Mathematatica Balkanica

Mathematical Society of South-Eastern Europe
A quarterly published by
the Bulgarian Academy of Sciences – National Committee for Mathematics

Mathematica Balkanica

New Series Vol.8, 1994, Fasc.4

Solution of Symmetric and Hermitian J-symmetric Eigenvalue Problem

Milko G. Petkov, Ivan G. Ivanov

Presented by P. Kenderov

New effective Jacobi modifications for solving of eigenvalue problems for symmetric J-symmetric matrices are proposed.

1. Introduction

Let $R^{mxn}(C^{nxn})$ be the set of all mxn real (complex) matrices and

$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \tag{1}$$

be 2×2 block matrix with A, B, C and $D \in C^{m \times n}$. Moreover $J \in R^{2n \times 2n}$ be a matrix of the form

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \tag{2}$$

where 0 is the zero matrix and I is the identity matrix of order n

Definition 1. A matrix M of the form (1) is said to be J-symmetric (simplectically symmetric) iff

$$J^T M J = M^T, \tag{3}$$

where T denotes transposition.

It is easy to see, that if the matrix (1) is J-symmetric, then it has the form

$$M = \begin{pmatrix} A & B \\ C & A^T \end{pmatrix} \tag{4}$$

with $B^T = -B$, $C^T = -C$.

Definition 2. A matrix M of (1) is said to be simplectic, iff

$$J^T M J = M^{-T}, \tag{5}$$

where - T denotes inverting and transposition in arbitrary order.

The J-symmetric matrices are invariant under similarity tranformations with simplectic matrices. That's the reason why in numerical solution of the spectral problem for J-symmetric matrices simplectic similarities are used. Otherwise the coresponding algorithms would require about twice more computing time and memory. In order to stabilize the algorithm, it is desireable the similarity transformation used to be both simplectic and ortogonal (or unitary).

If the matrix M from (1) is simplectic and ortogonal (unitary), then it has the form

$$M = \begin{pmatrix} A & -B \\ C & A \end{pmatrix} \tag{6}$$

As far as we know, the first use of ortogonal simplectic algorithm for solving the eigenproblem of real symmetric J-symmetric matrices is made in [5].

Moreover, such an algorithm solves in the same time the eigenproblem of complex Hermitian matrices in real arithmetic too. For the completeness sake start brietly with this algorithm.

2. Simplectic modification of the Jacobi method for real symmetric J-symmetric matrices.

Let we are to solve the eigenproblem for nxn Hermitian matrix $C = A + iB$ $(A = \Re C,\ B = \Im C)$

$$Cz = \lambda z \tag{7}$$

$z = x + iy$ $(x = \Re z,\ y = \Im z)$ with real λ. One option solve this problem is by a modification of the Jacobi process for solving eigenproblem of real symmetric matrix. In this modification it is used the following convergent sequence of unitary similar matrices

$$C_k = Z_k^H C_{k-1} Z_k \tag{8}$$

($k = 1, 2, 3, ..., C_0 = C$, H means copmlex conjugate and transposition in arbitrary order). The sequence (8) convergens to a diagonal matrix, i.e.

$$C_k \to Z^H ZCZ = diag[\lambda_1, \lambda_2, ..., \lambda_n] \tag{9}$$

where $Z^H Z = I$ and λ_s are the eigenvalues of C. If the colums of $Z = X + iY$ are $z_s = x_s + iy_s$ they are the corresponding eigenvectors of C. The rate of convergence is given by

$$\sigma_k^2 \le (1 - \frac{2}{n(n-1)})^k \sigma_0^2 \tag{10}$$

where σ_s^2 is the sum of the absolute values of the offdiagonal elements of C_s. The above scheme we denote C-scheme.

But the problem (7) can be solved in real arithmetic by its reducing to the eigenproblem (R-scheme)

$$\begin{pmatrix} A & -B \\ C & A \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \lambda \begin{pmatrix} x \\ y \end{pmatrix} \tag{11}$$

In such a way the eigenproblem of the Hermitian matrix C is transformed into the eigenproblem of the following real symmetric (J-symmetric too)

$$M = M(A, B) = \begin{pmatrix} A & -B \\ B & A \end{pmatrix} \tag{12}$$

It is dear, that the equation (11) can be solved by the classical Jacobi method. But proceeding in such a way one shall use up to twice more memory with respect to the C-scheme. Much will be the computing time too.

Now we propose more effective algorithm which consists in constructiy the following sequence of simplectically and ortogonally similar matrices

$$M_k = M(A_k, B_k) = S_k^T M_{k-1} S_k \tag{13}$$

where $k = 1, 2, 3, ..., M_0 = M, S_k^T S_k = I$. To give an idea for the iteration proces (13) we explain only the first iteration by which from matrix $M = M(A, B) = (m_{pq})$, $A = (a_{pq})$, $B = (b_{pq})$ the next matrix $M_1 = \tilde{M} = M(\tilde{A}, \tilde{B}) = S_{\alpha,\beta}^T(\varphi) M S_{\alpha,\beta}(\varphi) = (\tilde{m}_{pq})$, $\tilde{A} = (\tilde{a}_{pq})$, $\tilde{B} = (\tilde{b}_{pq})$ and $1 \le \alpha < \beta \le n$ is obtained.

$$\text{First case:} \quad \max_{p \ne q} |m_{pq}| = |a_{\alpha,\beta}| \tag{14}$$

In this case

$$S_{\alpha,\beta}(\varphi) = diag[U_{\alpha,\beta}(\varphi), U_{\alpha,\beta}(\varphi)]$$

where

$$u_{\alpha\alpha} = (u_{\beta\beta}) = \cos\varphi$$
$$U_{\alpha\beta}(\varphi) = (u_{pq})\ u_{\alpha\beta} = -u_{\beta\alpha} = -\sin\varphi$$
$$u_{pq} = \delta_{pq} \text{ in the remaining cases}$$

The parameter φ is to be found from the equation $\tilde{a}_{\alpha\beta} = 0$. So we get

$$\tilde{A} = U^T_{\alpha\beta}(\varphi)AU_{\alpha\beta}(\varphi) = \tilde{A}^T, \tilde{B} = U^T_{\alpha\beta}(\varphi)BU_{\alpha\beta}(\varphi) = -\tilde{B}^T \tag{15}$$

or

$$\begin{aligned}
\tilde{a}_{pq} &= a_{pq} && (p \neq \alpha,\beta,\ q \neq \alpha,\beta)\\
\tilde{a}_{\alpha q} &= a_{\alpha q}\cos\varphi + a_{\beta q}\sin\varphi && (q \neq \alpha,\beta)\\
\tilde{a}_{\beta q} &= -a_{\alpha q}\sin\varphi + a_{\beta q}\cos\varphi && (q \neq \alpha,\beta)\\
\tilde{a}_{\alpha\alpha} &= (a_{\alpha\alpha}\cos\varphi + a_{\beta\alpha}\sin\varphi)\cos\varphi &+& (a_{\alpha\beta}\cos\varphi + a_{\beta\beta}\sin\varphi)\sin\varphi\\
\tilde{a}_{\beta\beta} &= -(-a_{\alpha\alpha}\sin\varphi + a_{\beta\alpha}\cos\varphi)\sin\varphi &+& (-a_{\alpha\beta}\sin\varphi + a_{\beta\beta}\cos\varphi)\cos\varphi\\
\tilde{a}_{\alpha\beta} &= -(a_{\alpha\alpha}\cos\varphi + a_{\beta\alpha}\sin\varphi)\sin\varphi &+& (a_{\alpha\beta}\cos\varphi + a_{\beta\beta}\sin\varphi)\cos\varphi = 0
\end{aligned} \tag{16}$$

Similar are the formulas for the elements of the matrix $\tilde{B}$.
The last equation (16) gives

$$\text{tg}2\varphi = \frac{2a_{\alpha\beta}}{a_{\alpha\alpha} - a_{\beta\beta}} \tag{17}$$

In fact formulas (16) and (17) are the same, as for Jacobi method.

$$\text{Second case:}\quad \max_{p\neq q}|m_{pq}| = |b_{\alpha\beta}| \tag{18}$$

In this case the elements of $S_{\alpha\beta}(\varphi)$, respectively A, B are

$$S_{\alpha\beta}(\varphi) = (s_{pq}): \begin{aligned} &s_{\alpha\alpha} = s_{\beta\beta} = s_{n+\alpha n+\alpha} = s_{n+\beta n+\beta} = cos\varphi\\ &s_{\alpha n+\beta} = s_{\beta n+\alpha} = -s_{n+\alpha\beta} = -s_{n+\beta\alpha} = -sin\varphi\\ &s_{pq} = \delta_{pq} \text{ in the remaining cases}\end{aligned}$$

$$\begin{aligned}
\tilde{a}_{pq} &= a_{pq} && (p \neq \alpha,\beta q \neq \alpha,\beta)\\
\tilde{a}_{\alpha q} &= a_{\alpha q}\cos\varphi + b_{\beta q}\sin\varphi && (q \neq \alpha,\beta)\\
\tilde{a}_{\beta q} &= b_{\alpha q}\sin\varphi + a_{\beta q}\cos\varphi && (q \neq \alpha,\beta)\\
\tilde{a}_{\alpha\alpha} &= (a_{\alpha\alpha}\cos\varphi - b_{\alpha\beta}\sin\varphi)\cos\varphi &+& (a_{\beta\beta}\sin\varphi - b_{\alpha\beta}\cos\varphi)\sin\varphi\\
\tilde{a}_{\beta\beta} &= -(a_{\beta\beta}\cos\varphi + b_{\alpha\beta}\sin\varphi)\cos\varphi &+& (a_{\alpha\alpha}\sin\varphi + b_{\alpha\beta}\cos\varphi)\sin\varphi\\
\tilde{a}_{\alpha\beta} &= (a_{\alpha\beta}\cos\varphi + b_{\beta\beta}\sin\varphi)\cos\varphi &+& (a_{\alpha\beta}\sin\varphi - b_{\alpha\alpha}\cos\varphi)\sin\varphi = a_{\alpha\beta}
\end{aligned} \tag{19}$$

$$
(20)\qquad
\begin{aligned}
\tilde{b}_{pq} &= b_{pq} && (p \neq \alpha, \beta q \neq \alpha, \beta)\\
\tilde{b}_{\alpha q} &= b_{\alpha q}\cos\varphi - a_{\beta q}\sin\varphi && (q \neq \alpha, \beta)\\
\tilde{b}_{\beta q} &= b_{\beta q}\cos\varphi - a_{\alpha q}\cos\varphi && (q \neq \alpha, \beta)\\
\tilde{b}_{\alpha\alpha} &= \tilde{b}_{\beta\beta} = 0\\
\tilde{b}_{\alpha\beta} &= (a_{\alpha\alpha}\cos\varphi - b_{\alpha\beta}\sin\varphi)\sin\varphi && - \quad (a_{\beta\beta}\sin\varphi - b_{\alpha\beta}\cos\varphi)\cos\varphi = 0
\end{aligned}
$$

From (20):

$$
(21)\qquad \mathrm{tg}2\varphi = \frac{2b_{\alpha\beta}}{a_{\beta\beta} - a_{\alpha\alpha}}
$$

Now, substituting $A = A_k = (a_{pq}^{(k)})$, $B = B_k = (b_{pq}^{(k)})$, $S_{\alpha\beta}(\varphi) = S_{\alpha_k\beta_k}(\varphi_k) = S_k$, $M_{k+1} = M(\tilde{A}, \tilde{B}) = M(A_{k+1}, B_{k+1})$, we get the sequence $M_k = M(A_k, B_k)$ which is always convergent. Indeed if $V_k = S_1 S_2 ... S_K$, then

$$
(22)\qquad M_k = V_k^T M V_k \to M(L, 0) = V^T M(A, B) V
$$

where $V_k \to V$, $L = diag[\lambda_1, \lambda_2, ..., \lambda_n]$. The matrix V is ortogonal and simplectic and hence it has the form

$$
(23)\qquad V = \begin{pmatrix} X & -Y \\ Y & X \end{pmatrix}
$$

Therefore the matrix $M(A, B)$ has the eigenvalues $\lambda_1, \lambda_1, \lambda_2, \lambda_2, ..., \lambda_n, \lambda_n$ and corresponding eigenvectors

$$
(24)\qquad \begin{pmatrix} x_s \\ y_s \end{pmatrix}, \begin{pmatrix} y_s \\ x_s \end{pmatrix}, \quad s = 1, 2, \ldots, n,
$$

where x_s and y_s are the columns of matrix X and Y, i.e. we can put $Z = X + iY$.

One can prove that the rate of convergence of R-scheme is given by

$$
(25)\qquad \sigma_k^2 \le \left(1 - \frac{1}{n(n-1)}\right)^k \sigma_0^2
$$

where σ^2 are the same quantitis, introduced for the C-scheme.

Now we shall compare the above two schemes with respect to: memory, number of operations, convergence and rate of convergence.

For the two schemes the necessary memory is of the same order. As for the number of operations for one iteration of C-scheme are up to twice more but in both schemes the convergence is out of question. Now we shall show that the rate of convergence of R-scheme is about twice less.

Indeed let $\epsilon > 0$ be arbitrary after q iterations of the C-scheme it holds the inequality

$$\sigma_0(1 - \frac{2}{n(n-1)})^q \leq \epsilon. \tag{26}$$

In order to achieve at least the same accuracy in the R-scheme after p iterations, the inequality

$$\sigma_0^2(1 - \frac{1}{n(n-1)})^p \leq \sigma_0^2(1 - \frac{2}{n(n-1)})^q \tag{27}$$

should be satisfied. (Here p denotes the least positive integer with this property.) Denoting $1/(n^2 - n) = x$, we get

$$\frac{p}{q} \geq \frac{\ln(1-2x)}{\ln(1-x)} = y(x),\ 0 \leq x \leq \frac{1}{6} \tag{28}$$

The function $y(x)$ is increasing in $(0, \frac{1}{6}]$ and

$$2.5 > y_{max}(\frac{1}{6}) = \ln(\frac{2}{3})/\ln(\frac{5}{6}) > 2.$$

These estimates show that the rational number $\frac{p}{q}$ is of the interval $[y(x), \infty)$ and the choise of p is as better as $\frac{p}{q}$ is closer to $y(x)$. It is also clear that as smaller is x (n greater) so $\frac{p}{q}$ is closer to 2. For example if $n \geq 6$ then in order to achive by p iterations in R-scheme at least the same accuracy ϵ, attaible by q iterations in C-scheme it is sufficient $y(x) \leq \frac{p}{q} \leq 2.1$ to hold.

We will not consider other charactiristics of the effectiveness of the R-scheme and modification of this scheme since they are similar to that of the classical Jacobi method.

From the theoretical consideration of the R-scheme made here and from numerical experiments we may conclude that the advantages of the R-scheme are enough in order it to be preferable in comparision with the C-scheme.

3. Simplectic modifications of the Jacobi method for solving eigenproblems for Hermitian J-symmetric matrices.

In this section we propose two more modifications of the Jacobi method in complex and real arithmetic for solving of the eigenvalue problem for Hermitian and J-symmetric matrix of the form

$$\begin{pmatrix} A & B \\ -\bar{B} & \bar{A} \end{pmatrix}, (A, B \in C^{n \times n}) \tag{29}$$

Here and elsewhere the bar denotes the complex conjugate. Matrices of the form (29) arise in the calculation of electronic structure for molecules and solids containing heavy atoms [3,4].

3.1. Complex arithmetic

An idea of the method could be obtained considering the first iteration. Let for M of (29) we have $M = (m_{pq})$, $A = (a_{pq})$, $B = (b_{pq})$. Then M is subjected to an unitary simplectic similarity transformation by a matrix $S_{\alpha\beta}(\varphi, \psi)$ where both the natural parameters $\alpha, \beta (\alpha < \beta) \in [1, n]$ and φ, ψ are to be determineed. Let

$$\tilde{M} = S^H_{\alpha\beta}(\varphi, \psi) M S_{\alpha\beta}(\varphi, \psi) = \begin{pmatrix} \tilde{A} & \tilde{B} \\ -\bar{\tilde{B}} & \bar{\tilde{A}} \end{pmatrix}$$

with $\tilde{A} = (\tilde{a}_{pq})$, $\tilde{B} = (\tilde{b}_{pq})$. $S_{\alpha\beta}(\varphi, \psi)$ be the unitary simplectic matrix we are looking for.

We are considering 2 cases:

i) $max_{p \neq q} |m_{pq}| = |a_{\alpha\beta}|$ In this case

$$S_{\alpha\beta}(\varphi, \psi) = \begin{pmatrix} T_{\alpha\beta}(\varphi, \psi) & 0 \\ 0 & \bar{T}_{\alpha\beta}(\varphi, \psi) \end{pmatrix} \tag{30}$$

where $T_{\alpha\beta}(\varphi, \psi) = (t_{pq}) \in C^{n \times n}$ has the elements

$$\begin{aligned} t_{\alpha\alpha} &= t_{\beta\beta} = \cos\varphi \\ t_{\alpha\beta} &= -\bar{t}_{\beta\alpha} = -e^{i\psi} \sin\varphi \\ t_{pq} &= \delta_{pq} \text{ - in the remaining cases.} \end{aligned} \tag{31}$$

Till now we determined the form of $S_{\alpha\beta}(\varphi, \psi)$ and had show how to determine the parameters α, β. As for the other two parameters φ and ψ, they are to be obtained from the condition $\tilde{m}_{\alpha\beta} = 0$. In such a way we obtain

$$\psi = \arg a_{\alpha\beta}, \mathrm{tg} 2\varphi = \frac{2|a_{\alpha\beta}|}{a_{\alpha\alpha} - a_{\beta\beta}} \tag{32}$$

ii) $max_{p \neq q} |m_{pq}| = |b_{\alpha\beta}|$ In this case the elements of $S_{\alpha\beta}(\varphi, \psi) = (s_{pq})$ are

$$\begin{aligned} s_{\alpha\alpha} &= s_{\beta\beta} = s_{\alpha+n\alpha+n} = s_{\beta+n\beta+n} = \cos\varphi \\ s_{\alpha\beta+n} &= -\bar{s}_{\beta+n\alpha} = -e^{i\psi} \sin\varphi \\ s_{\beta\alpha+n} &= -\bar{s}_{\alpha+n\beta} = -e^{i\psi} \sin\varphi \\ s_{pq} &= \delta_{pq} \text{ - in the remaining cases} \end{aligned} \tag{33}$$

Now φ and ψ are to be obtained from the condition $\tilde{b}_{\alpha\beta} = 0$. This yields

$$(34) \qquad \psi = \arg b_{\alpha\beta}, \ \mathrm{tg} 2\varphi = \frac{2|b_{\alpha\beta}|}{a_{\alpha\alpha} - a_{\beta\beta}}$$

Denoting

$$A = A^{(k)} = (a_{pq}^{(k)}), \ B = B^{(k)} = (b_{pq}^{(k)}), \ M = M^{(k)} = (m_{pq}^{(k)})$$
$$\tilde{A} = A^{(k+1)}, \ \tilde{B} = B^{(k+1)}, \ \tilde{M} = M^{(k+1)}, \ S_{\alpha\beta}(\varphi, \psi) = S_{\alpha_k\beta_K}(\varphi_k, \psi_k)$$

the iteration process has the form

$$M^{(k+1)} = S^H_{\alpha_k\beta_k}(\varphi_k, \psi_k) M^{(k)} S_{\alpha_k\beta_k}(\varphi_k, \psi_k) \ (k = 0, 1, 2, ...)$$

In order to study the convergence of the process, let us introduce

$$(35) \qquad \sigma_k^2 = \sum_{p \neq q} |m_{pq}^{(k)}|^2 = 2 \sum_{p \neq q} (|a_{pq}^{(k)}|^2 + |b_{pq}^{(k)}|^2)$$

As in the classical Jacobi method, one can show that

$$(36) \qquad \sigma_{k+1}^2 \leq \sigma_0^2 (1 - \frac{1}{n(n-1)})^{k+1}.$$

Hence $M^{(k)}(A^{(k)})$ convergence to a diagonal matrix, and $B^{(k)}$ convergence to the zeromatrix, i.e.

$$(37) \qquad M^{(k)} \to \begin{pmatrix} D & 0 \\ 0 & D \end{pmatrix} = D_1$$

Here D is a diagonal matrix with the eigenvalues of M as diagonal elements.

Denoting $S_k = \prod_{r=1}^{k} S_{\alpha_r\beta_r}$, then $S_k \to S$, where S is a simplectic unitary matrix of the form

$$(38) \qquad S = \begin{pmatrix} U & V \\ -\bar{V} & \bar{U} \end{pmatrix}$$

with the eigenvectors of M as columns. Hence, $M^{(k)}$ is a good approximation of D_1, and S_k, for S for sufficiently big k.

Remark. If

$$(39) \qquad M = \begin{pmatrix} A & B \\ \bar{B} & -\bar{A} \end{pmatrix}$$

is an anti-Hetmitian matrix, then the spectral problem for matrix (39) can be reduced to the yet considered case for $N = iM$.

3.2. Real arithmetic

Let us write the spectral problem for the matrix M of (29) in the form

$$\begin{pmatrix} A & B \\ -\bar{B} & \bar{A} \end{pmatrix} \begin{pmatrix} x+iy \\ u+iv \end{pmatrix} = \lambda \begin{pmatrix} z+iy \\ u+iv \end{pmatrix} \tag{40}$$

with $x, y, u, v \in R^{n\times 1}$. Let us denote $A = H + iD$, $B = E + iF$ ($H, D, E, F \in R^{n\times n}$). From the assumptions for M it follows that H is a symmetric matrix, and D, E and F are anti-symmetric matrices. Then (40) can be transformed into the following $4n \times 4n$ real eigenvalue problem

$$Rz = \lambda z \tag{41}$$

with

$$R = \begin{pmatrix} H & -D & E & -F \\ D & H & F & E \\ -E & -F & H & D \\ F & -E & -D & H \end{pmatrix}, \quad z = \begin{pmatrix} x \\ y \\ u \\ v \end{pmatrix} \tag{42}$$

Since R is a real symmetric matrix, then (41) can be solved by the classical Jacobi method but not taking into account the special structure of R. It is easy to see that the equation (41) can be writen in the form

$$\tilde{R}\tilde{z} = \lambda\tilde{z} \tag{43}$$

with

$$\tilde{R} = \begin{pmatrix} H & -D & E & F \\ D & H & F & -E \\ -E & -F & H & -D \\ -F & E & D & H \end{pmatrix} = \begin{pmatrix} K & L \\ -L & K \end{pmatrix}, \quad \tilde{z} = \begin{pmatrix} u \\ y \\ u \\ -v \end{pmatrix} \tag{44}$$

where

$$K = \begin{pmatrix} H & -D \\ D & H \end{pmatrix}, L = \begin{pmatrix} E & F \\ F & -E \end{pmatrix}$$

Then the problem can be solved with any of the algorithms given in [1, 2]. These algorithms take into account that R is a symmetric and J-symmetric matrix.

The algorithm described below uses all the information for the structure of the matrix M of problem (41)–(42).

In order to describe the idea of the algorithm we consider again the first iteration for obtaining of $\hat{R} = Q^T_{\alpha\beta}(\varphi)RQ_{\alpha\beta}(\varphi)$ from R, where $Q_{\alpha\beta}(\varphi)$ is an apropriate ortogonal matrix. To this end we denote $R = (r_{pq})$, $H = (h_{pq})$, $D = (d_{pq})$, $E = (e_{pq})$, $F = (f_{pq})$ and

$$\hat{R} = \begin{pmatrix} \hat{H} & -\hat{D} & \hat{E} & \hat{F} \\ \hat{D} & \hat{H} & \hat{F} & -\hat{E} \\ -\hat{E} & -\hat{F} & \hat{H} & -\hat{D} \\ -\hat{F} & \hat{E} & \hat{D} & \hat{H} \end{pmatrix}$$

with $\hat{H} = (\hat{h}_{pq})$, $\hat{D} = (\hat{d}_{pq})$, $\hat{E} = (\hat{e}_{pq})$, $\hat{F} = (\hat{f}_{pq})$.

It remains to be shown how to choose the matrix $Q_{\alpha\beta}(\varphi)$. To this aim we consider 4 cases

1) $\max_{p\neq q} |r_{pq}| = |h_{\alpha\beta}|$. In this case

$$Q_{\alpha\beta}(\varphi) = diag[T_{\alpha\beta}(\varphi), T_{\alpha\beta}(\varphi), T_{\alpha\beta}(\varphi), T_{\alpha\beta}(\varphi)]$$

where the $n \times n$ matrix $T_{\alpha\beta}(\varphi)$ has the elements

$$\begin{aligned} t_{\alpha\alpha} &= t_{\beta\beta} = \cos\varphi \\ t_{\alpha\beta} &= -t_{\beta\alpha} = -sin\varphi \\ t_{pq} &= \delta_{pq} \text{ - in the remaining cases.} \end{aligned} \tag{45}$$

The parameter φ is to be determined from

$$\text{tg}2\varphi = \frac{2h_{\alpha\beta}}{h_{\alpha\alpha} - h_{\beta\beta}} \tag{46}$$

which follows from $\hat{h}_{\alpha\beta} = 0$.

2) $max_{p\neq q}|r_{pq}| = |d_{\alpha\beta}|$. In this case we introduce the $n \times n$ matrices $C = (c_{pq})$ and $S = (s_{pq})$ which elements are given by

$$\begin{aligned} c_{\alpha\alpha} &= c_{\beta\beta} = \cos\varphi \\ c_{pq} &= \delta_{pq} - \text{ in the remaining cases} \end{aligned} \tag{47}$$

and

$$\begin{aligned} s_{\alpha\beta} &= s_{\beta\alpha} = \sin\varphi \\ s_{pq} &= 0 \text{ - in the remaining cases.} \end{aligned} \tag{48}$$

Then

$$Q_{\alpha\beta}(\varphi) = \begin{pmatrix} C & -S & 0 & 0 \\ S & C & 0 & 0 \\ 0 & 0 & C & S \\ 0 & 0 & -S & C \end{pmatrix} \tag{49}$$

From $\hat{d}_{\alpha\beta} = 0$ one can obtain the eqiation

$$\text{tg}2\varphi = \frac{2d_{\alpha\beta}}{h_{\beta\beta} - h_{\alpha\alpha}} \tag{50}$$

for the parameter φ.

3) $\max_{p\neq q} |r_{pq}| = |e_{\alpha\beta}|$. In this case

$$Q_{\alpha\beta}(\varphi) = \begin{pmatrix} C & 0 & S & 0 \\ 0 & C & 0 & S \\ -S & 0 & C & 0 \\ 0 & -S & 0 & C \end{pmatrix} \tag{51}$$

and for φ from $\hat{e}_{\alpha\beta} = 0$ we get

$$\text{tg}2\varphi = \frac{2e_{\alpha\beta}}{h_{\beta\beta} - h_{\alpha\alpha}} \tag{52}$$

4) $\max_{p\neq q} |r_{pq}| = |f_{\alpha\beta}|$. In this case

$$Q_{\alpha\beta}(\varphi) = \begin{pmatrix} C & 0 & 0 & -S \\ 0 & C & S & 0 \\ 0 & -S & C & 0 \\ S & 0 & 0 & C \end{pmatrix} \tag{53}$$

and from $\hat{f}_{\alpha\beta} = 0$ we get

$$\text{tg}2\varphi = \frac{2f_{\alpha\beta}}{h_{\beta\beta} - h_{\alpha\alpha}} \tag{54}$$

By analogy to the complex arithmetic the considerations from $R = R^{(k)} = (r_{pq}^{(k)})$ and $\tilde{R} = R^{(k+1)} = (r_{pq}^{(k+1)})$ e.t.c. we get

$$\sigma_{k+1}^2 \leq \sigma_0^2(1 - \frac{1}{2n(n-1)})^{k+1}.$$

The last inequality implies the convergence of $R^{(k)}$ to the quasi-diagonal matrices $diag[L, L, L, L]$ with diagonal matrix $L \in R^{n\times n}$. Meanwhile, the matrix sequence $Q_{\alpha_k\beta_k}(\varphi_k)$ converges to a matrix of the form

$$\begin{pmatrix} X & -Y & U & -V \\ Y & X & V & U \\ -U & -V & X & Y \\ V & -U & -Y & X \end{pmatrix} \tag{55}$$

with columns determining the eigenvectors of R. Having on our disposal these eigenvectors, one can easily obtain the eigenvectors of M. In fact, all the information for the eigenvalues and eigenvectors could be obtained from the matrix L and a block column of (55) only.

4. Generalized eigenvalue problem

Practically, to a spectral problem of the form (29) one can arrive considering the foloowing generalized spectral problem

$$Mx = \lambda Nx \tag{56}$$

where each of the matrices M and N is of the form (29), and N is a positive definite matrix. In this section we propose an orthogonal simplectic algorithm for reducing of (56) to an ordinary spectral problem of the form

$$Py = \lambda y \tag{57}$$

where P is a matrix of the form (2) too. This can be achieved, applying the algorithm of 3.1 with respect to N. In such a way the matrix N can be represented in the form $N = G^H DG$ with an unitary simplectic matrix G and D is a diagonal J-symmetric matrix with positive diagonal elements. Thus (56) can be transfomed in the form (57) with a matrix P of the form (29)

$$P = D^{-1/2} GMG^H D^{-1/2}, \; y = D^{1/2} x$$

Here a variant in real arithmetic can be considered too.

5. Experiments

The algorithms proposed here are compared with an algorithm described in [1]. The comparison is made using a computer AT and the algorithmic language TURBO PASCAL. For the examples experimented, the algorithms proposed in this paper happened to be slower that the algorithm described in [1], but our algorithms are more accurate and have simpler computational schemes, giving better options for parallel modifications.

References

1. J.J. Dongarra, J.R. Gabriel, D.D. Koelling, J.H. Wilkinson. The eigenvalue problem for Hermitian matrices with time reversal symmetry, *Linear Alg. and Apl.* **60**, 1984, 27–42.
2. M. Petkov. Numerical solution of linear algebric problems in the complex case. *Annuaire of Sofia Unifersity "Kl. Okhridski"* **71**, 1976/1977, 15–26 (in Bulgarian)
3. P. Soveh. Relativistic band structure and form surface of thallimn., *Phys. Rev.* **137**, 1965, A1706.
4. E.P Wigner. Group theory and its application to the quantum mechanics of atomic spectra., Academic. New York, 1959.
5. J.H. Wilkinson. The algebric eigenvalue problem. London Oxford Unifersity Press, 1965.

Institute of Mathematics
Acad. G. Bonchev Str., bl.8
1113 Sofia
BULGARIA

Received 01.02.1993