

ON PARALLEL FAST JACOBI ALGORITHM FOR THE EIGENPROBLEM OF REAL SYMMETRIC MATRICES*

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Abstract

Jacobi algorithm has been developed for the eigenproblem of real symmetric matrices, singular value decomposition of matrices and least squares of the overdetermined system on a parallel computer. In this paper, the parallel schemes and fast algorithm are discussed, and the error analysis and a new bound are presented.

§1. Introduction

The accuracy of the classical Jacobi method [7] for the eigensystem of a real symmetric matrix is comparable with that of QR. Especially, the computed eigenvectors are almost exactly orthogonal and span a correct subspace. It is independent of the separation of the eigenvalues. For eigenvectors, QR is incomparable to the Jacobi method. If the matrix is close to the diagonal form, QR loses its advantage [8]. But in speed, the Jacobi method is too slow.

The algorithm has had several interesting developments, since Givens transformations without square roots were presented [3]. The Jacobi algorithm using Gentleman's technique has been developed, and an experimental code [1] produces a more accurate solution than the classical version. The fast algorithm requires only $4n$ multiplications for each two-sided transformations; apparently 50% of work can be reduced. But it is still not suitable for systems of which the order is larger than ten.

With the development of parallel computers, the parallel Jacobi algorithm has been given, and used to solve singular value decomposition problems and to find the least squares solution for the overdetermined system [4]–[6]. The parallel fast algorithm is nearly n times faster than the classical Jacobi method. We have reason to believe that the algorithm may be efficiently used for the parallel computing of larger order matrices. The error analysis of the Jacobi algorithm has been given by Wilkinson [7], and the error analysis of Givens transformations has been given by Gentleman [2], but they cannot be applied to the new algorithm directly, because there are some differences between the two algorithms. In fact, although their transformations are essentially orthogonal similar, the computed transformations are not in fast algorithm. In this paper, an error analysis and a new bound are presented.

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§2. Fast Rotation Transformations

In the fast Jacobi algorithm a real symmetric $n \times n$ matrix A is reduced to a diagonal form by a sequence of fast plane rotations R . Let A and R be the product of three matrices respectively:

$$A = DBD, \quad R = \tilde{D}BD^{-1} \quad (2.1)$$

where $\tilde{D} = \text{diag}(\tilde{d}_i)$, $D = \text{diag}(d_i)$, $d_i > 0$, $i = 1, 2, \dots, n$. A rotation similarity transformation in plane (p, q) of the classical method can be modified as

$$\tilde{A} = \tilde{D}\tilde{B}\tilde{D}, \quad \tilde{B} = HBH^T \quad (2.2)$$

where the nonzero elements of H are defined by

$$h_{pq} = \alpha, \quad h_{qp} = \beta, \quad h_{ii} = 1, \quad i = 1, 2, \dots \quad (2.3)$$

B differs from \tilde{B} only in the rows and columns p, q , as shown in (2.2). α, β can be computed by the following equations:

$$1 = d_p^2 b_{pp} - d_q^2 b_{qq},$$

$$g = 2b_{pq} / (1 + \text{sign}(1) \{1^2 + 4d_p^2 d_q^2 b_{pq}^2\}^{1/2}), \quad (2.4)$$

$$\alpha = g d_q^2, \quad \beta = -g d_p^2. \quad (2.5)$$

The diagonal elements in \tilde{D} can be defined by

$$\tilde{d}_p^2 = d_p^2 / (1 - \alpha\beta), \quad \tilde{d}_q^2 = d_q^2 / (1 - \alpha\beta). \quad (2.6)$$

The transformation defined by (2.1)–(2.6) saves 50% of work by comparison with the classical algorithm. Notice that $\tilde{A} = \tilde{D}\tilde{B}\tilde{D}$ is never produced before completion of the process; therefore the iteration requires only \tilde{B} and \tilde{D} . The transformation $\tilde{B} = HBH^T$ in (2.2) is no longer orthogonal similar; because the matrix H is not orthogonal but $\tilde{D}H\tilde{D}^{-1}$ is orthogonal.

§3. Parallel Scheme

In the Jacobi method each transformation affects only two rows and two columns. Consider a sweep consisting of $n(n-1)/2$ transformations, which should annihilate each off-diagonal elements only once. The transformations in a sweep can be divided into $n-1$ (or n) groups. Since all transformations in each group are disjoint plane rotations, they can be simultaneous when implemented. Hence the algorithm is $n/2$ times faster than the common one. Furthermore, an improved error bound can be obtained [2]. Some partition

regimes have been designed [6], [4]. For example, suppose A is an 8×8 matrix; a regime is

| | | | | |
|---|--------|--------|--------|--------|
| 1 | (1, 2) | (3, 4) | (5, 6) | (7, 8) |
| 2 | (1, 3) | (2, 4) | (5, 7) | (6, 8) |
| 3 | (1, 4) | (2, 3) | (5, 8) | (6, 7) |
| 4 | (1, 5) | (2, 6) | (3, 7) | (4, 8) |
| 5 | (1, 6) | (2, 5) | (3, 8) | (4, 7) |
| 6 | (1, 7) | (2, 8) | (3, 5) | (4, 6) |
| 7 | (1, 8) | (2, 7) | (3, 6) | (4, 5) |

In general, there is another scheme which is coded easily [1]. It can be shown as

| | | | | | |
|---------|-----------|---------------|---------------|---------------|-------|
| 1 | (1, 2) | (3, n) | (4, $n - 1$) | (5, $n - 2$) | |
| 2 | (1, 3) | (4, n) | (5, $n - 1$) | (6, $n - 2$) | |
| 3 | (1, 4) | (2, 3) | (5, n) | (6, $n - 1$) | |
| ⋮ | | | | | |
| $n - 1$ | (1, n) | (2, $n - 1$) | (3, $n - 2$) | (4, $n - 3$) | |
| n | (2, n) | (3, $n - 1$) | (4, $n - 2$) | (5, $n - 3$) | |

§4. Error Analysis

Assume that the mantissa length is t and let $\epsilon = 2^{-t}$. From (2.4) and (2.5), After much tiresome calculation, let \bar{H} denote the computed value of H . We show that

$$\bar{H} = H + F, \quad |F| \leq \delta \cdot H, \quad (1 + \delta) \leq (1 + \epsilon)^6. \tag{4.1}$$

Thus, if $a = (a_i, a_j)^T, b = (b_i, b_j)^T$ and $b = Ha$, then

$$\bar{b} = fl(\bar{H}a) \equiv b + f_b, \quad |f_b| \leq x|b|, \quad (1 + x) \leq (1 + \epsilon)^8. \tag{4.2}$$

Let v be an n -dimensional vector, where $n = 2k$. $H_i (i = 1, 2, \dots, k)$ denotes a sequence of disjoint transformations. Since the errors are independent, equation (4.1) gives

$$\bar{v}_k = fl(\bar{H}_k v) \equiv v_k + f_k, \quad H_k = H_k H_{k-1} \dots H_1, \quad |f_k| \leq x|v_k|. \tag{4.3}$$

Clearly, for an $n \times n$ matrix C , we may write

$$\bar{C}_k = fl(\bar{H}_k C) \equiv C_k + P_k, \quad |P_k| \leq x|C_k|.$$

For the two-sided transformation, if the higher order small quantity is negligible, the bound has only factor 2 extraneously. Thus

$$\bar{C}_{2k} = fl(\bar{H}_k C \bar{H}_k) \equiv C_{2k} + P_{2k}, \quad C_{2k} = H_k C H_k^T, \quad |P_{2k}| \leq x|C_{2k}|. \tag{4.4}$$

For convenience, we consider $n - 1$ groups consisting of n independent transformations in a sweep. Let T_i denote the product of the n transformation matrices $H_i, i = 1, 2, \dots, n$, in the i -th group. From (2.1)–(2.6), the general iteration is given by

$$D_i = D_{i-1} \Lambda_{i-1}^{-1}, \quad \Lambda_{i-1} = \text{diag} (d_j^{(i-1)}).$$

Then

$$\bar{D}_2 = fl(D_1 \bar{A}_1^{-1}) \equiv D_2 + G_2, \quad |G_2| \leq y|D_2|, \quad (1+y) \leq (1+\epsilon)^7. \quad (4.5)$$

Equation (4.4) gives

$$B_2 = fl(H_1 B_1 H_1^T) \equiv H_1 B_1 H_1^T + F_2 = B_2 + F_2, \quad |F_2| \leq 2x|B_2|. \quad (4.6)$$

The transformation becomes

$$A_2 = R_1 A_1 R_1^T = D_2 B_2 D_2, \quad R_1 = D_2 H_1 D_1^{-1}. \quad (4.7)$$

In fact, the higher order small quantity is negligible. From (4.5) and (4.6), we obtain

$$\bar{A}_2 = (D_2 + G_2)(B_2 + F_2)(D_2 + G_2) = A_2 + E_2, \quad \|E_2\| \leq e\|A\|, \quad e = 2x + 2y. \quad (4.8)$$

Thus

$$\bar{A}_2 \leq \|A_2\| + e\|A_2\| \leq (1+e)\|A\|. \quad (4.9)$$

In practice, $A'_3 = R'_2 \bar{A}_2 R_2'^T$ can be computed, where A'_3, R'_2 denote the values of A_3, R_2 obtained from \bar{A}_2 . We have reason to neglect the difference between R'_2 and R_2 , because only the similarity of A_2 and $A_3 = R_2 A_2 R_2^T$ is most important. By similar reasoning, from (4.7)-(4.9) we have

$$\bar{A}_3 = R_2 \bar{A}_2 R_2^T + E'_3, \quad |E'_3| \leq e|R_2 \bar{A}_2 R_2^T|.$$

Thus

$$\bar{A}_3 = A_3 + E_3, \quad \|E_3\| \leq [(1+e)^2 - 1]\|A\|. \quad (4.10)$$

The recursion can be implemented in sequence if r sweeps are applied. Then there are rn groups of transformations. Let $N = rn$. We have

$$\bar{A}_N = A_N + E_N, \quad \|E_N\| \leq [(1+e)^{N-1} - 1]\|A\|. \quad (4.11)$$

If the higher order small quantity is neglected, then

$$\|E_N\| \leq Ne\|A\|. \quad (4.12)$$

Note that the elements below the diagonal in each transformation are not computed but are assigned the same value as those above the diagonal. The matrices are exactly symmetric and so are the errors. Hence, according to the Weyl theorem [9] and equations (4.11), (4.12) we have

$$|\lambda_i - \mu_i| \leq Ne\|A\| \quad (4.13)$$

where $\lambda_i = \lambda_i(A), \mu_i = \mu_i(\bar{A}_N)$ and $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n, \mu_1 \leq \mu_2 \leq \dots \leq \mu_n$. In general, letting r equal six we have the bound

$$|\lambda_i - \mu_i| / (\sum \lambda_i^2)^{1/2} \leq 180 \cdot n2^{-t}. \quad (4.14)$$

If \bar{A}_N and A_N are diagonal in machine accuracy, then

$$(\sum(\lambda_i - \mu_i)^2)^{1/2} / (\sum(\lambda_i^2))^{1/2} \leq 180 \cdot n2^{-t}. \quad (4.15)$$

Now we consider the computational accuracy of the computed vectors. Equation (4.11) gives

$$\bar{A}_N = A_N + E_N = R_N(A + G)R_N^T \quad (4.16)$$

where $G = R_N^T E_N R_N$ is considered a perturbed matrix of A . This equation implies that the parallel fast Jacobi algorithm enables us to obtain the eigenvalues and eigenvector matrix R_N of perturbed matrix $A + G$ exactly. We also find a bound of G as $\|G\| = \|E_N\|$. Furthermore, there is an error in computing R_N since

$$R_N = R_{rn}R_{rn-1} \dots R_1 = D_{rn}H_{rn-1}H_{rn-2} \dots H_1.$$

Suppose $D_1 = I$. From equations (4.1) and (4.5) we obtain the following result:

$$\begin{aligned} \bar{D}_{rn} &= fl(I\bar{\lambda}_1^{-1}\bar{\lambda}_2^{-1} \dots \bar{\lambda}_{N-1}^{-1}) \equiv D_{rn}(1 + (rn - 1)y), \\ \bar{H}_N &= fl(\bar{H}_{rn-1}\bar{H}_{rn-2} \dots \bar{H}_1) \equiv H_N(1 + (rn - 1)x). \end{aligned}$$

Hence

$$\bar{R}_N = fl(\bar{D}_{rn}\bar{H}_N) \equiv D_{rn}H_N(1 + (rn - 1)(x + y) + \epsilon) = R_N(1 + 13rn \cdot \epsilon)$$

Let r equal six; we have

$$\|\bar{R}_N - R_N\| \leq 78n2^{-t}. \quad (4.17)$$

This bound shows that the computed eigenvector matrix is almost orthogonal, and is close to the exact eigenvector matrix of $A + G$.

§5. Comments

In order to solve an eigenproblem, generally the parallel fast Jacobi method discussed above needs 6 times sweeps. It means $6n$ steps will be taken. The same is required in QR $3n$ iterations. In addition, every iteration reducing a matrix to a tridiagonal one by the QR method contains about $n/2$ steps. It means that QR has $(3/2)n^2$ steps. In fact this does not mean that the Jacobi method is $n/4$ times faster than QR because communications are a heavy overhead in the machine.

On the other hand, a slight numerical instability might result from algorithm (2.1)–(2.6) with the growing of elements. We suggest that an alternative fast rotation should be used instead of the one presented in this paper when the rotation angle is larger than 45° , let transformation H be $\begin{bmatrix} \alpha & 1 \\ 1 & \beta \end{bmatrix}$ rather than $\begin{bmatrix} 1 & \alpha \\ \beta & 1 \end{bmatrix}$. The determination of rotation angle and the selection of computing formulas must be done before each transformation is carried out. We think it is not difficult to keep the numerical stability of the parallel fast Jacobi algorithm.

Appendix

Round-off error in Fast Rotation Transformation

Let mantissa length be t and unless otherwise specified, ε_i satisfy $(1 - 2^{-t}) \leq (1 + \varepsilon_i) \leq (1 + 2^{-t})$.

$$\begin{aligned}
 fl(l) &= d_p^2 b_{pp}(1 + \varepsilon_1) - d_q^2 b_{qq}(1 + \varepsilon_2) = l(1 + \varepsilon_3), (1 - 2^{-t})^2 \leq (1 + \varepsilon_3) \leq (1 + 2^{-t})^2; \\
 fl(l^2) &= l^2(1 + \varepsilon_3)^2(1 + \varepsilon_4) = l^2(1 + \varepsilon_5), (1 - 2^{-t})^5 \leq (1 + \varepsilon_5) \leq (1 + 2^{-t})^5; \\
 fl(4d_p^2 d_q^2 b_{pq}^2) &= 4d_p^2 d_q^2 b_{pq}^2(1 + \varepsilon_6), (1 - 2^{-t})^3 \leq (1 + \varepsilon_6) \leq (1 + 2^{-t})^3; \\
 fl(l^2 + 4d_p^2 d_q^2 b_{pq}^2) &= l^2(1 + \varepsilon_5) + 4d_p^2 d_q^2 b_{pq}^2(1 + \varepsilon_6) = (l^2 + 4d_p^2 d_q^2 b_{pq}^2)(1 + \varepsilon_7), \\
 &\quad (1 - 2^{-t})^6 \leq (1 + \varepsilon_7) \leq (1 + 2^{-t})^6; \\
 fl(l + \text{sig}(l) \sqrt{l^2 + 4d_p^2 d_q^2 b_{pq}^2}) &= (l(1 + \varepsilon_3) + \text{sig}(l)(l^2 + 4d_p^2 d_q^2 b_{pq}^2)^{1/2}(1 + \varepsilon_7)^{1/2})(1 + \varepsilon_8) \\
 &= (l + \text{sig}(l)(l^2 + 4d_p^2 d_q^2 b_{pq}^2)^{1/2})(1 + \varepsilon_9), (1 - 2^{-t})^4 \leq (1 + \varepsilon_9) \leq (1 + 2^{-t})^4; \\
 fl(g) &= 2b_{pq}(1 + \varepsilon_{10}) / (l + \text{sig}(l)(l^2 + 4d_p^2 d_q^2 b_{pq}^2)^{1/2}) = 9(1 + \varepsilon_{11}), \\
 &\quad (1 - 2^{-t})^5 \leq (1 + \varepsilon_{11}) \leq (1 + 2^{-t})^5; \\
 fl(\alpha) &= 9(1 + \varepsilon_{11})d_q^2(1 + \varepsilon_{12}) = \alpha(1 + \varepsilon_{13}), (1 - 2^{-t})^6 \leq (1 + \varepsilon_{13}) \leq (1 + 2^{-t})^6; \\
 fl(\beta) &= (1 + \varepsilon'_{13}), (1 - 2^{-t})^6 \leq (1 + \varepsilon'_{13}) \leq (1 + 2^{-t})^6; \\
 fl(\tilde{d}_p^2) &= d_p^2(1 + \varepsilon_{14}) / (1 - \alpha(1 + \varepsilon_{13})\beta(1 + \varepsilon_{13}))(1 + \varepsilon_{15}) = \tilde{d}_p^2(1 + \varepsilon_{16}), \\
 &\quad (1 - 2^{-t})^{14} \leq (1 + \varepsilon_{16}) \leq (1 + 2^{-t})^{14}; \\
 fl(\tilde{d}_q^2) &= \tilde{d}_q^2(1 + \varepsilon'_{16}), (1 - 2^{-t})^{14} \leq (1 + \varepsilon'_{16}) \leq (1 + 2^{-t})^{14}.
 \end{aligned}$$

References

- [1] Deng Jian-Xin, The Jacobi method of solving eigenvalue problem of a real symmetric matrix, *Journal on Numerical Method and Computer Applications*, 2 (1981), 122-128.
- [2] W.M. Gentleman, Error analysis of QR decompositions by Givens transformations, *Lin. Alg. Appl.*, 10 (1975), 188-197.
- [3] W.M. Gentleman, Least squares computations by Givens transformations without square roots, *J. Inst. Math. Appl.*, 12 (1973), 329-336.
- [4] G.H. Golub, Van C. F. Loan, *Matrix Computations*, The Johns Hopkins University Press, 1983.
- [5] F.T. Luk, Computing the Singular value decomposition on the ILLIAC, *ACM Transactions on Mathematics software*, 6 (1980), 524-539.
- [6] A.H. Sameh, On Jacobi and Jacobi-like algorithms for a parallel computer, *Math. of Comp.*, 25 (1971), 579-590.
- [7] J.H. Wilkinson, *The Algebraic Eigenvalue Problem*. Clarendon, Oxford, 1965.
- [8] J.H. Wilkinson, Almost diagonal matrices with multiple or close eigenvalues, *Lin. Alg. & Its Appl.*, 1 (1968), 1-12.
- [9] H. Wolkowicz, G. H. Styan, Bounds for eigenvalues using traces, *Lin. Alg. and Its appl.*, 29 (1980), 471-506.