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On the shifted eigenvalue problem

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Lanczos (1, 2) has considered the *shifted eigenvalue problem*

$$\begin{bmatrix} 0 & \mathbf{C} \\ \mathbf{C}^H & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix} = \lambda \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix}, \tag{1}$$

where $\mathbf{C}$ is a $(p \times q)$ matrix of rank r, $\mathbf{C}^H$ is its hermitean conjugate and $\mathbf{u}$, $\mathbf{v}$ are column vectors of orders p, q respectively. In this note we extend Lanczos' work to cover the more general eigenvalue problem

$$[\mathbf{M}] \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix} \equiv \begin{bmatrix} a\mathbf{I} & \mathbf{C} \\ \mathbf{C}^H & b\mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix} = \lambda \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix}, \tag{2}$$

which arises in certain problems in solid state physics (3). In (2), the $\mathbf{I}$'s are unit matrices of appropriate orders and the constants a, b are real; the partitioned matrix $\mathbf{M}$ is thus hermitean so that its eigenvalues λ are real.

Equation (2) may be decomposed into the relations

$$\mathbf{C}\mathbf{v} = (\lambda - a)\,\mathbf{u}, \tag{3a}$$

$$\mathbf{C}^H\mathbf{u} = (\lambda - b)\,\mathbf{v}. \tag{3b}$$

Premultiplying the first of these equations by $\mathbf{C}^H$ and the second by $\mathbf{C}$, we obtain

$$\mathbf{C}^H\mathbf{C}\mathbf{v} = \gamma^2\mathbf{v}, \tag{4a}$$

$$\mathbf{C}\mathbf{C}^H\mathbf{u} = \gamma^2\mathbf{u}, \tag{4b}$$

where the eigenvalues γ^2 of $\mathbf{C}^H\mathbf{C}$ and $\mathbf{C}\mathbf{C}^H$ are given by

$$\gamma^2 = (\lambda - a)(\lambda - b). \tag{5}$$

The matrices $\mathbf{C}^H\mathbf{C}$ and $\mathbf{C}\mathbf{C}^H$ are each of rank r, and they possess r eigenvalues, $\gamma^2 > 0$, in common. The remaining eigenvalue, $\gamma^2 = 0$, occurs with multiplicities $p - r$ and $q - r$ for $\mathbf{C}\mathbf{C}^H$ and $\mathbf{C}^H\mathbf{C}$ respectively.

It is not possible, in general, to satisfy (2) by combining, arbitrarily, the solutions of (4*a*) and (4*b*). As in the Lanczos problem, the $\mathbf{u}$'s must be normalized in a specific way relative to the $\mathbf{v}$'s (or vice versa), and to ensure this one needs to make use of the original inhomogeneous equations (3*a*) and (3*b*). In order to analyse the structure of the eigenvectors of (2) in detail, we consider separately the cases (i) $\lambda \neq a$ or b, (ii) $\lambda = a \neq b$, (iii) $\lambda = b \neq a$, (iv) $\lambda = a = b$.

(i) $\lambda \neq a$ *or* b. One may solve (4*a*) to obtain r vectors $\mathbf{v}$ corresponding to positive eigenvalues γ^2, and then find the appropriate $\mathbf{u}$'s from (3*a*); alternatively, one can use

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(4b) to obtain the $\mathbf{u}$'s and then construct the $\mathbf{v}$'s from (3b). According to (5), each γ^2 gives rise to a pair of eigenvalues

$$\lambda = \tfrac{1}{2}\{(a+b) \pm \sqrt{[(a-b)^2+4\gamma^2]}\} \tag{6}$$

of the original equation (2). If one choice of sign in (6) gives an eigenvalue λ and an eigenvector $(\mathbf{u}, \mathbf{v})$ of (2), it may be readily verified that the other choice corresponds to the eigenvalue λ' and the eigenvector $(\mathbf{u}', \mathbf{v}')$, where

$$\lambda' = a+b-\lambda \tag{7}$$

and, with a suitable choice of normalization,

$$\left.\begin{aligned} \mathbf{u}' &= (\lambda-a)\,\mathbf{u}, \\ \mathbf{v}' &= (b-\lambda)\,\mathbf{v}. \end{aligned}\right\} \tag{8}$$

The paired vectors $(\mathbf{u}, \mathbf{v})$ and $(\mathbf{u}', \mathbf{v}')$ constitute $2r$ solutions of (2) with $\lambda \neq a$ or b.

Vectors associated with different λ's are of course automatically orthogonal, but the case where $\mathbf{M}$ has a multiple eigenvalue merits separate mention: this corresponds to the situation where $\mathbf{C}^H\mathbf{C}$ has an eigenvalue ($\gamma^2 \neq 0$) associated, say, with L solutions $\mathbf{v}_l$ ($l = 1, 2, \ldots, L$) of 4(a). Provided the $\mathbf{v}_l$ are chosen to be mutually orthogonal, it can be shown that (3a) leads to L mutually orthogonal vectors $\mathbf{u}_l$. It follows almost immediately that the L eigenvectors $(\mathbf{u}_l, \mathbf{v}_l)$ of $\mathbf{M}$, given by this procedure, are automatically mutually orthogonal, as are the L vectors $(\mathbf{u}_l', \mathbf{v}_l')$.

Finally, we observe that (5) does not give eigenvalues between a and b.

(ii) $\lambda = a \neq b$. In this case, equations (3) become

$$\mathbf{C}\mathbf{v} = 0, \tag{9}$$

$$\mathbf{C}^H\mathbf{u} = (a-b)\,\mathbf{v}; \tag{10}$$

clearly, for non-trivial solutions, we require $\mathbf{u} \neq 0$. Now the well-known compatibility theorem for linear operators states that (10) is soluble if and only if the right-hand side is orthogonal to all the solutions $\mathbf{w}$ of the adjoint homogeneous equation

$$\mathbf{C}\mathbf{w} = 0. \tag{11}$$

However, $\mathbf{v}$ is not orthogonal to the $\mathbf{w}$'s; it is itself a solution of (11)! Clearly, then, the eigenvectors of (2) for $\lambda = a \neq b$ are given by

$$\mathbf{v} = 0, \quad \mathbf{C}^H\mathbf{u} = 0, \tag{12a}$$

there being $p-r$ such solutions. Here, the $\mathbf{u}$'s may be identified with the $p-r$ solutions of (4b) having $\gamma^2 = 0$. Obviously, then, not only can the vectors $(\mathbf{u}, 0)$ be chosen as mutually orthogonal, but they are also automatically orthogonal to the eigenvectors $(\mathbf{u}, \mathbf{v})$ and $(\mathbf{u}', \mathbf{v}')$ under category (i).

For the case $\lambda = a$ the relation (8) gives $\mathbf{u}'$, $\mathbf{v}' = 0$, so that we do not obtain paired eigenvectors of $\mathbf{M}$.

(iii) $\lambda = b \neq a$. The argument for $\lambda = b$ is analogous to that for $\lambda = a$. The eigenvectors of $\mathbf{M}$ are now given by

$$\mathbf{u} = 0, \quad \mathbf{C}\mathbf{v} = 0; \tag{12b}$$

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in this case there are $q-r$ vectors, the $\mathbf{v}$'s being identifiable with the solutions of (4a) for $\gamma^2 = 0$. Here, again, the eigenvectors $(0, \mathbf{v})$ can be chosen as mutually orthogonal, while their orthogonality to the $(\mathbf{u}, \mathbf{v})$ and $(\mathbf{u}', \mathbf{v}')$ under category (i) and the $(\mathbf{u}, 0)$ under (ii) is already automatically ensured.

In this case, too, the transformation (8) gives $\mathbf{u}', \mathbf{v}' = 0$, so that paired eigenvectors do not occur for $\lambda = b$.

(iv) $\lambda = a = b$. The results given for cases (ii) and (iii) together provide a solution to (2) even when $a = b$. Now, however, the eigenvectors of (2) need not be restricted to the form $(\mathbf{u}, 0)$ or $(0, \mathbf{v})$; we can obtain the $p+q-2r$ required vectors in the more general form $(\mathbf{u}, \mathbf{v})$, by combining appropriate solutions of $\mathbf{C}^H\mathbf{u} = 0$ and $\mathbf{C}\mathbf{v} = 0$.

Summarizing, there is a region between a and b where eigenvalues of $\mathbf{M}$ do not occur; if $p > r$ there are $p-r$ eigenvectors $(\mathbf{u}, 0)$ corresponding to $\lambda = a$, and if $q > r$ there are $q-r$ vectors $(0, \mathbf{v})$ corresponding to $\lambda = b$. The remaining $2r$ eigenvalues ($\lambda \neq a$ or b) occur in pairs λ and $\lambda' = a+b-\lambda$, and the corresponding paired eigenvectors are related by (8).

Finally, if the eigenvalues λ of (2) have been obtained for a pair of constants a and b, we observe from (5) that the corresponding eigenvalues $\bar{\lambda}$ for another choice of constants $\bar{a}$ and $\bar{b}$ are given simply by

$$(\bar{\lambda}-\bar{a})\,(\bar{\lambda}-\bar{b}) = \gamma^2 = (\lambda-a)\,(\lambda-b). \tag{13}$$

If $(\mathbf{u}, \mathbf{v})$ is the vector associated with λ for the constants a and b, it follows that the corresponding vector $(\bar{\mathbf{u}}, \bar{\mathbf{v}})$ for $\bar{a}$ and $\bar{b}$ is given by

$$\bar{\mathbf{u}} = \sigma\mathbf{u}, \quad \bar{\mathbf{v}} = \tau\mathbf{v}, \tag{14}$$

where

$$\left.\begin{aligned} \sigma/\tau &= (\lambda-a)/(\bar{\lambda}-\bar{a}) = (\bar{\lambda}-\bar{b})/(\lambda-b), && \lambda \neq a \text{ or } b, \\ &= 1, && \lambda = a \text{ or } b. \end{aligned}\right\} \tag{15}$$

The choice $\bar{a} = \bar{b} = 0$ corresponds to the Lanczos equation (1), so the relations (13), (14) and (15) demonstrate the connexion between solutions of the Lanczos problem and those of the more general eigenvalue equation (2).

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