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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 $V = (v_1, v_2, \dots, v_n)$ 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

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

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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.