Journal of Computational Mathematics, Vol.20, No.5, 2002, 519–524.

A REVERSE ORDER IMPLICIT Q-THEOREM AND THE ARNOLDI PROCESS*[1)]

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Abstract

Let A be a real square matrix and $V^{\mathrm{T}}AV = G$ be an upper Hessenberg matrix with positive subdiagonal entries, where V is an orthogonal matrix. Then the implicit Q-theorem states that once the first column of V is given then V and G are uniquely determined. In this paper, three results are established. First, it holds a reverse order implicit Q-theorem: once the last column of V is given, then V and G are uniquely determined too. Second, it is proved that for a Krylov subspace two formulations of the Arnoldi process are equivalent and in one to one correspondence. Finally, by the equivalence relation and the reverse order implicit Q-theorem, it is proved that for the Krylov subspace, if the last vector of vector sequence generated by the Arnoldi process is given, then the vector sequence and resulting Hessenberg matrix are uniquely determined.

Key words: Implicit Q-theorem, Reverse order implicit Q-theorem, Truncated version, Arnoldi process.

1. Introduction

It is well known [1] that for a general real square matrix A of order n there exists an orthogonal matrix $V = (v_1, v_2, \ldots, v_n)$ such that $V^{\mathrm{T}}AV = G$ is an upper Hessenberg matrix with nonnegative subdiagonal entries, where the superscript T denotes the transpose of a vector or matrix. This is called an upper Hessenberg decomposition of A. The implicit Q-theorem states that if the subdiagonal entries of G are positive then such a decomposition is unique once v_1 is given. That is, V and G are uniquely determined [4, 1]. For A symmetric, it can be trivially proved in the same way that V and G are also uniquely determined once the last column v_n of V is given [4], where G now reduces to a symmetric tridiagonal matrix. This is called the reverse order implicit Q-theorem. The Hessenberg decomposition is a commonly used tool in matrix computations. Its uniqueness is critical for efficiently implementing the QR algorithm to solve the eigenproblem of A [1]. When A is symmetric, the reverse order implicit Q-theorem plays a central role in the QL algorithm [4].

In this paper, we generalize the reverse order implicit Q-theorem and its truncated version to the unsymmetric case. It turns out that their proofs are nontrivial. Meanwhile, we prove that for a Krylov subspace, two formulations of the process are equivalent and in one to one correspondence. That is, let

$$AQ_m = Q_m H_m + r e_m^{\mathrm{T}} \tag{1}$$

* Received January 10, 2000.

1) Supported by the Special Funds for Major State Basic Research Projects (G1999032805), the Foundation for Excellent Young Scholars of the Ministry of Education, the Research Fund for the Doctoral Program of Higher Education and the Foundation for Key Teachers in Chinese Universities.

and

$$Q_m^{\mathrm{T}} A Q_m = H_m, \tag{2}$$

where e_i is the ith column of the $n \times n$ identity matrix I_n, $Q_m^{\mathrm{T}} r = 0$ and H_m is an upper Hessenberg matrix with positive subdiagonal entries and $Q_m = (q_1, q_2, \ldots, q_m)$ is orthonormal. Then (1) is equivalent to (2). Using the above relations and the truncated version of the reverse order implicit Q-theorem, we prove that for the Krylov subspace, Q_m and H_m generated by the Arnoldi process are uniquely determined if q_m of the vector sequence is given. One of the results in our paper plays a key role in characterizing a refined Ritz vector by polynomials [3].

Throughout, let A be an $n \times n$ real matrix and $\mathcal{K}_m(q_1, A) = \mathrm{span}\{q_1, Aq_1, \ldots, A^{m-1}q_1\}$ denote a m-dimensional Krylov subspace.

2. The implicit Q-theorem

Theorem 1 (the implicit Q-theorem [1]). *Assume that both $Q = (q_1, q_2, \ldots, q_n)$ and $V = (v_1, v_2, \ldots, v_n)$ are orthogonal matrices. Let*

$$Q^{\mathrm{T}} A Q = H \quad \text{and} \quad V^{\mathrm{T}} A V = G,$$

where H and G are upper Hessenberg matrices with positive subdiagonal entries. Then if $v_1 = q_1$, we have $V = Q$ and $G = H$.

This theorem has the following two truncated versions.

Theorem 2[1]. *Assume that $Q_m = (q_1, q_2, \ldots, q_m)$ and $V_m = (v_1, v_2, \ldots, v_m)$ are both orthonormal and satisfy*

$$Q_m^{\mathrm{T}} A Q_m = H_m, \ V_m^{\mathrm{T}} A V_m = G_m,$$

where H_m and G_m are $m \times m$ upper Hessenberg matrices with positive subdiagonal entries. If $v_1 = q_1$, then $V_m = Q_m$ and $G_m = H_m$.

Theorem 3. *Assume that $Q_m = (q_1, q_2, \ldots, q_m)$ and $V_m = (v_1, v_2, \ldots, v_m)$ satisfy the Arnoldi process*

$$\begin{aligned} AQ_m &= Q_m H_m + r e_m^{\mathrm{T}}, \\ AV_m &= V_m G_m + f e_m^{\mathrm{T}}, \end{aligned}$$

where $Q_m^{\mathrm{T}} Q_m = V_m^{\mathrm{T}} V_m = I_m$, $Q_m^{\mathrm{T}} r = V_m^{\mathrm{T}} f = 0$, and H_m and G_m are upper Hessenberg matrices with positive subdiagonal entries. If $v_1 = q_1$, then $V_m = Q_m$, $G_m = H_m$ and $f = r$.

3. The reverse order implicit Q-theorem

In this section we prove the reverse order implicit Q-theorem and its truncated version. To this end, we need the following lemma.

Lemma 1. *Assume that $Q = (q_1, q_2, \ldots, q_m)$ is orthonormal and $Q^{\mathrm{T}} A Q = H = (h_{ij})$ is an upper Hessenberg matrix with positive subdiagonal entries. Let $\hat{Q} = (q_m, q_{m-1}, \ldots, q_1)$ and*

$$\hat{H} = \begin{pmatrix} h_{mm} & h_{m-1m} & \cdots & \cdots & h_{1m} \\ h_{mm-1} & h_{m-1m-1} & \cdots & \cdots & h_{1m-1} \\ & \ddots & \ddots & \vdots & \vdots \\ & & h_{32} & h_{22} & h_{12} \\ & & & h_{21} & h_{11} \end{pmatrix}.$$

Then $\hat{Q}^{\mathrm{T}} A^{\mathrm{T}} \hat{Q} = \hat{H}$ is an upper Hessenberg matrix with positive subdiagonal entries.

Proof. Since $\hat{Q} = Q(e_m, e_{m-1}, \ldots, e_1)$, we have by $Q^{\mathrm{T}}AQ = H$ that

$$\hat{Q}^{\mathrm{T}}A\hat{Q} = \begin{pmatrix} h_{mm} & h_{mm-1} & & & \\ h_{m-1m} & h_{m-1m-1} & \ddots & & \\ \vdots & \vdots & \ddots & \ddots & \\ h_{2m} & h_{2m-1} & \ldots & \ldots & h_{21} \\ h_{1m} & h_{1m-1} & \ldots & \ldots & h_{11} \end{pmatrix},$$

which gives that $\hat{Q}^{\mathrm{T}}A^{\mathrm{T}}\hat{Q} = \hat{H}$. Obviously, the subdiagonal entries of $\hat{H}$ are positive. □

Theorem 4. *All the assumption are as above. If $v_n = q_n$, then $V = Q$ and $G = H$.*

Proof. Let

$$\begin{aligned} \hat{V} &= V(e_n, e_{n-1}, \ldots, e_1) = (v_n, v_{n-1}, \ldots, v_1), \\ \hat{Q} &= Q(e_n, e_{n-1}, \ldots, e_1) = (q_n, q_{n-1}, \ldots, q_1). \end{aligned}$$

By Lemma 1, we know $\hat{V}^{\mathrm{T}}A^{\mathrm{T}}\hat{V} = \hat{G}$ and $\hat{Q}^{\mathrm{T}}A^{\mathrm{T}}\hat{Q} = \hat{H}$ are upper Hessenberg matrices with positive subdiagonal entries. On the other hand, since $v_n = q_n$ is the first column of $\hat{V}$ and of $\hat{Q}$, we have from Theorem 1 that $\hat{V} = \hat{Q}$. Therefore, $V = Q$ and $G = H$. □

Analogously, we can derive the truncated version of Theorem 4, i.e., the reverse order truncated implicit Q-theorem.

Theorem 5. *The assumptions are as in Theorem 2. If $v_m = q_m$, then $V_m = Q_m$ and $G_m = H_m$.*

4. Uniqueness of the Arnoldi process in the reverse order

Given the m-dimensional Krylov subspace $\mathcal{K}_m(q_1, A)$, the Arnoldi process generates an orthonormal basis $\{q_i\}_1^m$ of the subspace [5]. Let $Q_m = (q_1, q_2, \ldots, q_m)$. Then the process can be written in the matrix form

$$AQ_m = Q_m H_m + r e_m^{\mathrm{T}}, \tag{3}$$

where H_m is an upper Hessenberg matrix with posive subdiagonal entries, and $Q_m^{\mathrm{T}} r = 0$.

Premultiplying (3) by Q_m^{T} immediately gives

$$Q_m^{\mathrm{T}} A Q_m = H_m, \tag{4}$$

which is called the matrix representation of A in $\mathcal{K}_m(q_1, A)$ with respect to the basis $\{q_i\}_1^m$.

For $m \le n$, Theorem 3 says that once q_1 is given then Q_m and G_m in (3) are uniquely determined. Naturally, we hope that for $m < n$ there holds the reverse order version of Theorem 3, namely, given q_m, then Q_m and H_m are uniquely determined. To do this, an important problem to be solved is whether or not we can derive unique (3) from (4), i.e., whether or not (3) and (4) are equivalent and in one to one correspondence. If the answer were positive, we would conclude from Theorem 5 that if q_m in (3) is given then Q_m and H_m in (3) can be uniquely determined. It is trivial and direct to derive (4) from (3), as seen above. This is a well-known fact in the field. However, it appears that no one has considered its opposite side: if an orthonormal basis Q_m of $\mathcal{K}_m(q_1, A)$ satisfies (4), must Q_m be generated by the Arnoldi process? The following theorem gives a positive answer to this question.

Theorem 6. *Assume $Q_m = (q_1, q_2, \ldots, q_m)$ to be an orthonormal basis of $\mathcal{K}_m(q_1, A)$. If $Q_m^{\mathrm{T}} A Q_m = H_m$ is an upper Hessenberg matrix with positive subdiagonal entries, then $AQ_m = Q_m H_m + r e_m^{\mathrm{T}}$, where $Q_m^{\mathrm{T}} r = 0$.*

Proof. By definition, $\pi_m = Q_m Q_m^{\mathrm{T}}$ is the orthogonal projector onto $\mathcal{K}_m(q_1, A)$. Since $Q_m^{\mathrm{T}} A Q_m = H_m$ and $Aq_1 \in \mathcal{K}_m(q_1, A)$, we have

$$Aq_1 = \pi_m A q_1 = Q_m Q_m^{\mathrm{T}} A q_1 = Q_m H_m e_1.$$

Therefore, we obtain from $A^2 q_1 \in \mathcal{K}_m(q_1, A)$ that

$$A^2 q_1 = \pi_m A^2 q_1 = \pi_m A A q_1 = \pi_m A \pi_m A q_1 = Q_m Q_m^{\mathrm{T}} A Q_m Q_m^{\mathrm{T}} A q_1 = Q_m H_m H_m e_1 = Q_m H_m^2 e_1.$$

Similarly, we can prove by induction that

$$A^i q_1 = Q_m H_m^i e_1, \quad i = 3, 4, \ldots, m-1.$$

Define the matrix $K_m(q_1, A) = (q_1, Aq_1, \ldots, A^{m-1} q_1)$. Then we get

$$\begin{aligned} K_m(q_1, A) &= (Q_m e_1, Q_m H_m e_1, \ldots, Q_m H_m^{m-1} e_1) \\ &= Q_m K_m(e_1, H_m). \end{aligned}$$

Clearly, $K_m(e_1, H_m)$ is upper triangular, and we can verify that its diagonal entries are 1, h_{21} $h_{21} h_{32}$, ..., $h_{21} h_{32} \cdots h_{mm-1}$, which all are positive. Hence $K_m(e_1, H_m)$ is nonsingular. Therefore, we get by letting $R = K_m(e_1, H_m)^{-1}$

$$Q_m = K_m(q_1, A) R \qquad \text{with} \quad R = \begin{pmatrix} 1 & r_{12} & \cdots & r_{1m} \\ 0 & r_{22} & \cdots & r_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & r_{mm} \end{pmatrix}. \tag{5}$$

We now have from (5) that

$$Aq_i \in \mathcal{K}_m(q_1, A), i = 1, 2, \ldots, m-1. \tag{6}$$

Noting that π_m is the orthogonal projector onto $\mathcal{K}_m(q_1, A)$, we have

$$\begin{aligned} \pi_m A q_i &= Aq_i, \ i = 1, 2, \ldots, m-1. \\ (I_m - \pi_m) A Q_m &= (0, 0, \ldots, (I_m - \pi_m) A q_m). \end{aligned} \tag{7}$$

On the other hand, it follows from $Q_m^{\mathrm{T}} A Q_m = H_m$ and $\pi_m = Q_m Q_m^{\mathrm{T}}$ that

$$\pi_m A Q_m = Q_m H_m. \tag{8}$$

Let $r = (I_m - \pi_m) A q_m$. Then $Q_m^{\mathrm{T}} r = 0$. Combining (7) with (8) yields

$$AQ_m - Q_m H_m = (0, \ldots, 0, r) = r e_m^{\mathrm{T}}, Q_m^{\mathrm{T}} r = 0.$$

This completes the proof. $\square$

Now, since (3) and (4) are equivalent, we have proved by Theorem 5 the uniqueness of the Arnoldi process and its reverse order form.

Theorem 7. *The assumptions are as in Theorem 3. If $v_m = q_m$, then $V_m = Q_m$, $G_m = H_m$ and $f = r$.*

We see that Theorem 6 requires Q_m to be an orthonormal basis of $\mathcal{K}_m(q_1, A)$. This condition is necessary. Otherwise, the assertion can be false, as shown below.

Proposition *Assume that* $Q_m = (q_1, q_2, \ldots, q_m)$ *is orthonormal such that*

$$Q_m^{\mathrm{T}} A Q_m = H_m,$$

is an $m \times m$ *upper Hessenberg matrix with positive subdiagonal entries. Then the columns of* Q_m *may not be a basis of* $\mathcal{K}_m(q_1, A)$.

Proof. Suppose the assertion does not hold, namely, Q_m must be an orthonormal basis of $\mathcal{K}_m(q_1, A)$. Then we know from Lemma 1 that if $\hat{Q}_m = Q_m(e_m, e_{m-1}, \ldots, e_1) = (q_m, q_{m-1}, \ldots, q_1)$ then $\hat{Q}_m^{\mathrm{T}} A^{\mathrm{T}} \hat{Q}_m = \hat{H}_m$, where $\hat{H}_m$ is an upper Hessenberg matrix with positive subdiagonal entries. So $\hat{Q}_m$ is an orthonormal basis of $\mathcal{K}_m(q_m, A^{\mathrm{T}})$. It follows from

$$\mathrm{span}\{Q_m\} = \mathrm{span}\{\hat{Q}_m\}$$

that

$$\mathcal{K}_m(q_1, A) = \mathcal{K}_m(q_m, A^{\mathrm{T}}). \tag{9}$$

In fact, (9) does not hold generally. For example, if

$$A = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \\ 0 & 4 & 0 \end{pmatrix}$$

and we take for $m = 2$

$$q_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix},$$

then

$$\mathcal{K}_2(q_1, A) = \mathrm{span}\{\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix}\}, \quad q_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}.$$

So

$$\mathcal{K}_2(q_2, A^{\mathrm{T}}) = \mathrm{span}\{\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 2 \\ 3 \\ 1 \end{pmatrix}\}.$$

It is easily verified that

$$\mathcal{K}_2(q_1, A) \neq \mathcal{K}_2(q_m, A^{\mathrm{T}}), \tag{10}$$

A contradication! □

5. Conclusion

We have considered the reverse order analogue of the implicit Q-theorem and of its truncated version for the unsymmetric A, and we have proved that the Arnoldi process has such a property: once the first or last one of the Arnoldi vectors is given, then the Arnoldi vectors and the upper Hessenberg matrix are uniquely determined. In the meanwhile, we have shown that the two formulations of the Arnoldi process are equivalent.

In recent years, the second author has proposed a refined Arnoldi method for large matrix eigenproblems. The resulting algorithms are considerably faster than their conventional counterparts [2, 3]. Theorem 4 of this paper was implicitly used for characterizing refined Ritz vectors by polynomials for a Krylov subspace.

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