Real Tridiagonalization of Hermitian Matrices by Modified Householder Transformation

By Osamu SHUKUZAWA, Toshio SUZUKI, and Ichiro YOKOTA

Department of Mathematics, Yamanashi University

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1. Introduction. In the numerical computations of eigenvalue-eigenvector pairs of real symmetric matrices, the process of tridiagonalization is of great importance to get results with various efficient methods for the tridiagonal matrices. It is convincing that the Householder method is the best one for tridiagonalization of real symmetric matrices. But for complex Hermitian matrices, it has been considered that the tridiagonalization by Householder algorithm could be accomplished only with complex off-diagonal elements (cf. Wilkinson [4] p342, Watkins [3], Godunov et al. [1]). In practical numerical computations, the real tridiagonalization of Hermitian matrices is carried out by operating a unitary matrix to the complex tridiagonal matrix. ([2])

In this paper, we obtain the result that any complex Hermitian matrix can be transformed to a real tridiagonal matrix by only transformations of Householder-type. Our result is based on the method using the extended reflection found by Yokota [5,6] which plays an important role in getting the cellular decomposition of unitary groups. The method of our real tridiagonalization of Hermitian matrices is a modification of the Householder method with a parameter introduced in Yokota's theory. It will be seen in section 2 that, because the essential algorithms are just the same, the programs for the Householder method is directly applicable to our method after rewriting the corresponding parts written for the case of real numbers into those of complex numbers. So the various efficient methods for computing eigenpairs of real symmetric matrices through tridiagonalization of them can be easily extended to apply to those of complex Hermitian matrices.

2. Extended reflection and real tridiagonalization of Hermitian matrix. The idea of extended reflection is so general that our theory stands for the field of quaternions. First, we confirm our notation in order to state the fundamental lemma on the extended reflection under the most general situation. Let K denote the field $\boldsymbol{R}$ of real numbers or the field $\boldsymbol{C}$ of complex numbers or the field $\boldsymbol{H}$ of quaternions. In a natural way, $\boldsymbol{R} \subset \boldsymbol{C} \subset \boldsymbol{H}$. The conjugate $\bar{q}$ and the norm $|q|$ of a quaternion $q = a + bi + cj + dk$ are defined respectively by $\bar{q} = a - bi - cj - dk$ and $|q| = \sqrt{\bar{q}q} = \sqrt{a^2 + b^2 + c^2 + d^2}$. Let K^n be the space of all column n-tuples with entries in K and $M(n, K)$ the space of (n, n) matrices with entries in K. The transpose and conjugate of a matrix X are denoted by ${}^tX$ and $\bar{X}$ respectively; X^* denotes ${}^t\bar{X}$. An inner product $(\ ,\ )$ on K^n and a norm $\|x\|$ of x in K^n are defined respectively by $(x, y) = x^*y$ and $\|x\| = \sqrt{(x, x)}$. A matrix $X \in M(n, K)$ such that $X^* = X$ is called Hermitian. We define $U(n, K)$ by $\{U \in M(n, K) \mid U^*U = I_n\}$, where I_n denotes the identity matrix of order n. Then $U(n, \boldsymbol{R}) = O(n)$, $U(n, \boldsymbol{C}) = U(n)$ and $U(n, \boldsymbol{H}) = Sp(n)$, in standard notation. Now, we shall define an extended reflection

(2.1) $$D = I_n + u(\kappa - 1)u^*$$

where $u \in K^n$ such that $\|u\| = 1$ and $\kappa \in K$ such that $|\kappa| = 1$. Then as easily seen D is a member of $U(n, K)$.

Lemma 2.1. *Let $x, y \in K^n$ such that $\|x\| = \|y\|$. Then there exists an extended reflection D such that $Dx = y$.*

Proof. We may assume that $x \neq y$. Noting that $\|x - y\| \neq 0$ and $(x - y, x) \neq 0$ under the conditions $\|x\| = \|y\|$ and $x \neq y$, put $u = \dfrac{x - y}{\|x - y\|}$ and $\kappa = (x - y, y)(x - y, x)^{-1} = (-\|y\|^2 + x^*y)(\|x\|^2 - y^*x)^{-1} = -(\|x\|^2 - x^*y)(\|x\|^2 - y^*x)^{-1}$. Then obviously $\|u\| = 1$, and it holds $|\kappa| = 1$. In fact, since $\overline{\|x\|^2 - x^*y} = \|x\|^2 - \overline{x^*y} = \|x\|^2 - y^*x$, it is immediate that $|\|x\|^2 - x^*y| = |\|x\|^2 - y^*x|$, which implies $|\kappa| = 1$. Therefore, operating the extended reflection defined by (2.1) on x, we obtain

$$
\begin{aligned}
Dx &= x + \frac{1}{\| x - y \|^2} (x - y)(\kappa - 1)(x - y)^* x \\
&= x + \frac{1}{\| x - y \|^2} (x - y)((x - y, y) \\
&\quad (x - y, x)^{-1} - 1)(x - y, x) \\
&= x + \frac{1}{\| x - y \|^2} (x - y)((x - y, y) \\
&\quad - (x - y, x))(x - y, x)^{-1}(x - y, x) \\
&= x + \frac{1}{\| x - y \|^2} (x - y)(x - y, y - x) \\
&= x + \frac{1}{\| x - y \|^2} (x - y)(- \| x - y \|^2) \\
&= x - (x - y) \\
&= y.
\end{aligned}
$$

Remark 2.2. *In the case $K = C$, it is stated in the books of Wilkinson* [4] (p. 49), *Watkins* [3] (p. 157) *and Godunov et al.* [1] (pp. 100–101) *that the same result of Lemma* 2.1 *holds under the additional condition that* (x, y) *is real.*

Let the i-th component of x be denoted by x_i. The following proposition is a direct consequence of Lemma 2.1.

Proposition 2.3. *Let m be a positive number smaller than $n - 1$. For any complex* (*resp. quaternionic*) *n-vector a, we can construct a unitary* (*resp. symplectic*) *extended reflection D_m which transforms a to a vector b such that $b_j = a_j$ for $1 \leq j \leq m$, b_{m+1} is real and $b_j = 0$ for $m + 2 \leq j \leq n$.*

Proof. Put $s = \sqrt{\sum_{j=m+1}^{n} | a_j |^2}$. Obviously, we have only to show the case that $s > 0$. Let x denote the vector such that $x_j = 0$ for $1 \leq j \leq m$ and $x_j = a_j$ for $m + 1 \leq j \leq n$. Let y be the vector such that $y_j = 0$ for all j but $m + 1$ and that $y_{m+1} = - s$. Put $\kappa = - (\| x \|^2 - x^* y)(\| x \|^2 - y^* x)^{-1} = - (\bar{a}_{m+1} + s)(a_{m+1} + s)^{-1}$. It is easily seen by Lemma 2.1 and its proof that defining the extended reflection D_m to be $I_n + (x - y) \frac{\kappa - 1}{\| x - y \|^2} (x - y)^* = I_n - (x - y) \frac{1}{s} (a_{m+1} + s)^{-1} (x - y)^*$, we complete our proof.

Owing to Proposition 2.3, the following theorem can be derived through the standard argument for tridiagonalization by Householder transformation. (Wilkinson [4], pp.290–292)

Theorem 2.4. *For any complex* (*resp. quaternionic*) *Hermitian* (n, n) *matrix H, there exists a unitary* (*resp. symplectic*) *matrix U with the following properties*:

1) *U is a product of extended reflections,*
2) *UHU^* is real, symmetric and tridiagonal.*

References

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