Linear Algebra and its Applications 555 (2018) 355–360

Contents lists available at ScienceDirect

Linear Algebra and its Applications

www.elsevier.com/locate/laa

Another orthogonal matrix, revisited

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ARTICLE INFO

Article history:
Received 7 August 2017
Accepted 24 June 2018
Available online 28 June 2018
Submitted by R. Brualdi

MSC:
15B10
65F30

Keywords:
Unitary
k-Hessenberg
Matrix completion
Quasiseparable
Semiseparable

ABSTRACT

A 2006 paper by Parlett and Barszcz [4] proposed the following problem: Given an unit vector q, compute the orthogonal Hessenberg matrix A with first column q. In complex form, this translates to completing the unitary Hessenberg matrix U with first column q. Looking at the matrix $I - qq^*$ in the special form $I - qq^* = LD^2L^*$, where L is $n \times (n-1)$ and lower triangular with 1's on its main diagonal and $D^2 = diag(\mu_1^2, \dots, \mu_{n-1}^2)$ is positive definite, Parlett observed that for $i > j$ the entries of $\tilde{L} = LD$ can be written as $\tilde{l}_{ij} = -q_i\overline{q}_j\mu_j/\rho_j$, where $\overline{q}_j$ denotes the complex conjugate of q_j and $\rho_i = \sum_{j=i+1}^{n} |q_j|^2$, $\rho_n = 0$, and $\mu_i = \sqrt{\rho_i/\rho_{i-1}}$, for $i = 1, \dots, n$. Furthermore, one solution to this problem is $U = [q\ \tilde{L}]$. Section 1 provides some background, as well as details on the derivation of Parlett's formula. Section 2 contains the main result, where Parlett's method is extended to "tall thin" matrices as suggested by Parlett in his original paper. In other words, using a repeated application of Parlett's method, a solution is given to the problem of completing the unitary k-Hessenberg matrix given its first k columns.

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https://doi.org/10.1016/j.laa.2018.06.029

1. Introduction

In 1971, Householder and Fox [1] introduced a method for computing an orthonormal basis for the range of a projection. Using a Cholesky decomposition on a symmetric idempotent matrix A produced $A = LL^T$, where the columns of the lower triangular matrix L form said basis. Moler and Stewart [3] performed an error analysis on the Householder–Fox algorithm in 1978, where it was shown that in most cases reasonable results can be expected. However, the 2006 paper by Parlett and Barszcz [4] included a numerical experiment by Kahan in which the Householder–Fox method performed poorly. Using the Cholesky factorization technique on $I - qq^T$ with the normalized version of $q = (1, 1/8, 1/8^2, \ldots, 1/8^{15})$ produced L such that $||L^TL - I|| \approx 1$. The source of this poor result is simply cancellation due to subtraction. Parlett suggested a method in which subtraction can be avoided. To begin, recall that if A_k is the $k \times k$ leading principal submatrix of $A = LU$, then $det(A_k) = u_{11} \cdots u_{kk}$ and the kth pivot is given by

$$u_{kk} = \begin{cases} det(A_1) = a_{11} & \text{for } k = 1 \\ det(A_k)/det(A_{k-1}) & \text{for } k = 2, \ldots, n \end{cases} \tag{1}$$

Let $p_0 = 1$ and $p_1, \ldots, p_{n-1}$ denote the leading principal minors of $I - qq^T$, where $p_n = det(I - qq^T) = 0$. Sylvester's determinant theorem states that if A is $n \times m$ and B is $m \times n$, then $det(I_n - AB) = det(I_m - BA)$, where I_n and I_m denote the $n \times n$ and $m \times m$ identity matrices respectively. Thus, for the leading principal minors, we have the formula

$$\begin{aligned} p_j &= det\left(1 - \begin{bmatrix} q_1 & \cdots & q_j \end{bmatrix} \begin{bmatrix} q_1 \\ \vdots \\ q_j \end{bmatrix}\right) \\ &= 1 - \sum_{i=1}^{j} q_i^2 \end{aligned} \tag{2}$$

Parlett however used the simple observation that since

$$\sum_{i=1}^{n} q_i^2 = 1$$

it follows that

$$p_j = 1 - \sum_{i=1}^{j} q_i^2 = \sum_{k=j+1}^{n} q_k^2$$

or defined recursively