}^n$, such that $(A - \lambda B)x = 0$. The same with $x \in S_B^+$ and with $x \in S_B^1$.

Problem IV: Find all real nonnegative numbers λ such that $\det(A - \lambda B) = 0$, where $\det(\cdot)$ is the *determinant* of a matrix.

Problem V: Find all square nonsingular W such that $W'AW$ and $W'BW$ are both *diagonal* matrices.

Our *procedure* in this paper is that we first solve problem V, and use the solution to that problem to find the solutions to the four other problems.

Solution of Problem V

The fact that problem V is solvable, i.e., that there exists a square nonsingular W that diagonalizes both A and B , is often attributed to Newcomb [1961]. The proof given by Newcomb is constructive; it shows how to construct a solution W . Our formulation of problem V, however, calls for the construction of *all possible* W that diagonalize A and B . Because of this we need a proof which is more explicit than Newcomb's. Our procedure is to construct all possible W that diagonalize both A and B , and that satisfy some additional identification conditions. The answer to problem V can then be easily found from this by dropping these identification conditions.

In order to make a more precise formulation of the identified diagonalization problem possible we partition W as $W = (U | V)$. We then write down the equations

$$U'BU = I, \tag{3a}$$

$$V'BV = 0, \tag{3b}$$

$$U'AU = \Psi, \tag{3c}$$

$$U'AV = 0, \tag{3d}$$

$$V'AV = \Phi, \tag{3e}$$

with

$$U \text{ an } n \times r \text{ matrix of rank } r, \tag{3f}$$

$$V \text{ an } n \times (n - r) \text{ matrix of rank } n - r, \tag{3g}$$

$$\Psi \text{ a diagonal matrix with elements nonincreasing along the diagonal,} \tag{3h}$$

$$\Phi \text{ a diagonal matrix with elements nonincreasing along the diagonal,} \tag{3i}$$

and

$$V'V = I. \tag{3j}$$

To state our main theorem we need some extra notation. Suppose $B = FF'$ is any fixed full-rank decomposition of B , thus F is $n \times \rho$ and of rank ρ , where $\rho \triangleq \text{rank}(B)$. Define F^+ , the Moore-Penrose inverse of F , by $F^+ \triangleq (F'F)^{-1}F'$. The notation F^- is used for any g -inverse of F , because F has full column rank, g -inverse are also left inverses, and satisfy

$F^-F = I$. We use K for some fixed orthonormal basis for the null-space of B . Thus K is $n \times (n - \rho)$, $K'K = I$, and $BK = 0$. We also define

$$\tilde{A}_{11} \triangleq F^+ A(F^+)', \quad (4a)$$

$$\tilde{A}_{22} \triangleq K'AK, \quad (4b)$$

$$\tilde{A}_{12} \triangleq \tilde{A}'_{21} \triangleq \overline{F^+ AK}. \quad (4c)$$

Using this notation we can now state our main theorem.

Theorem 1. 1: Existence : System (3a)–(3j) is solvable if and only if $r = \rho$.

2: *Solutions:* a: $V = KM$, with M a complete set of eigenvectors corresponding with ordered eigenvalues of \tilde{A}_{22} .

b: $U = (F^+)L - K\tilde{A}_{22}^{-1}\tilde{A}_{21}L + K(I - \tilde{A}_{22}^{-1}\tilde{A}_{22})S$, with S of order $(n - r) \times r$ but otherwise arbitrary, with \tilde{A}_{22}^{-1} any g -inverse of \tilde{A}_{22} , and with L a complete set of eigenvectors corresponding with ordered eigenvalues of $\tilde{A}_{11} - \tilde{A}_{12}\tilde{A}_{22}^{-1}\tilde{A}_{21}$.

c: Ψ are the ordered eigenvalues of $\tilde{A}_{11} - \tilde{A}_{12}\tilde{A}_{22}^{-1}\tilde{A}_{21}$.

d: Φ are the ordered eigenvalues of \tilde{A}_{22} .

3: *Uniqueness:* The solution to (3a)–(3j) with $r = \rho$ is unique if and only if the following three conditions are all satisfied.

a: The eigenvalues of $\tilde{A}_{11} - \tilde{A}_{12}\tilde{A}_{22}^{-1}\tilde{A}_{21}$ are different.

b: The eigenvalues of \tilde{A}_{22} are different.

c: $K(I - \tilde{A}_{22}^{-1}\tilde{A}_{22}) = 0$.

Proof. From (3a) and (3f) solvability implies $r \leq \rho$. From (3b) and (3g) it implies $r \geq \rho$. Thus $r = \rho$ is necessary for solvability. We prove sufficiency, and at the same time part 2 of Theorem 1, by constructing the general solution, assuming that $r = \rho$.

From (3b) it follows that $V = KN$, (3g) implies that N must be square and nonsingular, (3j) even implies that N must be orthonormal. Now (3e) gives $N'\tilde{A}_{22}N = \Phi$, which together with (3i) shows that parts 2:a and 2:d of Theorem 1 are true.

From (3a) we have $U'FF'U = I$, or $F'U = L$, with L square orthonormal. The general solution of $F'U = L$ for U , given L , is $U = (F^+)L + KT$, with T arbitrary of order $(n - r) \times r$. Thus $U = (F^+)L + KT$ gives the general solution to (3a) if we let L vary over the square orthonormal and T over the arbitrary $(n - r) \times r$ matrices. Another way to write U is $U = (F^-)L$, with F^- varying over the left inverses of F and L over the square orthonormals. From (3d) and our previous results $L'\tilde{A}_{12}M + T'\tilde{A}_{22}M = 0$, which is equivalent to $L'\tilde{A}_{12} + T'\tilde{A}_{22} = 0$. This is a consistent system of linear equations in T for given L , whose general solution is $T = -\tilde{A}_{22}^{-1}\tilde{A}_{21}L + (I - \tilde{A}_{22}^{-1}\tilde{A}_{22})S$, with S an arbitrary $(n - r) \times r$ matrix. We now substitute the expression for T in the remaining equation (3c). This gives $L'(\tilde{A}_{11} - \tilde{A}_{12}\tilde{A}_{22}^{-1}\tilde{A}_{21})L = \Psi$, which together with identification condition (3h) shows that part 2:c is true and that L is as stated in part 2:b of theorem 1. If we combine the general solutions for U and T and L we obtain the rest of part 2:b.

Part 3 of Theorem 1 follows directly from the expressions in part 2. This ends the proof of Theorem 1.

Observe that the solutions do not change if we start out with another full-rank decomposition of B and/or with another orthonormal basis for the null-space of B . The ensuing rotations of F and K are compensated for by the eigenvectors of

$\tilde{A}_{11} - \tilde{A}_{12} \tilde{A}_{22}^{-1} \tilde{A}_{21}$ and \tilde{A}_{22} , which are counter-rotated in such a way that the solution sets for U and V remain the same. Of course the eigenvalues do not change at all.

To solve problem V in complete generality we must drop identification condition (3j), relax (3a) to $U'BU = \Omega$, with Ω diagonal and nonsingular, and eliminate the ordering of the elements from (3h) and (3i). Eliminating the order constraints has a trivial and predictable effect, the solutions are determined only up to a permutation of dimensions. Relaxing (3a) gives the same general solution for U , but postmultiplied by an arbitrary diagonal matrix $\Omega^{1/2}$, the eigenvalues of $\tilde{A}_{11} - \tilde{A}_{12} \tilde{A}_{22}^{-1} \tilde{A}_{21}$ are then $\Psi \Omega^{-1}$. Dropping (3j) is somewhat more interesting, also from a computational point of view. V and Φ are now solutions of the equations $V = KN$ and $N' \tilde{A}_{22} N = \Phi$, these equations are easily solved by using any full-rank decomposition of \tilde{A}_{22} , not necessarily an orthogonal one. In most practical problems, however, we are not particularly interested in V and Φ . And, indeed, Φ is *very* arbitrary if we do not impose (3j). It can be any diagonal matrix of the same rank as \tilde{A}_{22} , suitably ordered if we impose (3i). In the remaining sections of the paper we shall see that in most practical problems we are only interested in U and Ψ .

This last remark suggests that we take another look at the formula $U = (F^-)'L$, with F^- varying over the left inverses of F and with L varying over the square orthonormals. Above, we used (3d) to determine which F^- we wanted, and then (3c) to determine L and Ψ . We now take a different route. Suppose we start with a fixed F^- , compute $A_{11} = F^- A (F^-)'$ instead of $\tilde{A}_{11} - \tilde{A}_{12} \tilde{A}_{22}^{-1} \tilde{A}_{21}$, and determine L and Ψ as eigenvectors and eigenvalues of A_{11} . It is clear that this procedure produces a solution to system (3a)–(3j) if and only if $F^- AK = 0$. The procedure thus works for the Moore-Penrose inverse F^+ if and only if $\tilde{A}_{12} = 0$. The procedure works for *all* choices of F^- if and only if $\tilde{A}_{22} = 0$, which implies of course that $\tilde{A}_{12} = 0$. The condition $\tilde{A}_{22} = 0$ can also be written as $x'Ax = 0$ for all $x \in \mathbb{R}^n$ such that $x'Bx = 0$, or in the notation of formula (2a) as S_B^0 is a subspace of S_A^0 . A simple sufficient condition for $\tilde{A}_{22} = 0$ is that $A \leq B$, by which we mean that $B - A$ is psd. It is sometimes convenient to know that the condition $\tilde{A}_{12} = 0$ is equivalent to $F'AK = 0$, which is equivalent to $BA(I - B^+B) = 0$.

Solution of the First Four Problems

We start out with problem IV. From the results of the previous section we have that $\det(A - \lambda B) = 0$ if and only if

$$(\psi_1 - \lambda)(\psi_2 - \lambda) \cdots (\psi_r - \lambda)\phi_1 \phi_2 \cdots \phi_{n-r} = 0. \tag{5}$$

If \tilde{A}_{22} is nonsingular, i.e., if the intersection of the null-spaces of A and B is the zero vector, then this polynomial equation of degree r with roots $\psi_1, \psi_2, \dots, \psi_r$. If \tilde{A}_{22} is singular, then $\det(A - \lambda B)$ is identically equal to zero.

For problem III we define y by $y \triangleq W^{-1}x$, where W has its first r columns equal to U and its last $n - r$ columns equal to V . Thus $(A - \lambda B)x = 0$ becomes $(A - \lambda B)Wy = 0$. Premultiplying by W' gives $(\Psi - \lambda I)y_1 = 0$ and $\Phi y_2 = 0$, where y_1 consists of the first r elements of y and y_2 consists of the $n - r$ last elements of y . We can now give the solution for the elements of y as a function of λ , using ψ_s and ϕ_s for the diagonal elements of Ψ and Φ again.

$$\text{If } \phi_s = 0 \text{ then } y_{r+s} \text{ is arbitrary.} \tag{6a}$$

$$\text{If } \phi_s > 0 \text{ then } y_{r+s} = 0. \tag{6b}$$

$$\text{If } \psi_s \neq \lambda \text{ then } y_s = 0. \tag{6c}$$

$$\text{If } \psi_s = \lambda \text{ then } y_s \text{ is arbitrary.} \tag{6d}$$

Thus if $\lambda \neq \psi_s$ for all $s = 1, \dots, r$ then the dimensionality of the solution space for y is equal to the nullity of \tilde{A}_{22} . If $\lambda = \psi_s$ for some s , then this dimensionality is equal to the multiplicity of ψ_s plus the nullity of \tilde{A}_{22} . If we translate these results back from y to x we find the following theorem, in which V_0 are the last $(n - r) - \text{rank}(\tilde{A}_{22})$ columns of V , and U_s are those columns of U for which $U'AU = \psi_s I$.

Theorem 2. a: If $\lambda \neq \psi_s$ for all s , then $(A - \lambda B)x = 0$ if and only if $x = V_0 z$ for some z .

b: If $\lambda = \psi_s$ for some s , then $(A - \lambda B)x = 0$ if and only if $x = U_s t + V_0 z$ for some z and t .

This theorem gives a complete solution to problem III, first part. The other two parts are now easy. $(A - \lambda B)x = 0$ has a solution in S_B^+ if and only if $\lambda = \psi_s$ for some s . The solution is of the form $x = U_s t + V_0 z$, with z arbitrary and t nonzero, but otherwise arbitrary. The solutions in S_B^1 are of the same form, but now $t't = 1$ must be true.

In problem II we start by observing that $x \in S_B^1$ is a critical point of $\alpha(x)$ on S_B^1 if $Ax = \lambda Bx$, where λ is an undetermined multiplier. Finding all critical points is consequently the same thing as solving problem III with $x \in S_B^1$. The critical values are the corresponding values of λ . The global maximizer of $\alpha(x)$ on S_B^1 is any vector of the form $x = U_1 t + V_0 z$, with $t't = 1$, the maximum is ψ_1 . In the same way the global minimizer is $x = U_r t + V_0 z$ with $t't = 1$, and the minimum is ψ_r .

Problem I is very similar to problem II, but slightly more complicated. The vector x is a critical point of $\lambda(x)$ on \mathbb{R}^n if $[A - \lambda(x)B]x = 0$ and $\beta(x) > 0$. Thus all critical points can be found by solving problem III on S_B^+ , which we have already done. To find the maximum and minimum we make the transformation $y = W^{-1}x$ again, which transforms $\lambda(x)$ to $(y'_1 \Psi y_1 + y'_2 \Phi y_2) / y'_1 y_1$. If Φ is nonzero, i.e., if \tilde{A}_{22} is nonzero, then we can make this function arbitrarily large by choosing y_2 in such a way that $y'_2 \Phi y_2 > 0$ and by making y_1 very small. Thus the maximum does not always exist, which makes problem I different from problem II. The basic difference is, of course, that S_B^1 is compact, while S_B^+ is unbounded and open. It is interesting that the minimum is always attained at $x = U_r t + V_0 z$ with $t \neq 0$. It is equal to ψ_r . For ease of reference we summarize the result which is most interesting in problem I in a theorem.

Theorem 3. The maximum of $\lambda(x)$ on S_B^+ is attained if and only if $\tilde{A}_{22} = 0$. In this case the maximizer is equal to $x = U_1 t + V_0 z$ with $t \neq 0$, and the maximum is ψ_1 .

We have now solved all five problems. The interesting ones are I, III, and of course V. Problem IV usually merely provides the information that $\det(A - \lambda B) = 0$ for all λ . Problem II is essentially identical with problem III, but something new is added in problem I. Theorem 3 can be interpreted as saying that we can solve the simultaneous diagonalization problem by diagonalizing $F^- A (F^-)'$ for arbitrary F^- if and only if $\lambda(x)$ is bounded on S_B^+ .

A Theorem by McDonald, Torii, and Nishisato

In our analysis of problem V we have seen that in some cases we can find the orthonormal matrix L in the expression for U (Theorem 1, part 2:b) by diagonalizing $A_{11} = F^- A (F^-)'$, where F^- is some left inverse of F . In McDonald, Torii, and Nishisato [1979] three sufficient conditions are given which guarantee that we can find L by diagonalizing $\tilde{A}_{11} = F^+ A (F^+)'$. Observe that these authors assume merely that B is psd, their A can be indefinite. The three conditions are, in our notation,

$$(I - BB^+)A = 0, \tag{7a}$$

there exists Q such that $A = BQ$, (7b)

there exist G, H such that $GHH'G' = A$ and $GG' = B$. (7c)

Theorem 4. The three conditions (7a), (7b), (7c) are all equivalent to $\tilde{A}_{22} = 0$.

Proof. McDonald, Torii, and Nishisato prove that (7c) implies (7a) and that (7b) implies (7a). We first prove that (7a) implies $\tilde{A}_{22} = 0$. In our notation (7a) is $KK'A = 0$, which implies $K'A = 0$, which implies $K'AK = 0$ or $\tilde{A}_{22} = 0$. We now prove that $\tilde{A}_{22} = 0$ implies (7b) and (7c). Now $A = BQ$ is solvable if and only if $Q = B^+A$ is a solution, which is true if and only if $A = BB^+A$. $\tilde{A}_{22} = 0$ implies that $KK'A = 0$, which is $A = BB^+A$, and thus (7b). To prove finally that $\tilde{A}_{22} = 0$ implies (7c) we observe that $FF^+A(FF^+)' = (I - KK')A(I - KK')$. Thus if $\tilde{A}_{22} = 0$ then $F\tilde{A}_{11}F' = A$. This implies (7c) with $G = F$ and H any Gram-factor of \tilde{A}_{11} . This ends the proof of Theorem 4.

In the more general case, discussed by McDonald, Torii, and Nishisato [1979] it remains true that (7a) and (7b) are equivalent. Moreover (7c), which is the only condition they actually use in their applications, implies that A is psd. If we assume directly that A is psd, we get a more compact and useful result. In the first place by using Theorem 4, which states that their sufficient conditions are all equivalent to $\tilde{A}_{22} = 0$. In the second place by our earlier result that $\tilde{A}_{22} = 0$ is *necessary and sufficient* for the solutions of

$$LA_{11}L = \Psi, \tag{8a}$$

$$U = (F^-)L \tag{8b}$$

with $LL = I$ and with F^- an arbitrary left inverse of F , to provide a solution to (3a)–(3j), *no matter how we choose F^-* . In the third place by our earlier result that a necessary and sufficient condition in Theorem 1 of McDonald, Torii, and Nishisato, which uses F^+ for F^- , is that $\tilde{A}_{12} = 0$. And finally by our earlier result that a necessary and sufficient condition for a fixed F^- to work in (8a) and (8b) is that $F^-AK = 0$.

In psychometric data analysis the condition $\tilde{A}_{22} = 0$ is very often true by construction of the problem, an easily verified condition is that there is a $\kappa > 0$ such that $A \leq \kappa B$. This condition is equivalent to $x'Ax \leq \kappa x'Bx$ for all $x \in \mathbb{R}^n$. This is equivalent to the two conditions that $x'Ax = 0$ for all $x \in \overline{S_B^0}$ and that $\lambda(x)$ is bounded on S_B^+ . But these two conditions are both equivalent to $\tilde{A}_{22} = 0$. Thus we have proved theorem 5.

Theorem 5. $\tilde{A}_{22} = 0$ if and only if there is a $\kappa > 0$ such that $A \leq \kappa B$ (i.e., such that $\kappa B - A$ is psd).

In a sense problems with $\tilde{A}_{22} \neq 0$ are ill-defined, because the data analytic problem is often to maximize $\lambda(x)$, and we have seen that this is unbounded if $\tilde{A}_{22} \neq 0$. Although the conditions used by MacDonald, Torii, and Nishisato are not necessary for their theorem, they are necessary and sufficient for the maximum to be well defined and they are necessary and sufficient for using any F^- that is convenient. Thus the practical consequences of our improved results are possibly fairly small. If one cannot prove $\tilde{A}_{12} = 0$ or $\tilde{A}_{22} = 0$ for the particular problem one is considering, however, then one must stay on the safe side and use the constructions of our Theorem 1, which are valid for all pairs of psd matrices.

Generalizations

In this paper we use the assumption that both A and B are psd. If this is not the case, there are various other possibilities. If A and B are merely semi-definite, nothing really

changes in our treatment of problem V. If A is psd and B is negative semi-definite, for example, we apply our proof to A and $-B$. This minor generalization was also mentioned by Newcomb [1961]. Another case which is easy is if either A or B is definite. If B is positive definite, for example, then $W = B^{-1/2}K$ with $K'K = KK' = I$ and with $K'B^{-1/2}AB^{-1/2}K = \Psi$ diagonalizes both A and B ($B^{-1/2}$ is the inverse of the symmetric square root of B). If B is negative definite, we work with $-B$ again. The case in which B is psd and A is unrestricted is somewhat more complicated. By checking the proof of Theorem I we find that a necessary and sufficient condition for simultaneous diagonalizability of A and B is solvability of the linear system $L\tilde{A}_{12} + T'\tilde{A}_{22} = 0$ or $\tilde{A}_{22}\tilde{A}_{22}^{-1}\tilde{A}_{21} = \tilde{A}_{21}$.

The next case which is interesting is the case in which we can find μ and η such that $\mu A + \eta B$ is positive definite. If W diagonalizes $\mu A + \eta B$ as well as A , then it clearly also diagonalizes B . A classical theorem, whose history has recently been reviewed by Uhlig [1979], states that if $n \geq 3$ then a positive definite linear combination of A and B exists if $x'Ax = x'Bx = 0$ implies that $x = 0$. This condition is sufficient for simultaneous diagonalizability, but not necessary. Necessary and sufficient conditions have been given by many authors. Most of them are mentioned by Uhlig [1979, p. 230], we add to his list the very nice paper by Mitra and Rao [1968]. Necessary and sufficient conditions for simultaneous diagonalizability if A and B are not necessarily symmetric have been given by Lee [1971], they are not very relevant however in the quadratic form context.

If the pair A and B is not simultaneously diagonalizable, then the situation becomes considerably more complicated. In this case we can use the canonical form for real symmetric matrix pairs discovered by Muth [1905], and modernized recently by Ng [1976] and Uhlig [1976]. Again the relevance of this case for practical data analysis is limited.

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Manuscript received 4/14/81

Final version received 12/22/81