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Solving Large Sparse Linear and Quadratic Generalized Eigenvalue Problems*

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We study the methods for solving the following large order eigenvelue problems occurring in the analysis of structural vibration[3,4,12]:

$$(K-\lambda M)x=0, \tag{1}$$

$$(M\lambda^2-C\lambda-K)x=0 \tag{2}$$

and

$$(M\lambda^2+\widetilde{C}\lambda+K)x=0, \tag{3}$$

where M and C are both symmetric matrices, while $\widetilde{C}$ is skew symmetric. Moreover, M is positive definite, and the matrix K in (2) and (3) is also assumed to be symmetric positive definite.

I The eigenvalue problem for normal matrices in generalized inner prduct

Let B be an $n\times n$ Hermitian positive definite matrix. Then

$$\langle x,y\rangle\equiv(x,By)\equiv y^HBx \tag{4}$$

is called B-inner product. We can define B-norm, B-normal matrix, B-Hermitian matrix, B-skew Hermitian matrix and B-unitary matrix as usual.

Theorem 1 $n\times n$ matrix G is B-normal if and only if

$$B^{-1}G^HBG=GB^{-1}G^HB. \tag{5}$$

While the fact that G is B-Hermitian, B-skew Hermitian or B-unitary is characterized by $G^HB=BG$, $G^HB=-BG$ or $G^HB=BG^{-1}$ respectively. If $n\times m$ matrix F consists of m B-orthonormal vectors as its columns, then the project matrix of G determined by F is F^HBGF. If G is B-normal, then it has a full B-orthonormal system of eigenvectors. If the B-unitary matrix with these eigenvectors as its columns is denoted by Q, and the diagonal matrix consisting of the corresponding eigenvalue is denoted by Λ, then

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$$Q^H BGQ = \Lambda, \qquad Q^H G^H BQ = \bar{\Lambda}. \tag{6}$$

Poof Suppose G corresponds to an operator and the matrix corresponding to the conjugate operator in the B-inner product is G^*, then from

$$\langle Gx, y\rangle_B = \langle x, G^* y\rangle_B,$$

we have

$$(Gx, By) = (x, BG^* y),$$

that is

$$G^* = B^{-1} G^H B. \tag{7}$$

From this we can easily arrive at all the conclusions of the theorem. Q. E. D.

Corollary If G is B-normal, then $G^* G$ and G have a common full B-orthonormal system of eigenvectors.

Theorem 2 Suppose X is the $n\times p$ matrix whose columns are composed of p vectors from a B-orthonormal basis of the invariant subspace for the B-normal matrix G. Then the B-orthogonal project matrix $X^H BGX$ of G determined by X is normal.

Proof Let the columns of the $n\times(n-p)$ matrix Y be the basis of the B-orthogonal complement to the space spanned by the columns of X. We have

$$Y^H BX = O, \quad X^H BY = 0,$$

$$\begin{bmatrix} X^H \\ Y^H \end{bmatrix} B[X, Y] = I \tag{8}$$

and

$$\begin{bmatrix} X^H \\ Y^H \end{bmatrix} BG[X, Y] = \begin{bmatrix} X^H BGX & \\ & Y^H BGY \end{bmatrix}. \tag{9}$$

Let $[X, Y] = B^{-1/2}[\tilde{X}, \tilde{Y}]$, then from (8) we have

$$\begin{bmatrix} \tilde{X}^H \\ \tilde{Y}^H \end{bmatrix} [\tilde{X}, \tilde{Y}] = I = [\tilde{X}, \tilde{Y}] \begin{bmatrix} \tilde{X}^H \\ \tilde{Y}^H \end{bmatrix}, \tag{10}$$

from (9) it follows that

$$R \equiv \begin{bmatrix} \tilde{X}^H \\ \tilde{Y}^H \end{bmatrix} B^{1/2} G B^{-1/2} [\tilde{X}, \tilde{Y}] = \begin{bmatrix} X^H BGX & \\ & Y^H BGY \end{bmatrix}. \tag{11}$$

But from (10) and (5) we get

$$R^H R = \begin{bmatrix} \tilde{X}^H \\ \tilde{Y}^H \end{bmatrix} B^{-1/2} G^H BGB^{-1/2} [\tilde{X}, \tilde{Y}] = \begin{bmatrix} \tilde{X}^H \\ \tilde{Y}^H \end{bmatrix} B^{1/2} GB^{-1} G^H B^{1/2} [\tilde{X}, \tilde{Y}] = RR^H.$$

By (11) we also have

$$(X^H BGX)^H (X^H BGX) = (X^H BGX)(X^H BGX)^H. \quad \text{Q. E. D.}$$

From theorem 1 and its corollary and theorem 2 we can derive the following

Algorithm I (Subspace Iteration Method for B-normal Matrices)

(1) Take p random initial vectors $(q \leqslant p < n)$, B-orthonormalize them, and denote the resulting $n \times p$ matrix by $X^{(0)}$, that is, $X^{(0)H}BX^{(0)} = I_p$.

(2) If the $(\nu-1)$-th matrix $X^{(\nu-1)}$ has been obtained, then the iterative procedure for finding $X^{(\nu)}$ is as follows

(i) Compute $Z^{(\nu)} = GX^{(\nu-1)}$,

(ii) Compute $p \times p$ Hermitian positive definite matrix $S^{(\nu)} = Z^{(\nu)H}BZ^{(\nu)}$,

(iii) Find all the eigenvalues and eigenvectors of $S^{(\nu)}$.

$$Q^{(\nu)H}S^{(\nu)}Q^{(\nu)} = (D^{(\nu)})^2,$$

where $Q^{(\nu)}$ is a $p \times p$ unitary matrix, $D^{(\nu)}$ is a diagonal matrix with positive diagonal elements which are ordered decreasingly.

(iv) Compute $X^{(\nu+1)} = Z^{(\nu)}Q^{(\nu)}(D^{(\nu)})^{-1}$,

(v) Test the convergence.

(3) Denote $X^{(\nu)}$ which has converged by X. Partition X as $X = [X_1, \cdots, X_m]$, where each X_l corresponds to the eigenvalues which have an equal modulus. Compute the B-project matrix $X_l^H BGX_l$ of G determined by X_l, and solve the eigenvalue problem of the lower order normal matrix:

$$P_l^H(X_l^H BGX_l)P_l = \Lambda_l.$$

At the end of this step we obtain eigenvector matrix X_lP_l and eigenvalue diagonal matrix Λ_l.

Remark The analysis of the convergence in [8,11] may be adopted to the present algorithm, provided that the usual norm is replaced by B-norm. It is the generalization of that in [8]. McCormick and Noe have made an analogous generalization [6]. Obviousely, our way of generalization is more straigtforword.

For some special B-normal matrix G we can derive the following algorithm (provided that they satisfy the condition: for any matrix Q with B-orthonormal columns Q^HBGQ is normal. For exemple, if G is B-Hermitian or B-skew Hermitian, then the condition is satisfied.)

Algorithm II (Subspace Iteration Method for B-normal Matrix)

(1) Take p random initial vectors $(q \leqslant p < n)$, B-orthonormalize them, and denote the resulting $n \times p$ matrix by $X^{(0)}$, that is, $X^{(0)H}BX^{(0)} = I_p$.

(2) If the $(\nu-1)$-th matrix $X^{(\nu-1)}$ has been obtained, then the iterative procedure for finding $X^{(\nu)}$ is as follows

(i) Compute $Z^{(\nu)} = GX^{(\nu-1)}$,

(ii) B-orthonormalize the columns of $Z^{(\nu)}$ and get $Q^{(\nu)}$:

$$Z^{(\nu)}=Q^{(\nu)}R^{(\nu)},$$

where the columns of $Q^{(\nu)}$ are B-orthonormal, and $R^{(\nu)}$ is a $p\times p$ upper triangular matrix.

(iii) Compute B-orthogonal project matrix $S^{(\nu)}$ of G determined by $Q^{(\nu)}$

$$S^{(\nu)}=Q^{(\nu)H}BGQ^{(\nu)}.$$

(iv) Solve the eigenvalue problem for the lower order normal matrix $S^{(\nu)}$:

$$P^{(\nu)H}S^{(\nu)}P^{(\nu)}=\Lambda^{(\nu)}.$$

(v) Compute $X^{(\nu)}=Q^{(\nu)}P^{(\nu)}$.

(iv) Test the convergence.

Remarks 1. When B is real and G is B-symmetric (or B-skew symmetric), then

$$S^{(\nu)}=Q^{(\nu)T}BGQ^{(\nu)}$$

is real symmetric (or skew symmetric). We can use the Jacobi-like algorithm in [10] to perform step (2) (iv). The whole procedure of computation can be performed with real arithmetic.

2. By an argument analogous to that used in [10] we can prove the convergence of algorithm II. When G is B-normal, the convergence rate is the same as when G is symmetric.

For general B-normal matrix G, the Lanczos algorithm follows the same procedure as that of algorithm I: First, by applying Lanczos algorithm to G^*G we obtain some extreme eigenvalues and their corresponding eigenvectors. Then, by using the B-orthogonal project metrices determined by the invariant subspaces spanned by the eigenvectors corresponding to the eigenvalures with equal modulus, we can obtain the eigenvalues and the eigenvectors of G.

The recurrence relation of Lanczos algorithm for G^*G is

$$\beta_{j+1}Bv_{j+1}=G^HBGv_j-\alpha_jBv_j-\beta_jBv_{j-1},$$

and the corresponding matrix form is

$$G^HBGV_j=BV_jT_j+\beta_{j+1}Bv_{j+1}e_j,$$

where $V_j=[v_1,\cdots,v_j]$ and T_j is a symmetric three diagonal matrix

$$T_j=V_j^HG^HBGV_j=\begin{pmatrix}\alpha_1 & \beta_2 & & & \\ \beta_2 & \alpha_2 & \beta_3 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \beta_j \\ & & & \beta_j & \alpha_j\end{pmatrix}$$

For B-Hermitian G we can implement Lanczos algorithm directly to G, the recurrence relation is

$$\beta_{j+1}v_{j+1} = Gv_j - \alpha_j v_j - \beta_j v_{j-1}.$$

The corresponding matrx form is

$$GV_j = V_j T_j + \beta_{j+1} v_{j+1} e_j,$$

and the three diagonal matrix T_j is

$$T_j = V_j^H BGV_j.$$

For B-skew Hermitian G, owing to the fact that iG is B-Hermitian, we can implement the Lanczos algorithm to iG.

Ⅱ Generalized eigenvalue problem

By taking M as the matrix B in the previous section we can trans form the linear generalized eigenvalue problem (1) into a standard eigenvalue problem in M-inner product:

$$G_1 X \equiv M^{-1}(K - \sigma M)x = \lambda x \tag{12}$$

or

$$G_2 X \equiv (K - \sigma M)^{-1} M x = \lambda x. \tag{13}$$

If K is such that G_1 or G_2 is M-normal, then we can apply the algorithm in the previous section in solving problems (12) and (13). Particularly, when K is Hemitian, and σ is a real scalar, G_1 and G_2 are M-Hermitian. When K is skew Hermitian and σ is a pure imaginary scalar, G_1 and G_2 are M-skew Hermitian.

For quadratic generalized eigenvalue problem (2) and (3), we can respectively transform them into the following linear generalized eigenvalue problems[3,4,12]

$$\begin{bmatrix} O & K \\ K & C \end{bmatrix}\begin{bmatrix} x \\ \lambda x \end{bmatrix} = \lambda \begin{bmatrix} K & \\ & M \end{bmatrix}\begin{bmatrix} x \\ \lambda x \end{bmatrix} \tag{14}$$

and

$$\begin{bmatrix} O & K \\ -K & -\tilde{C} \end{bmatrix}\begin{bmatrix} x \\ \lambda x \end{bmatrix} = \lambda \begin{bmatrix} K & \\ & M \end{bmatrix}\begin{bmatrix} x \\ \lambda x \end{bmatrix}. \tag{15}$$

The problem (14) in which $\begin{bmatrix} O & K \\ K & C \end{bmatrix}$ is symmetric has been studied in [9]. We now study the method for solving problem (3) i. e. problem (14), (15) may be abbreviated to

$$Ay = \lambda By, \tag{16}$$

where B is symmetric positive definite, A is skew symmetric and A and B are of the forms presented by (15).

Theorem 3 The eigenvalues of the quadratic problem (3) are all nonzero pure imaginary scalars with a half of them on the positive imaginary semi-axis and the other half on the negative imaginary semi-axis.

Proof Make Cholesky decomposition $B = LL^T$, where L is nonsingular lower triangular. (16) is equivalent to

$$(L^{-1}AL^{-T})\tilde{y} = \lambda\tilde{y}. \tag{17}$$

It is easy to show that A is nonsingular. Also,

$$iA = \begin{bmatrix} O & iK \\ -iK & -i\tilde{C} \end{bmatrix}$$

is Hermitian. By applying Poincaré separation theorem[1,5] and considering the fact that iA is nonsingular we can see that iA has n positive eigenvalues and n negative eigenvalues. From (17), we may apply the inertia theorem and the conclusion of the theorem follows. Q. E. D.

It is most advantageous to take B-skew Hermitian matrix

$$(A - i\sigma B)^{-1}B, \tag{18}$$

where σ is a real scalar, in finding some of the eigenvalues which are near $i\sigma$ by the subspace algorithm or Lanczos algorithm discussed in the previous section. We shall show that it is not necessary to invert or to factorize a $2n\times 2n$ matrix (c.f. (18)).

Let

$$W(\sigma) = \mathrm{K} + i\sigma\tilde{C} - \sigma^2 M. \tag{19}$$

Clearly, $W(\sigma)$ is an $n\times n$ Hermitian matrix. Then we may make the symmetric decomposition

$$W(\sigma) = LDL^H, \tag{20}$$

where D is a real diagonal matrix.

Theorem 4 Let σ be a real scalar such that the decomposition (20) is possible, then, (i) The number of the negative diagonal elements of D is equal to the number of the eigenvalues of problem (3) between 0 and $i\sigma$ on the imaginary axis.

(ii)
$$(A - i\sigma B)^{-1}B\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = i\begin{bmatrix} W^{-1}(\sigma)(i\tilde{C}x_1 - \sigma Mx_1 + iMx_2) \\ -W^{-1}(\sigma)(i\mathrm{K}x_1 + \sigma Mx_2) \end{bmatrix}. \tag{21}$$

Proof When $\sigma\neq 0$, we have

$$iA + \sigma B = \begin{bmatrix} \mathrm{I} & \\ -iI/\sigma & \mathrm{I} \end{bmatrix}\begin{bmatrix} \sigma\mathrm{K} & \\ & -W(\sigma)/\sigma \end{bmatrix}\begin{bmatrix} \mathrm{I} & iI/\sigma \\ & \mathrm{I} \end{bmatrix}. \tag{22}$$

By applying the inertia theorem and theorem 3 the first assertion follows.

By (22) it is easy to get

$$(A-i\sigma B)^{-1}B\begin{bmatrix}x_1\\x_2\end{bmatrix}=i\begin{bmatrix}I & -iI/\sigma\\ & I\end{bmatrix}\begin{bmatrix}K^{-1}/\sigma & \\ & -\sigma W^{-1}(\sigma)\end{bmatrix}\begin{bmatrix}I & \\ iI/\sigma & I\end{bmatrix}\begin{bmatrix}Kx_1\\Mx_2\end{bmatrix}$$

$$=i\begin{bmatrix}x_1/\sigma+W^{-1}(\sigma))(-Kx_1/\sigma+iMx_2)\\ W^{-1}(\sigma)(-iKx_1-\sigma Mx_2)\end{bmatrix}=i\begin{bmatrix}W^{-1}(\sigma)(i\widetilde{C}x_1-\sigma Mx_1+iMx_2)\\ -W^{-1}(\sigma)(iKx_1+\sigma Mx_2)\end{bmatrix}.$$

When $\sigma=0$, it is easy to check that (21) holds. Q. E. D.

From Theorem 4 it follows that for solving problem (3), if we take B-skew Hermitian $(A-i\sigma B)^{-1}B$ as the matrix G and apply subspace iteration algorithm I or II, or if we take B-Hermitiam $(iA+\sigma B)^{-1}B$ as the matrix G and apply subspace iteration algorithm II or Ianczos algorithm, then it is only necessary to compute the triangular decomposition of the $n\times n$ Hermitian matrix $W(\sigma)$. Hence the presented algorithms for solving quadratic eigenvalue problem are quite efficient.

Particularly, if we want to find some eigenvalues with minimal moduli, then we may take $\sigma=0$, and then $A^{-1}B$ is B-skew symmetric and $W(0)=K$. Thus we can use subspace iteration algorithm II and perform the whole procedure with real arithmetic.

Obviousely, the algorithms for B-normal matrix presented in this paper can be used efficiently to solve the quadratic eigenvalue problems of a wide variety.

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