On the quadratic convergence of the Jacobi method for normal matrices

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In this paper it is proved that the Jacobi method for normal matrices, due to Goldstine and Horwitz, after a certain stage in the process, is quadratically convergent. The pivot pair (p, q) is chosen so that the sum of the absolute squares of the elements in positions (p, q) and (q, p) is greatest. In this respect, the results obtained here supplement those of Ruhe who considered only the special row cyclic method of enumerating pivot elements.

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Recently, many papers have been written to show that the Jacobi and Jacobi-like methods (Eberlein, 1962; Seaton, 1969) converge, after a certain stage in the process, quadratically. Here the rate of convergence of the Jacobi method applied to general normal matrices is studied. Goldstine and Horwitz (1959) proved the global convergence of an optimal procedure in the sense that the pairs (p, q) are chosen so that the sum of the squares of the absolute values of the off-diagonal elements is minimised at each stage of the process. Here it is assumed that the pivot pair (p, q) is chosen so that the sum of the squares of the absolute values of the elements in positions (p, q) and (q, p) is largest, and no attempt is made to prove that the process then converges. The aim is to show that if convergence has taken place to a certain extent, thereafter its speed is quadratic. It is noted that normal matrices have practical applications in quantum mechanics.

Description of the method

The method produces a sequence of transformations of the form

$$A_{k+1} = U_k A_k U_k^H \tag{1}$$

starting with the normal $n \times n$ matrix $A = A_0$. A_k approaches a diagonal matrix as $k \to \infty$. U_k is unitary and U_k^H is its transposed conjugate. The elements of U_k are chosen in the following manner:

$$\begin{aligned} u_{ij}^{(k)} &= \delta_{ij} \quad (i, j \neq p_k, q_k;\ p_k < q_k) \\ u_{p_kp_k}^{(k)} &= u_{q_kq_k}^{(k)} = \cos\theta_k \\ u_{p_kq_k}^{(k)} &= e^{i\alpha_k}\sin\theta_k \\ u_{q_kp_k}^{(k)} &= -e^{-i\alpha_k}\sin\theta_k\,. \end{aligned} \tag{2}$$

From (1) and (2) the elements of A_{k+1} are found:

$$\left.\begin{aligned} a_{ij}^{(k+1)} &= a_{ij}^{(k)} & i, j \neq p_k, q_k, \\ a_{p_kj}^{(k+1)} &= \cos\theta_k\, a_{p_kj}^{(k)} + e^{i\alpha_k}\sin\theta_k\, a_{q_kj}^{(k)} & j \neq p_k, q_k, \\ a_{ip_k}^{(k+1)} &= \cos\theta_k\, a_{ip_k}^{(k)} + e^{-i\alpha_k}\sin\theta_k\, a_{iq_k}^{(k)} & i \neq p_k, q_k, \\ a_{q_kj}^{(k+1)} &= -e^{-i\alpha_k}\sin\theta_k\, a_{p_kj}^{(k)} + \cos\theta_k\, a_{q_kj}^{(k)} & j \neq p_k, q_k, \\ a_{iq_k}^{(k+1)} &= -e^{i\alpha_k}\sin\theta_k\, a_{ip_k}^{(k)} + \cos\theta_k\, a_{iq_k}^{(k)} & i \neq p_k, q_k, \\ a_{p_kp_k}^{(k+1)} &= a_{p_kp_k}^{(k)} + L_k, \\ a_{q_kq_k}^{(k+1)} &= a_{q_kq_k}^{(k)} - L_k, \\ a_{p_kq_k}^{(k+1)} &= [a_{p_kq_k}^{(k)} + (a_{q_kq_k}^{(k)} - a_{p_kp_k}^{(k)})\beta_k - a_{q_kp_k}^{(k)}\beta_k^2]\cos^2\theta_k, \\ a_{q_kp_k}^{(k+1)} &= [a_{q_kp_k}^{(k)} + (a_{q_kq_k}^{(k)} - a_{p_kp_k}^{(k)})\bar\beta_k - a_{p_kq_k}^{(k)}\bar\beta_k^{\,2}]\cos^2\theta_k, \end{aligned}\right\} \tag{3}$$

with θ_k chosen in $[-\pi/4, \pi/4]$ and

$$L_k = (a_{q_kq_k}^{(k)} - a_{p_kp_k}^{(k)})\sin^2\theta_k + \tfrac{1}{2}(a_{p_kq_k}^{(k)}e^{-i\alpha_k} + a_{q_kp_k}^{(k)}e^{i\alpha_k})\sin 2\theta_k,$$

$$\beta_k = e^{i\alpha_k}\tan\theta_k.$$

Let S_k be defined by

$$S_k^2 = \sum_{\substack{i,j=1\\ i\neq j}}^{n} |a_{ij}^{(k)}|^2 \geqslant 0\,.$$

Then it can be found that

$$S_{k+1}^2 = S_k^2 + |a_{p_kq_k}^{(k+1)}|^2 + |a_{q_kp_k}^{(k+1)}|^2 - M_k^2 \tag{4}$$

where $M_k = \max_{i \neq j} \{|a_{ij}^{(k)}|^2 + |a_{ji}^{(k)}|^2\}^{\frac{1}{2}}$, and it is assumed that $|a_{p_kq_k}^{(k+1)}|^2 + |a_{q_kp_k}^{(k+1)}|^2 = m_k M_k^2$, $0 \leqslant m_k < 1$ for each k.

Quadratic convergence

The following preliminary result is now established.

Theorem 1:
If B and C are $n \times n$ normal matrices with eigenvalues $\beta_1, \beta_2, \ldots, \beta_n$ and $\gamma_1, \gamma_2, \ldots, \gamma_n$ respectively, then there exists a suitable numbering of the eigenvalues such that

$$|\beta_i - \gamma_i| \leqslant \|B - C\|$$

where $\|\cdot\|$ denotes the Euclidean matrix norm.

Proof:
Consider the matrix $B = C + (B - C)$. Then by the Wielandt-Hoffman theorem (1953) there exists an appropriate numbering of the eigenvalues such that

$$\sum_{i=1}^{n} |\beta_i - \gamma_i|^2 \leqslant \|B - C\|^2$$

from which the result follows immediately.

Now, if $B = A_k$ and $C = \operatorname{diag}[a_{11}^{(k)}, a_{22}^{(k)}, \ldots, a_{nn}^{(k)}]$, it follows from Theorem 1, for an appropriate numbering of the eigenvalues, that

$$|\lambda_i - a_{ii}^{(k)}| \leqslant S_k \tag{5}$$

where λ_i are the eigenvalues of A_k and therefore of A_0 as well.

Let the normal matrix A_0 have distinct eigenvalues and put

$$2\delta = \min_{i \neq j} |\lambda_i - \lambda_j|\,.$$

Now if

$$2S_k < \delta/\sqrt{N} \leqslant \delta, \text{ where } N = n(n-1)/2\,, \tag{6}$$

then from (5) and (6)

$$|a_{ii}^{(k)} - a_{jj}^{(k)}| \geqslant \delta > 0\,. \tag{7}$$

Also, since S_k decreases, (6) and (7) hold true for the rest of the process.

Since A is normal the matrix $C = AA^H - A^HA$ is null. Consequently

$$c_{pq} = (a_{pp} - a_{qq})\bar a_{qp} - (\bar a_{pp} - \bar a_{qq})a_{pq} + \sum_{j \neq p,q} (a_{pj}\bar a_{qj} - \bar a_{jp}a_{jq}) = 0$$

and

$$|(a_{pp} - a_{qq})\bar{a}_{qp} - (\bar{a}_{pp} - \bar{a}_{qq})a_{pq}| \leqslant \sum_{j \neq p,q} (|a_{pj}|\,|a_{qj}| + |a_{jp}|\,|a_{jq}|) \qquad (8)$$
$$\leqslant \tfrac{1}{2} \sum_{j \neq p,q} (|a_{pj}|^2 + |a_{qj}|^2 + |a_{jp}|^2 + |a_{jq}|^2)\,.$$

If at the $(k + 1)$th iteration β_k is chosen as one of the solutions to the equation

$$a^{(k)}_{q_k p_k} \beta_k^2 - (a^{(k)}_{q_k q_k} - a^{(k)}_{p_k p_k}) \beta_k - a^{(k)}_{p_k q_k} = 0$$

then $a^{(k+1)}_{p_k q_k} = 0$ and from (8), (3) and (7) the inequality

$$|a^{(k+1)}_{q_k p_k}| \leqslant (n-2) \frac{M_k^2}{\delta}$$

is obtained. However, the optimal choice of parameters yields the minimal value of

$$|a^{(k+1)}_{p_k q_k}|^2 + |a^{(k+1)}_{q_k p_k}|^2$$

which implies

$$|a^{(k+1)}_{p_k q_k}|^2 + |a^{(k+1)}_{q_k p_k}|^2 \leqslant (n-2)^2 M_k^4/\delta^2 < (n-1)^2 M_k^4/\delta^2. \quad (9)$$

In the case considered here θ_k is determined by (see, for example, Eberlein, 1962)

$$\tan 4\theta_k = \frac{2Re(\xi_k \bar{d}_k)}{|d_k|^2 - |\xi_k|^2}\,, \cos 4\theta_k = \frac{|d_k|^2 - |\xi_k|^2}{|d_k^2 + \xi_k^2|}$$

where

$$d_k = a^{(k)}_{p_k p_k} - a^{(k)}_{q_k q_k}\,,$$
$$\xi_k = a^{(k)}_{p_k q_k} \exp(-i\alpha_k) + a^{(k)}_{q_k p_k} \exp(i\alpha_k)\,,$$

so

$$|\sin \theta_k|^2 \leqslant \frac{2M_k^2}{\delta^2}\,. \qquad (10)$$

Theorem 2:
If (6) holds then

$$S_{k+N} < \frac{\sqrt{2}(n-1)}{1-m} \frac{S_k^2}{\delta} \qquad (11)$$

where $m = \max m_{k+\rho}$, $\rho = 0, 1, 2, \ldots, N-1$.

Proof:
It is first shown inductively that for certain r pairs of off-diagonal elements $a^{(k+r)'}_{ij}, a^{(k+r)'}_{ji}$ $(r \leqslant N)$

$$\sum (|a^{(k+r)'}_{ij}|^2 + |a^{(k+r)'}_{ji}|^2) < 2(n-1)^2 \left(\frac{\sum_{\rho=0}^{r-1} M^2_{k+\rho}}{\delta} \right)^2. \quad (12)$$

For $r = 1$ and $i = p_k, j = q_k$ (12) is obviously true, because of (9).

It is now assumed that (12) is valid for $r < N$ and that the r pairs of off-diagonal elements are chosen so that $a^{(k+r)}_{p_{k+r}q_{k+r}}$, $a^{(k+r)}_{q_{k+r}p_{k+r}}$ do not occur among them. When r is replaced by $r + 1$ the left-hand side of (12) yields

$$\sum (|a^{(k+r+1)'}_{ij}|^2 + |a^{(k+r+1)'}_{ji}|^2) \leqslant \sum (|a^{(k+r)'}_{ij}|^2 + |a^{(k+r)'}_{ji}|^2)$$
$$+ \left| \sum (|a^{(k+r+1)'}_{ij}|^2 + |a^{(k+r+1)'}_{ji}|^2 - |a^{(k+r)'}_{ij}|^2 - |a^{(k+r)'}_{ji}|^2) \right|. \qquad (13)$$

Because of

$$a^{(k+r+1)'}_{ij} = a^{(k+r)'}_{ij},\ i, j \neq p_{k+r}, q_{k+r},$$

and the fact that

$$|a^{(k+r+1)'}_{ip_{k+r}}|^2 + |a^{(k+r+1)'}_{iq_{k+r}}|^2 = |a^{(k+r)'}_{ip_{k+r}}|^2 + |a^{(k+r)'}_{iq_{k+r}}|^2, \quad (i \neq p_{k+r}, q_{k+r})$$

$$|a^{(k+r+1)'}_{p_{k+r}j}|^2 + |a^{(k+r+1)'}_{q_{k+r}j}|^2 = |a^{(k+r)'}_{p_{k+r}j}|^2 + |a^{(k+r)'}_{q_{k+r}j}|^2, \quad (j \neq p_{k+r}, q_{k+r})$$

there are at most $n - 1$ possible cases which are of interest as far as the latter sum of the right-hand side of (13) is concerned. Such elements as may be involved are denoted by $''$ and for $i = p_{k+r}, j \neq p_{k+r}, q_{k+r}$

$$\left| |a^{(k+r+1)''}_{p_{k+r}j}|^2 + |a^{(k+r+1)''}_{jp_{k+r}}|^2 - |a^{(k+r)''}_{p_{k+r}j}|^2 - |a^{(k+r)''}_{jp_{k+r}}|^2 \right|$$
$$\leqslant |(|a^{(k+r)''}_{p_{k+r}j}|\,|\cos \theta_{k+r}| + |a^{(k+r)}_{q_{k+r}j}|\,|\sin \theta_{k+r}|)^2$$
$$+ (|a^{(k+r)''}_{jp_{k+r}}|\,|\cos \theta_{k+r}| + |a^{(k+r)}_{jq_{k+r}}|\,|\sin \theta_{k+r}|)^2$$
$$- |a^{(k+r)''}_{p_{k+r}j}|^2 - |a^{(k+r)''}_{jp_{k+r}}|^2|$$
$$\leqslant \left| |a^{(k+r)}_{jq_{k+r}}|^2 + |a^{(k+r)}_{q_{k+r}j}|^2 - |a^{(k+r)''}_{p_{k+r}j}|^2 - |a^{(k+r)''}_{jp_{k+r}}|^2 \right| \sin^2 \theta_{k+r}$$
$$+ 2(|a^{(k+r)''}_{p_{k+r}j}|\,|a^{(k+r)}_{q_{k+r}j}| + |a^{(k+r)''}_{jp_{k+r}}|\,|a^{(k+r)}_{jq_{k+r}}|)\,|\sin \theta_{k+r}|$$
$$\leqslant \frac{2M^4_{k+r}}{\delta^2} + \frac{2\sqrt{2}\,M^2_{k+r}}{\delta} (|a^{(k+r)''}_{p_{k+r}j}|^2 + |a^{(k+r)''}_{jp_{k+r}}|^2)^{\frac{1}{2}}$$

on using (10) and the formula $ac + bd \leqslant (a^2 + b^2)^{\frac{1}{2}} (c^2 + d^2)^{\frac{1}{2}}$, a, b, c and d assumed non-negative. Also from (9) and the hypothesis

$$|a^{(k+r+1)''}_{p_{k+r}q_{k+r}}|^2 + |a^{(k+r+1)''}_{q_{k+r}p_{k+r}}|^2 < (n-1)^2 \frac{M^4_{k+r}}{\delta^2}\,.$$

Hence

$$\left| \sum (|a^{(k+r+1)'}_{ij}|^2 + |a^{(k+r+1)'}_{ji}|^2 - |a^{(k+r)'}_{ij}|^2 - |a^{(k+r)'}_{ji}|^2) \right|$$
$$< [(n-1)^2 + 2(n-2)] \frac{M^4_{k+r}}{\delta^2} + 2\sqrt{2} \frac{M^2_{k+r}}{\delta}$$
$$\sum (|a^{(k+r)''}_{ij}|^2 + |a^{(k+r)''}_{ji}|^2)^{\frac{1}{2}}\,. \quad (14)$$

Now from the Cauchy-Schwarz inequality

$$\sum (|a^{(k+r)''}_{ij}|^2 + |a^{(k+r)''}_{ji}|^2)^{\frac{1}{2}}$$
$$\leqslant \sqrt{n-2}\, (\sum (|a^{(k+r)''}_{ij}|^2 + |a^{(k+r)''}_{ji}|^2))^{\frac{1}{2}}$$
$$< (n-1) (\sum (|a^{(k+r)'}_{ij}|^2 + |a^{(k+r)'}_{ji}|^2))^{\frac{1}{2}}\,.$$

Therefore, from (13) and (14), and since $(n-1)^2 + 2(n-2) < 2(n-1)^2$

$$\sum (|a^{(k+r+1)'}_{ij}|^2 + |a^{(k+r+1)'}_{ji}|^2) < \sum (|a^{(k+r)'}_{ij}|^2 + |a^{(k+r)'}_{ji}|^2)$$
$$+ 2 \frac{\sqrt{2}\, M^2_{k+r}(n-1)}{\delta} (\sum (|a^{(k+r)'}_{ij}|^2 + |a^{(k+r)'}_{ji}|^2))^{\frac{1}{2}}$$
$$+ 2(n-1)^2 \frac{M^4_{k+r}}{\delta^2}$$
$$= \left(\sqrt{2}\,(n-1) \frac{M^2_{k+r}}{\delta} + (\sum (|a^{(k+r)'}_{ij}|^2 + |a^{(k+r)'}_{ji}|^2))^{\frac{1}{2}} \right)^2$$
$$= 2(n-1)^2 \left(\frac{\sum_{\rho=0}^{r} M^2_{k+\rho}}{\delta} \right)^2,$$

namely (12) holds for $r + 1$. In order to prove the theorem, r in (12) is replaced by N, so that

$$S^2_{k+N} = \sum (|a^{(k+N)'}_{ij}|^2 + |a^{(k+N)'}_{ji}|^2)\,.$$

Also from (4)

$$S^2_{k+N} = S_k^2 - \sum_{\rho=0}^{N-1} (1 - m_{k+\rho}) M^2_{k+\rho}$$

or

$$\sum_{\rho=0}^{N-1} M^2_{k+\rho} \leqslant \frac{1}{1-m} S_k^2\,. \qquad (15)$$

Now, from (12) and (15), (11) follows immediately.

Since $S_k^2 \leqslant NM_k^2$, it follows from (6) and the fact that $|a_{p_kq_k}^{(k+1)}|^2 + |a_{q_kp_k}^{(k+1)}|^2 \leqslant \frac{S_k^4}{4\delta^2}$ (Ruhe, 1967), that

$$\frac{1}{1-m} \leqslant \frac{16}{15} N .$$

Thus Theorem 2 proves that convergence is ultimately quadratic.

In practice, choosing the pivot pairs maximally requires a lot of computing time, due to the *scanning*. This can be cut down considerably by choosing the pivot pairs maximally not over the whole matrix (at each stage of the process), but over a row and the corresponding column. Similarly, the row cyclic enumeration of pivots is, in practical applications, carried out by a *threshold strategy*.

Multiple eigenvalues

It is assumed that diagonal elements which converge to the same eigenvalue occupy successive positions on the diagonal (see, for example, Kempen, 1966a). For convenience of notation it is also assumed, without loss of generality, that only the eigenvalue λ_1 is not simple, its multiplicity being $l \geqslant 2$, and that $a_{11}^{(k)}, a_{22}^{(k)}, \ldots, a_{ll}^{(k)}$ converge to λ_1. Because of (6) no $a_{ii}^{(k)}$ can change its affiliation thereafter in the process (Forsythe and Henrici, 1960). Let

$$S_{k+r}^{(1)^2} = \sum_{\substack{i,j=1 \\ i \neq j}}^{l} |a_{ij}^{(k+r)}|^2 .$$

To obtain an estimate of this quantity A_{k+r} is partitioned in the form

$$A_{k+r} = \begin{bmatrix} A_{k+r}^{(1)} & A_{k+r}^{(2)} \\ A_{k+r}^{(3)} & A_{k+r}^{(4)} \end{bmatrix}$$

such that only the diagonal elements of $A_{k+r}^{(1)}$ converge to λ_1. Hence (see, for example, Wilkinson, 1968)

$$S_{k+r}^{(1)} \leqslant \frac{\sqrt{n-l}}{2\delta}(\|A_{k+r}^{(2)}\|^2 + \|A_{k+r}^{(3)}\|^2) = \frac{\sqrt{n-l}}{2\delta}\varepsilon^2, \text{ say.} \quad (16)$$

Assume now that M_{k+r}^2 is in $A_{k+r}^{(1)}$. From (16) it follows that

$$M_{k+r}^2 \leqslant (n-l)(\varepsilon^2/2\delta)^2 .$$

If $L_{k+r}^2 = \max_{i \neq j} (|a_{ij}^{(k+r)}|^2 + |a_{ji}^{(k+r)}|^2)$,

$i = l + 1(1)n, j = 1(1)l$, then $L_{k+r}^2 \geqslant \varepsilon^2/(l(n-l))$.

Now, if $S_{k+r} << \delta$, in particular, $2S_{k+r} \leqslant \frac{\delta}{(n-l)\sqrt{l}}$, then no M_{k+r}^2 can lie in $A_{k+r}^{(1)}$, for in such a case

$$M_{k+r}^2 \leqslant (n-l)\frac{\varepsilon^4}{4\delta^2} < \frac{\varepsilon^2}{l(n-l)} \leqslant L_{k+r}^2 .$$

Therefore, for each vth transformation ($v > k$) the affected diagonal elements have distance larger than δ, which quantity is positive, and so the proof of quadratic convergence in the absence of multiple eigenvalues given above remains valid when such are present.

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Correspondence

To the Editor
The Computer Journal

Sir,

In the paper 'The formal definition of the BASIC language' by J. A. N. Lee (this *Journal*, Vol. 15, No. 1), the structure defined by the meta symbol ⟨expression⟩ allows any number of prefix operators and thus, for instance, the expression + −3.

This deficiency can be remedied by defining expression as

<expression> : : = { <prefix op > $\}_0^1$ <multiply factor> |
<expression> { + | − $\}_1^1$ <multiply factor>

Yours faithfully,

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