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On certain methods for expanding the characteristic polynomial

By

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A number of methods are available for expanding the characteristic polynomial of a matrix, symmetric, Hermitian, or otherwise, some obviously similar, others apparently quite disparate in principle. One of us (F. L. BAUER) has pointed out that the method of DANILEVSKIĬ is in principle an extension of the method of KRYLOV. The purpose of this paper is to show systematically that this applies equally to a wider class of methods. Briefly, KRYLOV forms a sequence of vectors

$$v_1, v_2 = A v_1, \quad v_3 = A v_2, \ldots \tag{1}$$

and by means of these obtains a set of linear equations satisfied by the coefficients of the minimal polynomial, or by some divisor of it, an idea previously used for theoretical purposes for example by TURNBULL and AITKEN. The methods to be discussed will be shown to amount to the application of particular methods for solving the system.

The methods may therefore be considered mathematically equivalent. This is not to say, of course, that they are computationally equivalent, or equivalent from the point of view of the programmer. Obviously the superficial disparities would ordinarily be reflected in differences in the organization of the computations. Moreover, there are efficient and inefficient ways of solving equations. Nevertheless, the recognition of genetic relationships will serve to exhibit common strengths and weaknesses and, perhaps, permit greater flexibility of application.

Perhaps the oldest method, other than that of direct evaluation of principal minors, is due to LEVERRIER (1840). This method has been rediscovered, and somewhat elaborated, in much more recent times: HORST, FADDEEV and SOMINSKIĬ, SOURIAU, FRAME, WEGNER. These methods are based upon the Newton identities relating the coefficients of an equation with sums of powers of the roots, and require repeated powers of the matrix. These methods will be considered to be a distinct family, and not be discussed here, although KRYLOV refers back to Leverrier in the development of his own method. Also excluded from present consideration will be escalator methods, or methods of enlargement, including Samuelson's method. Other methods possess novelty only in handling the equation and not in its explicit development, hence are not of present concern. All references will be found in the list at the end and need not be mentioned individually, except where attention is called to a particular exposition.

If the matrix A is of order n, and its minimal polynomial of degree m, it can be shown that there exists a vector v_1 such that in the sequence (1), the

first m will be linearly independent and the first $m+1$ linearly dependent. In fact, this is true of "almost every" vector in the space. Then if V is the matrix of order m whose columns are $v_1, \ldots, v_m$:

$$V = (v_1, v_2, \ldots, v_m), \tag{2}$$

this matrix is of rank m, and v_{m+1} is expressible by

$$Vf + v_{m+1} = 0, \tag{3}$$

where the elements of f are the coefficients of the minimal polynomial $\psi(\lambda)$. In fact, if the vector $l = l(\lambda)$ is defined by

$$l^T = (1, \lambda, \ldots, \lambda^{m-1}), \tag{4}$$

then the minimal equation is precisely

$$\psi(\lambda) \equiv l^T f + \lambda^m = 0. \tag{5}$$

In case $m = n$, and the matrix is nonderogatory, one can eliminate the elements of f from (5) and (3) to obtain the determinantal equation

$$\det \begin{pmatrix} 1 & \lambda & \lambda^2 \ldots \lambda^n \\ v_1 & v_2 & v_3 \ldots v_{n+1} \end{pmatrix} = 0 \tag{6}$$

in which λ occurs only in the first row instead of along the diagonal. Furthermore, if one takes $v_1 = e_1$, the first column of the identity I, the determinant is immediately reducible to one of order n. This KRYLOV does. In case $m < n$, one drops rows from V so that the determinant is of order $m+1$, reducible to one of order m. Following KRYLOV, LUZIN and HLODOVSKIĬ discussed the method extensively in a series of papers listed below.

Observe, now, that when the equations are solved, one has

$$AV = VF, \tag{7}$$

where

$$F = J - f e_n^T, \qquad J = (e_2, e_3, \ldots, e_n, 0). \tag{8}$$

That is to say, F is the matrix with ones along the subdiagonal, with $-f$ in the last column, and zeros elsewhere. Almost any method for solving (3) would amount to the determination of a matrix U such that UV has some simple form, generally either a diagonal (possibly I), or a triangular matrix. Moreover, the matrix U is ordinarily generated as a product of matrices

$$U = \cdots U_2 U_1, \tag{9}$$

each matrix being of simple form and effecting a partial reduction of the matrix V. As one of us (F. L. BAUER) has shown, the DANILEVSKIĬ method applies the JORDAN reduction to reduce V to the identity:

$$UV = I.$$

The first step in this process is to take U_1 in the form

$$U_1 = I - \sigma_1 u_1 e_1^T, \tag{10}$$

where u_1 is a column vector, e_1 the first column of I, and σ_1 a scale factor introduced here for convenience. The vector u_1 and scalar σ_1 are to be selected so that

$$(I - \sigma_1 u_1 e_1^T) v_1 = e_1,$$

hence

$$u_1 = v_1 - e_1, \quad \sigma_1 e_1^T v_1 = 1. \tag{11}$$

This is always possible if $e_1^T v_1$, the first element of v_1, is non-null. The usual choice is, in fact, $v_1 = e_1$, whence $\sigma_1 = 1$ and this initial step in the reduction appears unnecessary.

In any case, let

$$V_1 = U_1 V, \quad A_1 = U_1 A U_1^{-1},$$

where $U_1 = I$ if $v_1 = e_1$, and the first column of V_1 is e_1. Next, form

$$U_2 = I - \sigma_2 u_2 e_2^T \tag{12}$$

so that

$$U_2 v_2' = e_2,$$

hence

$$u_2 = v_2' - e_2, \quad \sigma_2 e_2^T v_2' = 1, \tag{13}$$

where, of course, v_2' is the second column in V_1. If

$$V_2 = U_2 V_1, \quad A_2 = U_2 A_1 U_2^{-1},$$

then

$$A_2 V_2 = V_2 F \tag{14}$$

or, schematically,

$$\begin{pmatrix} * & * & * & \dots \\ * & * & * & \dots \\ * & * & * & \dots \end{pmatrix} \begin{pmatrix} 1 & 0 & * & \dots \\ 0 & 1 & * & \dots \\ 0 & 0 & * & \dots \\ . & . & . & . \end{pmatrix} = \begin{pmatrix} 1 & 0 & * & \dots \\ 0 & 1 & * & \dots \\ 0 & 0 & * & \dots \\ . & . & . & . \end{pmatrix} \begin{pmatrix} 0 & 0 & \dots \\ 1 & 0 & \dots \\ 0 & 1 & \dots \\ . & . & . \end{pmatrix}.$$

One verifies readily that on the right, the first column in the product is e_2 and, for this to be so, the first column of the first matrix on the left must be also e_2. Continuing, therefore, if

$$V_i = U_i V_{i-1} \quad A_i = U_i A_{i-1} U_i^{-1}, \tag{15}$$

where the first i columns of V_i agree with those of I, then the first $i-1$ columns of A_i agree with those of F. Moreover, the inverse of a matrix of the form $I - \sigma u v^T$ is easily written down: It is of the form $I - \tau u v^T$, with

$$\sigma^{-1} + \tau^{-1} = v^T u.$$

Eventually, $V_n = I$, and $A_n = F$.

In the actual application of Danilevskiĭ's method the explicit formation of the matrix V is unnecessary. Instead, if A_i agrees with F in its first $i-1$ columns, one can ask for a matrix U_{i+1} such that $U_{i+1} A_i U_{i+1}^{-1}$ agrees also in the ith column. The above discussion is intended to show, however, that this is entirely equivalent to the inversion of V. Moreover, as remarked above, if $v_1 = e_1$, then $U_1 = I$, and the first step in the reduction is evaded. On the other hand, the stability

of the system (3) to be solved, or the condition of the matrix V, will vary with the initial choice of v_1, as shown by one of us (F. L. BAUER), and the initial selection of a $U_1 \doteq I$ is equivalent to the selection of a $v_1 \doteq e_1$.

Since Danilevskii's method, in principle, applies the JORDAN method to the inversion of V, it is natural to consider the application of other methods of inversion. Chronologically Hessenberg's method comes next, and to facilitate subsequent developments it will be described in somewhat greater generality than would ordinarily be used. The method develops a sequence of vectors $b_1 = v_1$, b_2 as a linear combination of v_1 and $v_2, \ldots$, b_i a linear combination of $v_1, v_2, \ldots, v_i$. This leads to a matrix

$$B = V\,Q \tag{16}$$

of columns b_i, with Q an upper triangular matrix. The determination of Q is made after selecting a matrix C of linearly independent columns such that

$$C^T B = P \tag{17}$$

is lower triangular. It follows from this that

$$V^{-1} = Q\,P^{-1} C^T.$$

However, (7) can be written

$$A(V\,Q) = (V\,Q)\,(Q^{-1} F\,Q),$$

$$A\,B = B\,T, \tag{18}$$

where T has the HESSENBERG form

$$T = \begin{pmatrix} \tau_{11} & \tau_{12} & \tau_{13} & \cdots \\ \tau_{21} & \tau_{22} & \tau_{23} & \cdots \\ 0 & \tau_{32} & \tau_{33} & \cdots \\ . & . & . & . \end{pmatrix}, \tag{19}$$

and, indeed, if Q is unit upper triangular, then

$$\tau_{i+1,i} = 1.$$

The generalized HESSENBERG method, however, forms T and B (but not V) directly, and in fact, on considering (18) column by column, one has, first,

$$A\,b_1 = b_1 \tau_{11} + b_2,$$

the orthogonality condition leading to

$$c_1^T A\,b_1 = c_1^T b_1 \tau_{11}.$$

Hence if c_1 and b_1 are not themselves orthogonal, then τ_{11} and hence b_2 can be found. Next

$$A\,b_2 = b_1 \tau_{12} + b_2 \tau_{22} + b_3,$$

orthogonality providing that

$$c_1^T A\,b_2 = c_1^T b_1 \tau_{12},$$
$$c_2^T A\,b_2 = c_2^T b_1 \tau_{12} + c_2^T b_2 \tau_{22}.$$

If c_2 and b_2 are not orthogonal, one can obtain τ_{12}, τ_{22} and b_3 in that order. Subsequent steps are obvious, and can fail only if $c_i^T b_i = 0$ for some $b_i \neq 0$. But automatically some b_{m+1} will vanish (except for the presence of rounding errors) for some $m \leqq n$.

Since Q has not been formed explicitly it remains to obtain F from T. One method for transforming T into F is given by SCHWARZ. Another arises from the observation that Q^{-1} is the KRYLOV sequence for T with the initial vector e_1. Still otherwise, Q may be calculated recursively. Let

$$Q = \begin{pmatrix} 1 & q_{12} & q_{13} & \cdots & q_{1m} \\ 0 & 1 & q_{23} & \cdots & q_{2m} \\ 0 & 0 & 1 & \cdots & q_{3m} \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & & 1 \end{pmatrix}.$$

Then,

$$\begin{pmatrix} q_{1,k+1} \\ q_{2,k+1} \\ \vdots \\ q_{k,k+1} \end{pmatrix} = \begin{pmatrix} 0 \\ q_{1k} \\ \vdots \\ q_{k-1,k} \end{pmatrix} - \begin{pmatrix} 1 & q_{12} & \cdots & q_{1k} \\ 0 & 1 & \cdots & q_{2k} \\ \vdots & \vdots & & \vdots \\ 0 & 0 & & 1 \end{pmatrix} \cdot \begin{pmatrix} \tau_{1k} \\ \tau_{2k} \\ \vdots \\ \tau_{kk} \end{pmatrix}.$$

But, $QT = FQ$. Therefore

$$q_{\mu,m+1} = a_{m+1-\mu}$$

the a_ν being the coefficients of the characteristic polynomial of T. More commonly, it is observed that the characteristic polynomial

$$\det(\lambda I - T)$$

is easily expanded and can be obtained by means of a well known recursion.

Clearly the selection of the triangular matrix Q in (16) could be made so that B itself is lower triangular, and this is the result obtained when $c_i = e_i$, $C = I$, as in the original HESSENBERG method. It amounts to applying ordinary GAUSSIAN elimination to V^T. This is the method of LOPŠIC, who, indeed, applies it explicitly to the vectors v_i as they are developed. The suggestion occurs naturally as a device for testing at each stage whether or not the vector just obtained is linearly dependent upon the preceding ones. It amounts also to a DANILEVSKIĬ sequence of transformations $A_{i+1} = L_{i+1} A_i L_i^{-1}$ with lower triangular L_i, which occurs in the method of SAIBEL and BERGER (and SCHWARZ).

The restrictions upon the vectors c_i in the HESSENBERG method are quite mild, being first linear independence, and, second, that $c_i^T b_i = 0$ only when $b_i = 0$. Hence it is natural to seek a criterion for selecting them. The particular selection $c_i = e_i$ is fortuitous, and not necessarily suitable for all matrices. LANCZOS and RUTISHAUSER made the suggestion that, in retrospect, seems entirely natural, which was that the c_i be chosen in essentially the same manner as the b_i, but by using A^T instead of A. Thus one seeks a matrix S, of the same form as T, such that

$$A^T C = C S. \tag{20}$$

But c_i will be selected orthogonal to $b_{i-1}, b_{i-2}, \ldots$, whereas $b_{i+1}, b_{i+2}, \ldots$, will be selected orthogonal to c_i, from which it follows that the matrix P in (17) is diagonal. Hence, by (18) and (20),

$$C^T A B = P T = S^T P, \tag{21}$$

and since T is null below the subdiagonal, and S^T above the superdiagonal, therefore both are tridiagonal, and a little further analysis shows that, in fact,

$$S = T. \tag{22}$$

Hence the recursions to be solved for the b_i and c_i never require more than three terms in each, and those for the c_i contain the same coefficients as those for the b_i.

The method again requires that $c_i^T b_i \neq 0$ unless either $b_i = 0$ or else $c_i = 0$. RUTISHAUSER has shown that b_1 and c_1 can be so chosen that $c_i^T b_i = 0$ only when both $b_i = c_i = 0$, and this only for $i = m+1$. Moreover, this will be true of "almost every" choice of b_1 and c_1. Unfortunately, there is no assurance in advance that such a choice has been made, and still less, that $c_i^T b_i$ may not become quite small while c_i and b_i remain relatively large. Should this happen one can, of course, start over, but again with no advance assurance of success. For Hermitian matrices the choice $c_1 = b_1$ implies $c_i = b_i$. For semi-definite matrices the LANCZOS method coincides with the method of STIEFEL and HESTENES.

But it is quite legitimate to select $c_i = b_i$, even for a non-Hermitian matrix A, in which case $c_i^T b_i = 0$ automatically implies $c_i = b_i = 0$. This suggestion has been made by ARNOLDI and by WARGA (described by SCHACKNOW). Again P in (17) is a diagonal with strictly positive diagonal elements. Hence one can write, in place of (17),

$$B^T B = D^{-2}, \tag{23}$$

the matrix being automatically nonsingular since one stops on the appearance of the first zero. Evidently, then, BD is orthogonal in the nonderogatory case when $m = n$ and B is square. Then (18) can be written

$$A(BD) = (BD)(D^{-1} T D), \tag{24}$$

where $D^{-1} T D$ no longer has a unit subdiagonal, but has the more general form of the T of (19). In the nonderogatory case (24) can be written

$$\Omega^T A \Omega = T', \quad \Omega = BD, \quad T' = D^{-1} T D, \tag{25}$$

where Ω is orthogonal, and T' is of the form (19).

This in effect shows, and it is otherwise known, that a matrix A can be reduced to HESSENBERG form by an orthogonal transformation (25), and one might seek to build it up in other ways. In fact, any orthogonal matrix can be expressed as a product of plane rotations, and this DANILEVSKII type sequence of transformations gives the method proposed by GIVENS. The method is to develop a sequence of plane rotations, the typical one being Ω_{ij} in the (i, j)-plane, such that in

$$\Omega_{23}^T A \Omega_{23}$$

the element in the (3, 1) position is annihilated; in

$$\Omega_{24}^T \Omega_{23}^T A \Omega_{23} \Omega_{24}$$

the element in the (4, 1) position can be annihilated without thereby disturbing the zero already obtained. One continues in this way, ultimately annihilating all elements below the subdiagonal, at which time the form T' is obtained and the product of all the Ω_{ij} forms Ω. Attacked in this way the method requires a square rooting for each element annihilated. When the form (24) is used only one per column is required.

In the light of the foregoing analysis a further variant, based on a paper by one of us (A. S. HOUSEHOLDER), may be presented that seems to differ slightly from all these. Returning to the form (7), consider again the possibility of forming an orthogonal matrix W such that

$$W V = S \tag{26}$$

is upper triangular. Then (7) can be written in the form

$$W A W^T = T, \qquad T = S F S^{-1}, \tag{27}$$

where T is subtriangular of form (19) again.

The matrix W will be constructed as a product of simpler orthogonal matrices, but not plane rotations. In fact, they are of the form

$$W_i = I - 2 w_i w_i^T, \qquad w_i^T w_i = 1, \qquad W_i^{-1} = W_i.$$

Consider the product $W_1 v_1$ where

$$W_1 = I - 2 w_1 w_1^T$$

and let the last $n-1$ elements of w_1 be proportional to those of v_1, the factor of proportionality to be determined, along with the first element. These two scalars will be chosen so that $W_1 v_1$ is null except in the first element. To secure this, the two scalars must satisfy a pair of simultaneous quadratics which are easily solved in terms of two square roots. For details see also a forthcoming paper by one of us (F. L. BAUER). At the next step the product $W_2 W_1 v_2$ is required to vanish in all but the first two elements. The process can terminate only with a v_{m+1} that is a linear combination of the preceding ones. As with the method of DANILEVSKIĬ, it is unnecessary to form V explicitly. Instead, one can make successive transformations of the matrix A. The first, $W_1 A W_1$ has the effect only of selecting the initial vector v_1. The next matrix W_2 is chosen so that $W_2 W_1 A W_1 W_2$ is null in the first column below the second element, and w_2 itself is null in its first element. If w_3 is null in its first two elements, W_3 can be selected so that the product $W_3 W_2 W_1 A W_1 W_2 W_3$ retains its zeros in the first column, and, in addition, is null in the second column below the third element. Eventually, W will be the product of all the W_i so formed.

It is not the purpose here to consider the detailed programming of any of the methods here described. It is the purpose to exhibit the fact that all these methods rest mathematically upon the formation of a KRYLOV sequence (1), where usually e_1 is taken for v_1. But if V is formed explicitly, then the efficacy

of the sequence depends upon the extent to which components of the proper vectors are represented in the vector v_i of the sequence, and they will not be well represented unless the proper vectors belonging to proper values of small modulus are strongly represented in v_1, since successive iterations with the matrix A have the effect of suppressing these components progressively. This cannot be expected from the choice $v_1 = e_1$. If these minor axes were not represented at all in v_1, this would be an advantage since the sequence would terminate early and one would obtain a polynomial divisor of the minimal polynomial. One could then find from this the larger proper values and their vectors. But this cannot be expected from this choice either. Instead, one can expect that the minor axes will be represented to some degree in the early terms, and completely suppressed in the later ones to within machine error. Hence numerical instability results.

However, the choice $v_1 = e_1$ is not necessary. It only provides a slight reduction in the number of computations formally required, and a better v_1 can be found. For a positive-definite matrix, a preparatory vector iteration with the matrix $\gamma E - A$, where γ is given by a bound for the greatest proper value, will give a v_1 with predominant minor axes. For a normal matrix, $\gamma^2 E - AA^T$ may be used, where γ is an upper bound for the moduli of the proper values of A. And, besides this, if the proper vectors of A group into symmetric $\left((x)_\mu = (x)_{n-\mu}\right)$ and antisymmetric $\left((x)_\mu = -(x)_{n-\mu}\right)$ ones, a symmetric or an antisymmetric v_1 may be used, to obtain the corresponding divisors of the minimal polynomial.

In any case, it seems to be worth while, because of the optimal condition of orthogonal transformations, to obtain the HESSENBERG transform by orthogonalization of V, or by means of the generalized HESSENBERG method with orthogonalization $(C = B)$, or by a sequence of orthogonal similarity transformations. The latter may be done in the GIVENS way by plane rotations, or by using the matrices W_i. These methods should show optimal numerical stability.

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