Kronecker's Canonical Form and the QZ Algorithm

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Dedicated to Alston S. Householder
on the occasion of his seventy-fifth birthday.

Submitted by G. W. Stewart

ABSTRACT

This paper examines the behavior of the QZ algorithm which is to be expected when $A-\lambda B$ is close to a singular pencil. The predicted results are fully confirmed by practical experience of using the QZ algorithm on examples of this kind.

1. INTRODUCTION

In a recent paper [5] we dicussed the derivation of the Kronecker canonical form (K.c.f.) of the λ matrix $A-\lambda B$ (usually referred to as a linear *pencil*) using the system of differential equations

$$B\dot{x} = Ax + f(t) \tag{1.1}$$

as the motivation. A related and in some respects more detailed treatment has been given by van Dooren [1], though there a direct attack was made on the derivation of the Kronecker canonical form.

In recent years the generalized eigenvalue problem

$$Au = \lambda Bu \tag{1.2}$$

has been the subject of intensive research. The importance of this problem

*Supported in part by National Aeronautics and Space Administration Grant N SG 1443.

0024-3795/79/060285+19$01.75

stems primarily from the fact that if λ and u are an eigenvalue and eigenvector of (1.2), then

$$x = ue^{\lambda t} \tag{1.3}$$

is a solution of the homogeneous system

$$B\dot{x} = Ax. \tag{1.4}$$

One of the most effective methods for dealing with the generalized eigenvalue problem is the QZ algorithm developed by Moler and Stewart [4]. This reduces B and A simultaneously to triangular matrices $\tilde{B}$ and $\tilde{A}$ such that

$$\tilde{B} = QBZ \quad \text{and} \quad \tilde{A} = QAZ, \tag{1.5}$$

where Q and Z are derived as the product of elementary unitary transformations. The problem

$$\tilde{A}v = \lambda\tilde{B}v \tag{1.6}$$

is therefore "equivalent" to (1.2) in that the eigenvalues are the same and corresponding u and v are such that $u = Zv$. If there are no zero values of $\tilde{b}_{ii}$, then the eigenvalues are given by

$$\lambda_i = \tilde{a}_{ii}/\tilde{b}_{ii}. \tag{1.7}$$

A zero value of $\tilde{b}_{ii}$ presents no special problem unless the corresponding $\tilde{a}_{ii}$ is also zero; it merely implies that the corresponding λ_i is infinite. It is simpler to regard such an infinite eigenvalue as a zero eigenvalue of

$$Bu = \mu Au. \tag{1.8}$$

However, if for any value of i we have $\tilde{a}_{ii} = \tilde{b}_{ii} = 0$, then

$$0 \equiv \det(\tilde{A} - \lambda\tilde{B}) = \det Q(A - \lambda B)Z = \det Q \det\,(A - \lambda B)\det Z, \tag{1.9}$$

and hence $\det(A - \lambda B) \equiv 0$, since Q and Z are unitary. Conversely if $\det(A - \lambda B) \equiv 0$ and $\tilde{A} - \lambda\tilde{B}$ is an equivalent triangular pencil, then since $\det(\tilde{A} - \lambda\tilde{B}) = \prod(\tilde{a}_{ii} - \lambda\tilde{b}_{ii})$, this cannot give the null polynomial unless $\tilde{a}_{ii} = \tilde{b}_{ii} = 0$ for at least one i.

2. THE KRONECKER CANONICAL FORM

Kroneckers's canonical form applies to general pencils $A-\lambda B$, where A and B may be rectangular matrices. The pencil is said to be *singular* if either

(i) $m \neq n$ or
(ii) $m = n$ and $\det(A-\lambda B \equiv 0$.

Otherwise the pencil is said to be *regular*; note that regular pencils necessarily involve square matrices. The pencil $A-\lambda\tilde{B}$ is said to be *strictly equivalent* to $A-\lambda B$ if there exist nonsingular matrices P and Q (not necessarily unitary) such that

$$\tilde{A} = PAQ, \qquad \tilde{B} = PBQ. \tag{2.1}$$

In the remainder of this paper we shall omit the qualification "strictly," since we shall not be concerned with any broader concept of equivalence.

Kronecker showed that $A-\lambda B$ could be reduced to an equivalent $\tilde{A}-\lambda\tilde{B}$ in which the $\tilde{A}$ and $\tilde{B}$ are of block diagonal form, the blocks in A and B being conformal. The blocks in the K.c.f. are of three types. In general there will be a number of blocks of each type in the K.c.f.

(i) *Those corresponding to elementary divisors of the form* $(\alpha-\lambda)^r$ *where* α *is finite (possibly zero)*. For these the blocks in $\tilde{A}$ and $\tilde{B}$ are $J_r(\alpha)$ and I_r respectively, where $J_r(\alpha)$ is the elementary Jordan matrix of order r associated with α, and I_r is the identity matrix of order r. These blocks are said to correspond to *finite* elementary divisors of $A-\lambda B$. They are of course square and of dimension $r \times r$. For reasons which become obvious when we discuss the other blocks, it is often more convenient to think in terms of the homogeneous pencil $\mu A-\lambda B$ and of the elementary divisor $(\alpha\mu-\lambda)^r$ rather than $(\alpha-\lambda)^r$.

(ii) *Those corresponding to elementary divisors* μ^r *of the homogeneous pencil* $\mu A-\lambda B$. For these the blocks in $\tilde{A}$ and $\tilde{B}$ are I_r and $J_r(0)$ respectively. Notice that the identity matrix is now in $\tilde{A}$ and the elementary Jordan matrix is in $\tilde{B}$. These blocks are said to correspond to *infinite* elementary divisors. Again they are square.

(iii) *Elementary Kronecker blocks*, usually denoted by $L_\varepsilon(\lambda,\mu)$ and $L_\eta^T(\lambda,\mu)$. These are of dimensions $\varepsilon \times (\varepsilon+1)$ and $(\eta+1)\times\eta$ respectively. They are adequately illustrated by $L_2(\lambda,\mu)$, for which the blocks in $\mu\tilde{A}-\lambda\tilde{B}$, $\tilde{A}$ and $\tilde{B}$ are

$$\begin{bmatrix} \mu & -\lambda & 0 \\ 0 & \mu & -\lambda \end{bmatrix}, \quad \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \text{ and } \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{2.2}$$

respectively. There are no elementary divisors of $\mu A-\lambda B$ corresponding to these blocks, or perhaps we should say that the corresponding elementary divisor is unity, which is independent of μ or λ.

We make the following comments. If all of the blocks are of types (i) and (ii), then $\tilde{A}$ and $\tilde{B}$ (and hence A and B) are square. Further, since $\det(\mu\tilde{A}-\lambda\tilde{B})$ is the product of the determinants of the diagonal blocks in $\mu\tilde{A}-\lambda\tilde{B}$ and

$$\det[\,\mu J_r(\alpha)-\lambda I_r\,]=(\,\mu\alpha-\lambda)^r, \tag{2.3}$$

$$\det[\,\mu I_r-\lambda J_r(0)\,]=\mu^r, \tag{2.4}$$

we see that $\det(\mu\tilde{A}-\lambda\tilde{B})$ [and hence $\det(\mu A-\lambda B)$] is not null. In this case then the pencil is regular.

The blocks corresponding to infinite elementary divisors seem to be decisively different from those corresponding to finite elementary divisors. This is deceptive and rather unsatisfactory when we come to practical algorithms. In a block of type (i) corresponding to a zero value of α the matrix $\tilde{A}$ has a $J_r(0)$ and $\tilde{B}$ has an I_r. In a block of type (ii) $\tilde{A}$ has an I_r and $\tilde{B}$ has a $J_r(0)$; this is quite natural if we think in terms of a zero elementary divisor of $B-\mu A$. In computational terms it would perhaps be more satisfactory to make the distinction between values for which $|\alpha|\leqslant 1$ and those for which $|\alpha|>1$. For the former we could take blocks $J_r(\alpha)$ in $\tilde{A}$ and I_r in $\tilde{B}$; for the latter we take blocks I_r in $\tilde{A}$ and $J_r(\beta)$ in $\tilde{B}$, where $\beta=1/\alpha$. Now $\alpha=\infty$ corresponds to $\beta=0$, and the whole range is treated in a uniform manner. Strictly speaking if $\|A\|_2$ and $\|B\|_2$ are very disparate in size, then we should distinguish between those α for which $|\alpha|\leqslant\|A\|_2/\|B\|_2$ and those for which $|\alpha|>\|A\|_2/\|B\|_2$. Notice that for the standard eigenvalue problem $\|B\|_2=\|I\|_2=1$; since all eigenvalues satisfy the condition $|\alpha|\leqslant\|A\|_2$, the second set is always empty. This pinpoints an essential difference between the generalized problem and the standard problem. For simplicity of notation we shall assume that $\|A\|_2$ and $\|B\|_2$ are of comparable orders of magnitude; this is, after all, merely a matter of scaling. Accordingly we shall distinguish between $|\alpha||\leqslant 1$ and $|\alpha|>1$. When $m\neq n$ there must, of course, be some rectangular blocks in $\tilde{A}$ and $\tilde{B}$. Indeed, if $m<n$ there must be $n-m$ more blocks of type L_ε than of type L_η^T, while if $m>n$ there must be $m-n$ more blocks of types L_η^T than of type L_ε. When $m=n$ and $\det(A-\lambda B)\equiv 0$, we have already remarked that not all the blocks could be of type (i) and (ii). Hence in this case too, blocks of type (iii) must occur, and clearly there must be an equal number of L_ε and L_η^T blocks; otherwise $\tilde{A}$ and $\tilde{B}$ would not be square. However, the dimensions of the L_ε blocks need bear no relation to those of the L_η^T blocks.

It is well known that classical similarity theory, which is concerned with the standard eigenvalue problem $Au = \lambda u$, is dominated by the Jordan canonical form (J.c.f.) J of A. The corresponding K.c.f. of $A - \lambda I$ is $J - \lambda I$; in this simple case the K.c.f. never contains any blocks of type (iii). Now in *numerical* linear algebra the J.c.f. is not generally regarded as quite so important, for the following reason. Elementary Jordan blocks of dimension greater than unity can arise only if A has multiple eigenvalues. However, arbitrary perturbations in A then lead, in general, to a matrix having distinct eigenvalues and hence having a strictly diagonal J.c.f. Moreover, blocks of order greater than unity *usually* correspond to very sensitive eigenavlues. Thus if the block $J_2(a)$ is perturbed to

$$\begin{bmatrix} a & 1 \\ \varepsilon & a \end{bmatrix}, \tag{2.5}$$

the eigenvalue becomes $a \pm \varepsilon^{1/2}$.

However, it is salutary to remember that the use of unity elements in the standard Jordan form is for convenience only. The matrix

$$A = \begin{bmatrix} a & \varepsilon \\ 0 & a \end{bmatrix} \tag{2.6}$$

has the J.c.f.

$$\begin{bmatrix} a & 1 \\ 0 & a \end{bmatrix}, \tag{2.7}$$

but perturbations *of order* ε in A give perturbations of order ε in the eigenvalues. This remark is sometimes important in practice when we are not concerned with perturbations that are arbitrarily small.

In numerical linear algebra it is the insight provided by the J.c.f. into the perturbation of eigenvalues which is its more important aspect. The actual determination of the J.c.f. plays a much less important role, and indeed in the presence of rounding errors it is an unattainable goal except in special cases. An important feature is that if A has an eigenvalue α which is very sensitive to perturbations in the matrix elements, then A is to that extent close to a defective matrix, i.e. a matrix having a block of order greater than unity in its J.c.f. Hence extreme sensitivity is always related to defectiveness or near-defectiveness.

Since the K.c.f. is the generalization of the J.c.f., the comments we have made above will obviously apply to the K.c.f. However, there are new and important considerations. As we showed in [5], the number of Kronecker blocks and their dimensions are determined by considerations of rank; small perturbations in A and B may well change the ranks of the submatrices involved.

3. REGULAR PENCILS

Our main concern in this note is with the relevance of the K.c.f. for the QZ algorithm. Accordingly we concentrate on square A and B of order n and assume for the moment that $\det(A-\lambda B)\not\equiv 0$, i.e., that the pencil is regular, and therefore its K.c.f. contain no L_ε or L_η^T blocks. We write

$$\det(A-\lambda B)=a_r\lambda^r+a_{r-1}\lambda^{r-1}+\cdots+a_0 \qquad (r\leqslant n), \tag{3.1}$$

where a_r is the first nonvanishing coefficient. Notice that r could be zero, in which case $\det(A-\lambda B)=a_0\neq 0$. The equation $\det(A-\lambda B)=0$ has r finite roots, some of which may be zero, though these should not be regarded as special. For the homogeneous pencil we have

$$\det(\mu A-\lambda B)=\mu^{n-r}(a_r\lambda^r+a_{r-1}\lambda^{r-1}\mu+\cdots+a_0\mu^r), \tag{3.2}$$

and $\det(A-\lambda B)=0$ may accordingly be regarded as a polynomial equation of degree n having $n-r$ infinite roots. Adopting this convention, there are always n roots $\alpha_1,\alpha_2,\ldots,\alpha_n$. Following the convention suggested above, we may regard these α_i as divided into two sets, those for which $|\alpha_i|\leqslant 1$ and those for which $|\alpha_i|>1$. For the latter we shall work with $\beta_i=1/\alpha_i$, and hence infinities are avoided. Corresponding to each α_i there is at least one unit eigenvector u_i. We write

$$Au_i=\alpha_i u_i \quad (|\alpha_i|\leqslant 1), \quad \beta_i Au_i=Bu_i \quad (|\alpha_i|>1). \tag{3.3}$$

Let us consider the simultaneous reduction of A and B to upper triangular matrices $\tilde{A}$ and $\tilde{B}$. This can be done entirely by unitary equivalences, and it is upon this theorem that the feasibility of the QZ algorithm depends. We give an elementary proof of it which sheds light on the nature of the diagonal elements in $\tilde{A}$ and $\tilde{B}$. We state the theorem in the following form.

If $\det(A-\lambda B)\not\equiv 0$ *and* $Au=\lambda Bu$ *has eigenvalues* α_i *(reciprocals* β_i*), then there exist unitary* Q *and* Z *such that*

$$QAZ=\tilde{A}, \qquad QBZ=\tilde{B}, \tag{3.4}$$

where $\tilde{A}$ and $\tilde{B}$ are upper-triangular with

$$\tilde{a}_{ii} = \alpha_i k_i, \quad \tilde{b}_{ii} = k_i(|\alpha_i| \leqslant 1), \tag{3.5}$$

$$\tilde{a}_{ii} = k_i, \tilde{b}_{ii} = \beta_i k_i \qquad (|\alpha_i| > 1), \tag{3.6}$$

and the k_i are nonzero. The α_i may be taken to be in any order.

The proof is by induction. It is obviously true when $n = 1$; we assume it is true for matrices of order up to $n-1$ and then prove it is true for matrices of order n.

Corresponding to α_1 we have a unit vector u_1 such that

$$Au_1 = \alpha_1 Bu_1 \quad (|\alpha_1| \leqslant 1), \qquad \beta_1 Au_1 = Bu_1 \quad (|\alpha_1| > 1). \tag{3.7}$$

Let

$$u_1 = Z_1 e_1, \tag{3.8}$$

where Z_1 is unitary and e_1 is the first column of the identity. Then

$$AZ_1 e_1 = \alpha_1 BZ_1 e_1 \quad \text{or} \quad \beta_1 AZ_1 e_1 = BZ_1 e_1. \tag{3.9}$$

Writing

$$AZ_1 = G \quad \text{and} \quad BZ_1 = H, \tag{3.10}$$

we have

$$Ge_1 = \alpha_1 He_1 \quad \text{or} \quad \beta_1 Ge_1 = He_1. \tag{3.11}$$

Now $Ge_1 = g_1$ and $He_1 = h_1$, where g_1 and h_1 are the first columns of G and H respectively. At least one of g_1 and h_1 is nonnull, because if both were, then

$$0 \equiv \det(G - \lambda H) = \det(A - \lambda B)\det(Z_1), \tag{3.12}$$

and hence $\det(A - \lambda B) \equiv 0$, contrary to hypothesis. From Eq. (3.11) we have certainly

$$h_1 = He_1 \neq 0 \quad (|\alpha_1| \leqslant 1), \qquad g_1 = Ge_1 \neq 0 \quad (|\alpha_1| > 1). \tag{3.13}$$

Let Q_1 be a unitary matrix such that

$$Q_1 h_1 = k_1 e_1 \quad (|\alpha_1| \leqslant 1), \qquad Q_1 g_1 = k_1 e_1 \quad (|\alpha_1| > 1), \tag{3.14}$$

where $k_1 \neq 0$. We have

$$Q_1 H = Q_1 B Z_1 = \left[\begin{array}{c|c} k_1 & b_1^T \\ \hline 0 & B_2 \end{array}\right], \qquad Q_1 G = Q_1 A Z_1 = \left[\begin{array}{c|c} \alpha_1 k_1 & a_1^T \\ \hline 0 & A_2 \end{array}\right] \quad (|\alpha_1| \leqslant 1), \tag{3.15}$$

$$Q_1 G = Q_1 A Z_1 = \left[\begin{array}{c|c} k_1 & a_1^T \\ \hline 0 & A_2 \end{array}\right], \qquad Q_1 H = Q_1 B Z_1 = \left[\begin{array}{c|c} \beta_1 k_1 & b_1^T \\ \hline 0 & B_2 \end{array}\right] \quad (|\alpha_1| > 1), \tag{3.16}$$

where A_2 and B_2 are square matrices of order $n-1$. Since

$$\begin{aligned} \det Q_1 \det(A - \lambda B) \det Z_1 &= \det(Q_1 A Z_1 - \lambda Q_1 B Z_1) \\ &= k_1(\alpha_1 - \lambda) \det(A_2 - \lambda B_2) \qquad (|\alpha_1| \leqslant 1) \\ &= k_1(1 - \beta_1 \lambda) \det(A_2 - \lambda B_2) \qquad (|\alpha_1| > 1), \end{aligned} \tag{3.17}$$

it is clear that the eigenvalues of $A_2 u = \lambda B_2 u$ must be $\alpha_2, \alpha_3, \ldots, \alpha_n$ whatever the distribution of finite and infinite values this set may have. From the inductive hypothesis A_2 and B_2 may be reduced to upper-triangular form with the required diagonal elements using unitary equivalences, the proof follows in the obvious way.

Notice that the α_i could have been listed in any order and would then occur in that order in the triangular matrices. Corresponding to each infinite α_i, we work with a zero β_i and hence obtain a zero diagonal element $\tilde{b}_{ii}$ in $\tilde{B}$. We cannot have a zero $\tilde{a}_{ii}$ coupled with a zero $\tilde{b}_{ii}$; this is because $k_i \neq 0$, which is itself a consequence of the regularity of the pencil.

4. SQUARE SINGULAR PENCILS

Suppose now that $\det(A - \lambda B) \equiv 0$, so that the pencil $A - \lambda B$ is singular. Let us attempt to follow through the proof of the simultaneous reducibility of A and B to triangular form. If now α_1 is any number whatever, we have

$\det(A-\alpha_1 B)=0$, and hence there is a nonnull unit vector u_1 such that

$$Au_1=\alpha_1 Bu_1 \quad (|\alpha_1|\leqslant 1) \quad \text{or} \quad \beta_1 Au_1=Bu_1 \quad (|\alpha_1|<1). \tag{4.1}$$

The argument proceeds as before until we reach the comment that "at least one of the vectors g_1 and h_1 must be nonnull." We can no longer make this assertion, since it depended on the hypothesis $\det(A-\lambda B)\not\equiv 0$.

If nevertheless one or other (or both) *is* nonnull, then exactly as before we have a reduction to one or other of the forms (3.15) or (3.16) with $k_1\neq 0$. Clearly $\det(A_2-\lambda B_2)\equiv 0$, since if not, this would imply $\det(A-\lambda B)\not\equiv 0$. Hence in this case an arbitrary α_2 would satisfy $\det(A_2-\alpha_2 B_2)=0$ and we can continue with the next step of the reduction.

When, on the other hand, both g_1 and h_1 are null, we have

$$AZ_1=\left[\begin{array}{c|c} 0 & a_1^T \\ \hline 0 & A_2 \end{array}\right], \qquad BZ_1=\left[\begin{array}{c|c} 0 & b_1^T \\ \hline 0 & B_2 \end{array}\right]. \tag{4.2}$$

Since the equations (4.2) imply that

$$0\equiv \det Z_1 \det(A-\lambda B) = 0\det(A_2-\lambda B_2) \tag{4.3}$$

we cannot claim that $\det(A_2-\lambda B_2)\equiv 0$ in this case. It may or may not be true. Notice though that the first stage of the reduction has already assured final triangular forms in which $\tilde{a}_{11}=\tilde{b}_{11}=0$.

If we think of the reduction to triangular form as taking place in $n-1$ stages, then there must be at least one stage at which the current reduced matrices have $\tilde{a}_{ii}=\tilde{b}_{ii}=0$, since if we could complete the reduction without this happening it would imply $\det(A-\lambda B)\not\equiv 0$. Notice that if at any stage we reach matrices A_r and B_r such that $\det(A_r-\lambda B_r)\not\equiv 0$, then from that stage onwards we cannot choose the values of α_i arbitrarily.

The above discussion gives some insight into the degree of arbitrariness of the ratios of the $\tilde{a}_{ii}$ and $\tilde{b}_{ii}$ that can arise when $\det(A-\lambda B)\equiv 0$. Not only must $\tilde{A}$ and $\tilde{B}$ have $\tilde{a}_{ii}=\tilde{b}_{ii}=0$ for at least one i, but it appears highly probable that there will be some nonzero pairs $\tilde{a}_{jj}$ and $\tilde{b}_{jj}$ (which are not in any sense small) with arbitrary ratios.

We have not quite proved this, because although α_1 was indeed arbitrary, and could in particular have been taken to be zero or infinity, when k_1 is zero we do not obtain nonzero values for the 1,1 elements of the reduced A and B. However, it is easy to see that when $\tilde{a}_{ii}=\tilde{b}_{ii}=0$ for some i, then in general we can have nonzero diagonal elements $\tilde{a}_{jj}$ and $\tilde{b}_{jj}$ with arbitrary ratios. Consider, for example, the two triangular matrices

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ & 0 & a_{23} & a_{24} \\ & & a_{33} & a_{34} \\ & & & a_{44} \end{bmatrix}, \quad B = \begin{bmatrix} b_{11} & b_{12} & b_{13} & b_{14} \\ & 0 & b_{23} & b_{24} \\ & & b_{33} & b_{34} \\ & & & b_{44} \end{bmatrix}, \tag{4.4}$$

for which $a_{22} = b_{22} = 0$. If all the other elements in the upper triangles are full-sized numbers, it might be thought that a_{ii}/b_{ii} $(i = 1, 3, 4)$ are necessarily bona fide eigenvalues, or at least have some meaningful relationship with the problem $Au = \lambda Bu$.

However, let us consider the matrices AR_{12} and BR_{12}, where R_{12} is a rotation in the $(1, 2)$ plane. In the regular case this transformation certainly leaves the eigenvalues unaltered. The matrices AR_{12} and BR_{12} are of the form

$$\begin{bmatrix} a'_{11} & a'_{12} & a_{13} & a_{14} \\ & 0 & a_{23} & a_{24} \\ & & a_{33} & a_{34} \\ & & & a_{44} \end{bmatrix} \text{ and } \begin{bmatrix} b'_{11} & b'_{12} & b_{13} & b_{14} \\ & 0 & b_{23} & b_{24} \\ & & b_{33} & b_{34} \\ & & & b_{44} \end{bmatrix}, \tag{4.5}$$

where

$$\begin{aligned} a'_{11} &= a_{11}c - a_{12}s, \qquad & a'_{12} &= a_{11}s + a_{12}c, \\ b'_{11} &= b_{11}c - b_{12}s, \qquad & b'_{12} &= b_{11}s + b_{12}c, \end{aligned} \tag{4.6}$$

in which c and s are the cosine and sine associated with the rotation.

The zero diagonal elements persist, and we now have

$$\frac{a'_{11}}{b'_{11}} = \frac{a_{11}c - a_{12}s}{b_{11}c - b_{12}s}. \tag{4.7}$$

Unless $a_{11}/a_{12} = b_{11}/b_{12}$, the right-hand side of (4.7) can be made to take any given value by a suitable choice of c and s; in particular it can be made to take the value zero or infinity. Similarly if we premultiply by a rotation in the $(2, 3)$ plane, we can produce values of a'_{33} and b'_{33} having arbitrary ratios. By premultiplication with more complicated matrices (they need not, of course, be unitary) one can produce equivalent triangular matrices A' and B' with $a'_{22} = b'_{22} = 0$ and having an arbitrary value of a'_{44}/b'_{44}.

The apparently well-determined ratios are therefore of no true significance. Note however that if the zero elements a_{22} and b_{22} are replaced by nonzero elements, however small, the pencil $A-\lambda B$ becomes regular and now has four eigenvalues given by the four ratios a_{ii}/b_{ii}. In practical applications of the QZ algorithm one will rarely obtain an exactly zero pair of a_{ii} and b_{ii}. However, if $a_{ii}=\varepsilon_1$ and $b_{ii}=\varepsilon_2$, then perturbations $-\varepsilon_1$ in A and $-\varepsilon_2$ in B will give a singular pencil. This means that if the original data were not exact or if rounding errors are involved in the execution of the QZ algorithm, the emergence of negligible pair of $\tilde{a}_{ii}$ and $\tilde{b}_{ii}$ will usually imply that even those eigenvalues based on apparently satisfactory pairs of $\tilde{a}_{jj}$ and $\tilde{b}_{jj}$ may be of little true significance.

So far we have merely shown that when $\det(A-\lambda B)\equiv 0$ the ratios $\tilde{a}_{ii}/\tilde{b}_{ii}$ cannot be taken at their face value. A natural question to ask is the following:

Suppose the Kronecker canonical form really does have a regular part; this will correspond to true elementary divisors, finite and/or infinite. Will equivalent triangular $\tilde{A}$ and $\tilde{B}$ give the corresponding eigenvalues?

It is easy to see that they will not necessarily do so. Consider for example a pencil $A-\lambda B$ with the K.c.f.

$$A=\left[\begin{array}{cc|c|c} 2 & 1 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ \hline 0 & 0 & 3 & 0 \\ \hline 0 & 0 & 0 & 0 \end{array}\right], \qquad B=\left[\begin{array}{cc|c|c} 1 & & & \\ & 1 & & \\ \hline & & 1 & \\ \hline & & & 0 \end{array}\right]. \tag{4.8}$$

This is obviously singular, the elements in its K.c.f. corresponding to an L_0 and L_0^T and elementary divisors $(2-\lambda)^2$ and $(3-\lambda)$. However, multiplying A and B on the right with a matrix which permutes columns 1, 2, 3, 4 to 2, 3, 4, 1 respectively, the matrices become

$$\left[\begin{array}{c|cc|c} 0 & 2 & 1 & 0 \\ 0 & 0 & 2 & 0 \\ \hline 0 & 0 & 0 & 3 \\ \hline 0 & 0 & 0 & 0 \end{array}\right] \quad \text{and} \quad \left[\begin{array}{c|cc|c} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \\ \hline 0 & 0 & 0 & 0 \end{array}\right]. \tag{4.9}$$

The matrices are still upper-triangular, but all diagonal elements are zero. Examination of the diagonal elements gives no indication of the perfectly genuine elementary divisors. If we consider A and B in the form given in (4.9), it is obvious that nonzero perturbations $\varepsilon_1,\varepsilon_2,\varepsilon_3,\varepsilon_4$ in the diagonal element of A and nonzero perturbations $\eta_1,\eta_2,\eta_3,\eta_4$ in the diagonal element of B make the pencil $A-\lambda B$ regular, with eigenvalues ε_i/η_i. Indeed, provided we do not have $\varepsilon_i = \eta_i = 0$ for any value of i, we can permit zero values among the ε_i and η_j, and these merely lead to zero and infinite eigenvalues respectively.

This means, somewhat disappointingly, that when $\det(A - \lambda B) \equiv 0$ even quite respectable elementary divisors may be completely destroyed by arbitrarily small perturbations. Clearly, when $A - \lambda B$ is not exactly singular but merely very close to singular, small perturbations may cause the eigenvalues to move about almost arbitrarily. However, the situation is not quite as bad as that. Consider the matrices

$$A = \begin{bmatrix} 2 & 0 \\ 0 & 0 \end{bmatrix}, \qquad B = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \tag{4.10}$$

which correspond to a singular pencil but with a true elementary divisor $2-\lambda$ and an eigenvalue of 2. Consider now the neighboring problem with

$$\tilde{A} = \begin{bmatrix} 2+\varepsilon_1 & \varepsilon_2 \\ \varepsilon_3 & \varepsilon_4 \end{bmatrix}, \qquad B = \begin{bmatrix} 1+\eta_1 & \eta_2 \\ \eta_3 & \eta_4 \end{bmatrix}, \tag{4.11}$$

for which

$$\det(\tilde{A} - \lambda\tilde{B}) = [(2+\varepsilon_1) - (1+\eta_1)\lambda](\varepsilon_4 - \eta_4\lambda) - (\varepsilon_2 - \eta_2\lambda)(\varepsilon_3 - \eta_3\lambda). \tag{4.12}$$

For almost all small perturbations ε_i and η_i the equation $\det(\tilde{A} - \lambda\tilde{B}) = 0$ has a root which is very close to 2. Only very special perturbations affect this root at all seriously; e.g. if $\varepsilon_4 = \eta_4 = 0$, then the roots are ε_2/η_2 and ε_3/η_3, and these values may be arbitrarily different from 2.

5. NUMERICAL EXAMPLES

The points discussed in the previous section are illustrated by the performance of the QZ algorithm on a number of simple examples. In Examples 1 and 2 we have taken a pair of matrices A and B of order four and have applied the QZ algorithm

(i) to A and B themselves,
(ii) to AP and BP,
(iii) to PAP and PBP,

where P is the permutation matrix

$$\begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}.$$

When $A-\lambda B$ is a regular pencil, the eigenvalues are identical for all three problems, but when $A-\lambda B$ is a singular pencil we shall expect some (or all) of the "alleged" eigenvalues to be quite different for the three cases. The computations were performed on KDF9, which is a binary floating-point computer with a 39-digit mantissa. For convenience of presentation and of comparison, we give only ten decimal digits, although $2^{39} \doteqdot 10^{11.7}$. This effectively suppresses the effect of rounding errors, which are, in any case, of negligible significance in most of these examples.

EXAMPLE 1.

$$A=\begin{bmatrix} 4 & 3 & 2 & 5 \\ 6 & 4 & 2 & 7 \\ -1 & -1 & -2 & -2 \\ 5 & 3 & 2 & 6 \end{bmatrix}, \quad B=\begin{bmatrix} 3 & 1 & 3 & 4 \\ 3 & 3 & 3 & 5 \\ 0 & 0 & -3 & -2 \\ 3 & 1 & 3 & 5 \end{bmatrix}.$$

The matrix A is singular, and the matrix B is non-singular and well-conditioned with respect to inversion. We give the values of the diagonal elements $\tilde{a}_{ii}$ and $\tilde{b}_{ii}$ of the triangular matrices produced by the QZ algorithm and the ratios $\tilde{a}_{ii}/\tilde{b}_{ii}$ for each of the cases (i), (ii) and (iii).

CASE (i). MATRICES A AND B THEMSELVES

$\tilde{a}_{ii}$	$\tilde{b}_{ii}$	$\lambda_i=\tilde{a}_{ii}/\tilde{b}_{ii}$
$-2.7009\,97936_{10}-11$	$+6.6666\,66667_{10}-1$	$-4.0514\,96904_{10}-11$
$+1.3391\,28080_{10}+1$	$+9.3367\,27217_{10}+0$	$+1.4342\,58546_{10}+0$
$+1.5125\,58290_{10}+0$	$+2.2688\,37435_{10}+0$	$+6.6666\,66667_{10}-1$
$+2.9622\,17979_{10}-1$	$+1.2745\,75935_{10}+0$	$+2.3240\,81208_{10}-1$

CASE (ii). MATRICES AP AND BP

$\tilde{a}_{ii}$	$\tilde{b}_{ii}$	$\lambda_i=\tilde{a}_{ii}/\tilde{b}_{ii}$
$-5.9674\,39491_{10}-12$	$+6.6666\,66667_{10}-1$	$-8.9511\,59237_{10}-12$
$+1.3391\,28080_{10}+1$	$+9.3367\,27216_{10}+0$	$+1.4342\,58546_{10}+0$
$+4.7223\,08852_{10}-1$	$+2.0319\,03548_{10}+0$	$+2.3240\,81207_{10}-1$
$+9.4880\,01526_{10}-1$	$+1.4232\,00229_{10}+0$	$+6.6666\,66667_{10}-1$

Case (iii) Matrices PAP and PBP

$\tilde{a}_{ii}$	$\tilde{b}_{ii}$	$\lambda_P \tilde{a}_{ii}/\tilde{b}_{ii}$
$-2.4209\,14657_{10}-12$	$+6.6666\,66667_{10}-1$	$-3.6313\,71985_{10}-12$
$1.3391\,28080_{10}+1$	$+9.3367\,27216_{10}+0$	$+1.4342\,58546_{10}+0$
$4.7223\,08852_{10}-1$	$+2.0319\,03548_{10}+0$	$+2.3240\,81208_{10}-1$
$9.4880\,01525_{10}-1$	$+1.4232\,00229_{10}+0$	$+6.6666\,66667_{10}-1$

In each case one of the elements $\tilde{a}_{ii}$ is negligible and the three sets of eigenvalues agree almost to the working accuracy. One of the eigenvalues is negligible, which is to be expected, since A is singular and of rank three and B is nonsingular. The computed vectors were also in very close agreement, and all residuals were negligible.

Example 2.

$$A=\begin{bmatrix}4 & 3 & 2 & 5\\ 6 & 4 & 2 & 7\\ -1 & -1 & -2 & -2\\ 5 & 3 & 2 & 6\end{bmatrix},\quad B=\begin{bmatrix}2 & 1 & 3 & 4\\ 3 & 3 & 3 & 5\\ 0 & 0 & -3 & -2\\ 3 & 1 & 3 & 5\end{bmatrix}.$$

The matrix A is identical with that in Example 1, while B differs from that in Example 1 only in its (1,1) element and is now singular. Further, it may be verified that $\det(A-\lambda B)\equiv 0$, so that the pencil $A-\lambda B$ is singular. The computed results for the three cases are as follows. Since some of the a_{ii} and some of the "alleged" λ_i are now complex, the layout is slightly different for cases (i) and (iii):

Case (i). matrices A and B themselves

$\tilde{a}_{ii}$	$\tilde{b}_{ii}$
$+1.9332\,24953_{10}+0$	$+2.4138\,04758_{10}+0$
$+3.7405\,52679_{10}-10$	$+1.9956\,68463_{10}-10$
$+3.2187\,03829_{10}-1+(1.9076\,54397_{10}-1)i$	$+4.6918\,93487_{10}-1$
$+4.7604\,90373_{10}-2-(2.8214\,37099_{10}-1)i$	$+6.9393\,50421_{10}-1$

'λ'$_i=\tilde{a}_{ii}/\tilde{b}_{ii}$
$+8.0090\,36139_{10}-1$
$+1.8743\,35717_{10}+0$
$+6.8601\,38319_{10}-2+(4.0658\,51884_{10}-1)i$
$+6.8601\,38319_{10}-2-(4.0658\,51884_{10}-1)i$

Case (ii). matrices *AP* and *BP*

$\tilde{a}_{ii}$	$\tilde{b}_{ii}$	$'\lambda$
$9_i = \tilde{a}_{ii}/\tilde{b}_{ii}$		
$+4.1298\,40501_{10}+0$	$+6.2714\,90903_{10}+0$	$+6.5851\,01637_{10}-1$
$+1.7169\,30977_{10}-10$	$+1.1900\,68398_{10}-10$	$+1.4427\,16217_{10}+0$
$-1.8933\,16041_{10}-1$	$+5.3216\,43685_{10}-1$	$-3.5577\,65520_{10}-1$
$-2.8853\,97811_{10}-1$	$+2.8902\,71747_{10}-1$	$-9.9831\,36757_{10}-1$

Case (iii). matrices *PAP* and *PBP*

$\tilde{a}_{ii}$	$\tilde{b}_{ii}$
$+6.2346\,91954_{10}-1+(2.2113\,96258_{10}-1)i$	$+4.0831\,93280_{10}-1$
$+9.9724\,17516_{10}-10-(3.5371\,38152_{10}-10)i$	$+6.5310\,85815_{10}-10$
$+4.1156\,63077_{10}-1$	$+7.3322\,18461_{10}-1$
$-1.9986\,46939_{10}-1$	$+5.5039\,91337_{10-1}$

$'\lambda'_i = \tilde{a}_{ii}/\tilde{b}_{ii}$
$+1.5269\,15707_{10}+0+(5.4158\,50063_{10}-1)i$
$+1.5269\,15707_{10}+0-(5.4158\,50063_{10}-1)i$
$+5.6131\,21184_{10}-1$
$-3.6312\,68322_{10}-1$

In each case there is a value of i for which both $\tilde{a}_{ii}$ and $\tilde{b}_{ii}$ are negligible, as was to be expected. Naturally there is no agreement between the λ_i computed from the ratios of these negligible quantities. However, the λ_i computed from the other ratios are also in total disagreement, even though they came from full-sized $\tilde{a}_{ii}$ and $\tilde{b}_{ii}$. Cases (i) and (iii) each give a pair of complex λ_i (though they bear no relation to each other), while case (ii) gives four real λ_i. Nevertheless, all residuals were negligible to working accuracy.

Example 3.

Case (i). For this example we took as our basic matrices

$$A = \begin{bmatrix} 3 & 1 & 1 & 0 \\ 0 & 2 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \qquad B = \begin{bmatrix} 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

The pencil $A-\lambda B$ is obviously singular, but there are three genuine elementary divisors $3-\lambda$, $2-\lambda$ and $1-\lambda$. The QZ algorithm recognized that both A

and B were upper-triangular and therefore skipped all stages in the reduction and produced exact answers.

Case (ii). The matrices

$$A=\begin{bmatrix}0 & 3 & 1 & 1\\ 0 & 0 & 2 & 1\\ 0 & 0 & 0 & 1\\ 0 & 0 & 0 & 0\end{bmatrix}, \quad B=\begin{bmatrix}0 & 1 & 1 & 1\\ 0 & 0 & 1 & 1\\ 0 & 0 & 0 & 1\\ 0 & 0 & 0 & 0\end{bmatrix}$$

were obtained by permuting columns of the basic A and B conformally. Again the QZ algorithm recognized that the matrices were already upper-triangular and skipped all steps. However, since all diagonal elements of the A and B are zero, it naturally decided that all eigenvalues were indeterminate and failed to recognize the genuine elementary divisors.

Case (iii). The matrices

$$A=\begin{bmatrix}1 & 1 & 3 & 0\\ 1 & 2 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{bmatrix}, \quad B=\begin{bmatrix}1 & 1 & 1 & 0\\ 1 & 1 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{bmatrix}$$

were again obtained by permuting the columns of the basic A and B. The QZ algorithm now involved genuine computation with rounding errors. The diagonal elements of the computed upper-triangular matrices and the computed eigenvalues were

$\tilde{a}_{ii}$	$\tilde{b}_{ii}$	$\lambda_i = \tilde{a}_{ii}/\tilde{b}_{ii}$
$3.0000\,00000_{10}+0$	$1.0000\,00000_{10}+0$	$3.0000\,00000_{10}+0$
$1.4142\,13562_{10}+0$	$1.4142\,13562_{10}+0$	$1.0000\,00000_{10}+0$
$1.4142\,13562_{10}+0$	$7.0710\,67812_{10}+0$	$2.0000\,00000_{10}+0$
$0.0000\,00000$	$0.0000\,00000$	Indeterminate

The eigenvalues were given correct to working accuracy.

Case (iv). The matrices

$$A=\begin{bmatrix}1 & 1 & 3 & \varepsilon\\ 1 & 2 & \varepsilon & 0\\ 1 & \varepsilon & 0 & 0\\ \varepsilon & 0 & 0 & 0\end{bmatrix}, \quad B=\begin{bmatrix}1 & 1 & 1 & \varepsilon\\ 1 & 1 & 2\varepsilon & 0\\ 1 & 3\varepsilon & 0 & 0\\ 4\varepsilon & 0 & 0 & 0\end{bmatrix}$$

were derived from the A and B of case (iii) by adding perturbations in the secondary diagonal. For any nonzero value of ε the matrices A and B are nonsingular and the eigenvalues are (exactly) 1, $\frac{1}{2}$, $\frac{1}{3}$ and $\frac{1}{4}$. For $\varepsilon = 0$ the pencil is singular, but there are three true eigenvalues 3, 2 and 1. Values of $\varepsilon = 10^{-9}$, 10^{-7}, 10^{-3} and 10^{-1} were tried, and the results were as follows:

$\varepsilon = 10^{-9}$

$\tilde{a}_{ii}$	$\tilde{b}_{ii}$	$\lambda_i = \tilde{a}_{ii}/\tilde{b}_{ii}$
$-2.0002\,54759_{10}-8$	$+0.0000\,00000$	Infinite
$+3.0734\,74417_{10}-4$	$+1.0244\,82499_{10}-4$	$+3.0000\,26277_{10}+0$
$+5.7046\,43522_{10}-1$	$+5.7040\,49228_{10}-1$	$+1.0001\,04188_{10}+0$
$+9.4117\,54580_{10}-4$	$+4.7058\,77290_{10}-4$	$+2.0000\,00000_{10}+0$

$\varepsilon = 10^{-7}$

$\tilde{a}_{ii}$	$\tilde{b}_{ii}$	$\lambda_i = \tilde{a}_{ii}/\tilde{b}_{ii}$
$-2.0000\,17373_{10}-6$	$+0.0000\,00000$	Infinite
$+1.5688\,66556_{10}-4$	$+7.9511\,36649_{10}-5$	$+1.9731\,34944_{10}+0$
$+6.7693\,15682_{10}-2$	$+2.2164\,49806_{10}-2$	$+3.0541\,25415_{10}+0$
$+6.0001\,68768_{10}-6$	$+2.9992\,68091_{10}-6$	$+2.0005\,44328_{10}+0$

$\varepsilon = 10^{-3}$

$\tilde{a}_{ii}$	$\tilde{b}_{ii}$	$\lambda_i = \tilde{a}_{ii}/\tilde{b}_{ii}$
$+2.5055\,38348_{10}-3$	$+7.5052\,69298_{10}-3$	$+3.3383\,72347_{10}-1$
$+3.4300\,70603_{10}-3$	$+1.3738\,17575_{10}-2$	$+2.4967\,43865_{10}-1$
$+1.1393\,32748_{10}-3$	$+2.2795\,05214_{10}-3$	$+4.9981\,58114_{10}-1$
$+1.0211\,23529_{10}+0$	$+1.0211\,16748_{10}+0$	$+1.0000\,06640_{10}+0$

$\varepsilon = 10^{-1}$

$\tilde{a}_{ii}$	$\tilde{b}_{ii}$	$\lambda_i = \tilde{a}_{ii}/\tilde{b}_{ii}$
$+4.3852\,90097_{10}-1$	$+8.7705\,80193_{10}-1$	$+5.0000\,00000_{10}-1$
$+2.2803\,50850_{10}+0$	$+2.2803\,50850_{10}+0$	$+1.0000\,00000_{10}+0$
$+1.0000\,00000_{10}+0$	$+3.0000\,00000_{10}+0$	$+3.3333\,33333_{10}-1$
$+1.0000\,00000_{10}+0$	$+4.0000\,00000_{10}+0$	$+2.5000\,00000_{10}-1$

This is perhaps the most interesting example. If we think of the matrices of case (iii) as the basic matrices, then those of case (iv) are affected by two sets of perturbations: First, the highly specific perturbations of order ε which we have added to the secondary diagonal. Second the perturbations equivalent to the rounding errors made in the course of the QZ algorithms; on KDF9 these are relative errors of the order of magnitude 2^{-39}. The rounding errors are not randomly distributed over the whole of A and B, since the last row and column of both A and B contain only one nonzero element and that is of order ε. When ε is small, the matrices to which the computed results correspond may be regarded as very close to those of case (iii). As ε becomes larger, a point must be reached at which the effective matrices behave as though they were close to an A and B with eigenvalues 1, $\frac{1}{2}$, $\frac{1}{3}$ and $\frac{1}{4}$.

The results show this behavior very clearly. When $\varepsilon = 10^{-9}$ there are still eigenvalues very close to 1, 2 and 3, and there is one infinite eigenvalue, though this comes from an a_{ii} which is of order 10^{-8} coupled with a zero b_{ii}. Notice that $\tilde{a}_{22}$, $\tilde{b}_{22}$, $\tilde{a}_{44}$ and $\tilde{b}_{44}$ are all of magnitude 10^{-4}, i.e. quite small. With $\varepsilon = 10^{-7}$ the matrix is already losing touch with the original; there are eigenvalues reasonably close to 2 and 3, but the eigenvalue 1 has been lost. Most of the $\tilde{a}_{ii}$ and $\tilde{b}_{ii}$ are quite small.

With $\varepsilon = 10^{-3}$ we have moved decisively to the regime with eigenvalues 1, $\frac{1}{2}$, $\frac{1}{3}$ and $\frac{1}{4}$. The computed values now have three figures correct and are derived from $\tilde{a}_{ii}$ and $\tilde{b}_{ii}$, which are all at least as large as 10^{-3}. With $\varepsilon = 10^{-1}$ the computed eigenvalues are correct to working accuracy and the $\tilde{a}_{ii}$ and $\tilde{b}_{ii}$ are of full size. As is to be expected, all residuals corresponding to all eigenvalues of all matrices are negligible to working accuracy.

Case (v). As a final example we took

$$A = \begin{bmatrix} 1 & 1 & 3 & 5 \\ 2 & 3 & 3 & 8 \\ 2 & 1 & 3 & 6 \\ 1 & 1 & 3 & 5 \end{bmatrix}, \qquad B = \begin{bmatrix} 1 & 1 & 1 & 3 \\ 2 & 2 & 1 & 5 \\ 2 & 1 & 1 & 4 \\ 1 & 1 & 1 & 3 \end{bmatrix},$$

which are derived from exact elementary transformations of the matrix of case (i). The computed $\tilde{a}_{ii}$, $\tilde{b}_{ii}$ and λ_i were

$\tilde{a}_{ii}$	$\tilde{b}_{ii}$	$\lambda_i = \tilde{a}_{ii}/\tilde{b}_{ii}$
$+3.1622\,77660_{10}+0$	$+3.1622\,77660_{10}+0$	$+1.0000\,00000_{10}+0$
$+1.0259\,78352_{10}-1$	$+3.4199\,27841_{10}-2$	$+2.9999\,99999_{10}+0$
$+1.7592\,67639_{10}+0$	$+8.7963\,38193_{10}-1$	$+2.0000\,00000_{10}+0$
$+1.3520\,61076_{10}-11$	$+0.0000\,00000$	Infinite

The genuine eigenvalues are preserved to full working accuracy; there is one infinite eigenvalue, but this is derived from an $\tilde{a}_{ii}$ of order 10^{-11} coupled with a zero $\tilde{b}_{ii}$ and clearly shows that the pencil is singular.

6. GENERAL COMMENTS

The material presented in this paper should in no way be regarded as constituting an adverse criticism of the QZ algorithm. In all of our examples, however pathological, the QZ algorithm has given exact eigenvalues and eigenvectors of matrices differing from A and B by perturbations of the order of magnitude of rounding errors. In that sense it continues to give best possible results.

Our purpose has been to expose the properties of singular pencils and their consequences for practical algorithms. P. van Dooren [1] has suggested that the QZ algorithm should be preceded by an algorithm which extracts the singular part (if any) of the pencil, and we strongly support this recommendaiton. It should be appreciated that when an attempt is made to recognize the singular part by means of an algorithm which, in general, will involve rounding errors, decisions concerning the ranks of matrices are necessarily involved. If van Dooren's policy is adopted, these decisions are made in the most favorable context.

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Received 18 December 1978