

AN ABSTRACT OF THE THESIS OF

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This thesis confronts the problem of determining eigenvalues for matrices. Because symmetric and non-symmetric matrices respond differently to manipulation, the two cases are presented separately. More than one method exists for handling each type of matrix; however, one method for each situation is presented in this paper.

DETERMINING EIGENVALUES FOR REAL MATRICES

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CHAPTER I

For a square matrix A the question arises whether or not there is a nonzero vector x which, on multiplication by A , is transformed into a multiple of itself. That is, if A is an $n \times n$ matrix and \mathbb{R}^n denotes the n -dimensional vector space over the real numbers \mathbb{R} , define the linear transformation $L: \mathbb{R}^n \rightarrow \mathbb{R}^n$ by $L(x) = Ax$ for x in \mathbb{R}^n . A fairly important task in many applied problems is the seeking of vectors x such that x and $L(x)$ are parallel. This situation occurs in all applications involving vibrations: aerodynamics, elasticity, nuclear physics, mechanics, chemical engineering, biology, and differential equations.

Consider a system of n first order linear differential equations with constant coefficients to be solved simultaneously:

$$\begin{aligned}(1.1) \quad u_1'(t) &= a_{11}u_1(t) + a_{12}u_2(t) + \dots + a_{1n}u_n(t) \\ u_2'(t) &= a_{21}u_1(t) + a_{22}u_2(t) + \dots + a_{2n}u_n(t) \\ &\cdot \\ &\cdot \\ &\cdot \\ u_n'(t) &= a_{n1}u_1(t) + a_{n2}u_2(t) + \dots + a_{nn}u_n(t)\end{aligned}$$

In standard form, the system (1.1) may be written as

$$(1.2) \quad du/dt = Au$$

where $u = (u_1(t), u_2(t), \dots, u_n(t))^T$ and $du/dt = (u_1'(t), u_2'(t), \dots, u_n'(t))^T$. If $u = xe^{\lambda t}$ is a solution to (1.2), then $du/dt = \lambda xe^{\lambda t} = Au$

and $Axe^{\lambda t} = \lambda xe^{\lambda t}$. Thus, $Ax = \lambda x$. Conversely, if there exists λ and $x \neq 0$ such that $Ax = \lambda x$, then $d/dt(xe^{\lambda t}) = \lambda xe^{\lambda t} = Axe^{\lambda t}$, and we select u to be $xe^{\lambda t}$. The practical importance of studying these particular transformations is now realized. Determining λ and $x \neq 0$ which satisfy $Ax = \lambda x$ will give rise to a solution for the system (1.2).

We now officially formulate the algebraic eigenvalue-eigenvector problem. Let A be a matrix of order n with complex entries. Find a complex number λ such that there exists a complex vector x , $x \neq 0$, where $Ax = \lambda x$. The eigenvalues of A are defined to be those numbers λ for which the equation $Ax = \lambda x$ has a solution $x \neq 0$. Each nonzero vector x satisfying $Ax = \lambda x$ for a given eigenvalue λ is called an eigenvector of A corresponding to λ . The word "eigenvalue" is a hybrid one ("eigen" in German means "proper"). Eigenvalues are also called proper values, characteristic values, and latent values; eigenvectors are correspondingly called proper vectors, etc. In this study the terminology used will be eigenvalue and eigenvector.

When determining the values of λ for which the equation $Ax = \lambda x$ has nontrivial solutions, $Ax = \lambda x$ can be written in the equivalent forms:

$$(1.3) \quad (A - \lambda I)x = 0$$

and

$$(1.4) \quad \begin{bmatrix} (a_{11} - \lambda_1) & a_{12} & \dots & a_{1n} \\ a_{21} & (a_{22} - \lambda_2) & \dots & a_{2n} \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ a_{n1} & a_{n2} & \dots & (a_{nn} - \lambda_n) \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ x_n \end{bmatrix} = 0.$$

The matrix equation (1.4) represents a homogeneous system of linear algebraic equations. An obvious solution is the zero vector. Since this is seldom of interest, we call $x = 0$ the trivial solution and seek $x \neq 0$ such that $Ax = \lambda x$.

Nontrivial solutions exist for equations such as (1.4) if, and only if, the coefficient matrix is singular; in other words, if, and only if, the determinant of the coefficient matrix vanishes. Since $(A - \lambda I)$ contains the parameter λ , we can find nonzero vectors to satisfy (1.4) if, and only if, we can find values of λ satisfying $\det(A - \lambda I) = 0$. The definition of a determinant implies that λ satisfies a polynomial equation

$$(1.5) \quad f(\lambda) = \det(A - \lambda I) = \begin{vmatrix} (a_{11} - \lambda_1) & a_{12} & \dots & a_{1n} \\ a_{21} & (a_{22} - \lambda_2) & \dots & a_{2n} \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ a_{n1} & a_{n2} & \dots & (a_{nn} - \lambda_n) \end{vmatrix}$$

$$= (-1)^n (\lambda^n + a_1 \lambda^{n-1} + a_2 \lambda^{n-2} + \dots + a_{n-1} \lambda + a_n) = 0$$

which has exactly n roots $\lambda_1, \lambda_2, \dots, \lambda_n$. The equation (1.5) is known as the characteristic equation of A . The polynomial determined by the $\det(A - \lambda I)$ is the characteristic polynomial of A . Also, the spectrum of A is defined as $\sigma(A) = \{\lambda \mid Ax = \lambda x \text{ for some } x \neq 0\}$. In other words, $\sigma(A)$ is the set of distinct roots of the characteristic equation of the matrix A . Consequently, $\sigma(A)$ does not reveal the multiplicity of each root.

Although the algebraic eigenvalue-eigenvector problem occurs in many practical situations, the scope of this study is limited to presenting methods to determine the spectrum of a real matrix A . General properties of eigenvalues are stated in Chapter II to lay the groundwork for the study. Before actually determining eigenvalues of the matrix A , the usual initial procedure is a reduction step where A is transformed to a "similar" matrix B which has the same eigenvalues as A . The matrix B has a simpler structure than A , thereby reducing the number of computations necessary to determine the eigenvalues. Reduction methods are described in Chapter III. The algorithm to actually compute the eigenvalues, presented in Chapters IV and V, is the powerful QR algorithm of Francis [3, p. 315]. Remember, we shall restrict our attention to real square matrices only.

CHAPTER II

In order to form a basis for further study, in this chapter we will consider some basic eigenvalue properties and also define terminology to be used. Again, this study is restricted to real matrices because computations for real matrices are simpler than for matrices with complex entries, and results can easily be adapted.

At this point we have not yet placed any restrictions on the structure of a matrix other than requiring that it is a real $n \times n$ matrix. The form an eigenvalue takes, given a certain structure for the matrix to which it is associated, is not unexpected. For example, we can determine whether the eigenvalues of a symmetric matrix are real or complex. Recall that A is Hermitian if it is equal to the transpose of its conjugate (i.e., $A^* = \bar{A}^T = A$).

THEOREM 2.1 The eigenvalues of a Hermitian matrix are real.

Proof. Let A be a Hermitian matrix with the eigenvalue λ . Then there exists a vector $x \neq 0$ such that

$$(2.2) \quad Ax = \lambda x.$$

Thus, taking conjugates and transposing both sides, we have

$$(2.3) \quad x^*A = \bar{\lambda}x^*,$$

where x^* denotes the vector whose elements are the respective conjugates of the elements of the vector x and $\bar{\lambda}$ is the conjugate of λ . Because A is Hermitian, the conjugate transpose of A is A . Premultiply (2.2) by

x^* which results in $x^*Ax = \lambda x^*x$. Postmultiply (2.3) by x which results in $x^*Ax = \bar{\lambda}x^*x$. We find that $\lambda x^*x = \bar{\lambda}x^*x$. Since $x \neq 0$, $x^*x > 0$ and it follows that $\lambda = \bar{\lambda}$. ■

Because the set of symmetric matrices is a subset of the set of Hermitian matrices, we now know the roots of symmetric matrices are real.

Continuing to examine the structure of eigenvalues under specific conditions, we consider the relationship of the eigenvalues of A to the eigenvalues of A^2 or of the inverse of A . Or the question arises as to how eigenvalues are affected if the same constant is added to each diagonal element of A .

LEMMA 2.4 If the matrix A is nonsingular and if $Ax = \lambda x$ for $x \neq 0$, then $A^{-1}x = (1/\lambda)x$.

Proof. We are given that $Ax = \lambda x$ for $x \neq 0$. If $\lambda = 0$, then $Ax = 0$. Since $x \neq 0$, then A must be singular, contradicting the hypothesis. Therefore, $\lambda \neq 0$. Then premultiplication of $Ax = \lambda x$ by the inverse of A results in $A^{-1}Ax = A^{-1}\lambda x$ or $x = \lambda A^{-1}x$. Thus, $(1/\lambda)x = A^{-1}x$. ■

This states that the matrix A and the inverse of A have reciprocal eigenvalues. Interestingly, though, the eigenvector of A corresponding to λ is the same as the eigenvector of A^{-1} corresponding to $1/\lambda$.

LEMMA 2.5 If there exists λ such that $Ax = \lambda x$ for some $x \neq 0$, then $A^n x = \lambda^n x$ for $x \neq 0$.

Proof. 1) We are given that $Ax = \lambda x$ for some $x \neq 0$.

2) Assume that $A^{n-1}x = \lambda^{n-1}x$ for some $x \neq 0$. Then $AA^{n-1}x = A^{n-1}x$ and $A^n x = \lambda^{n-1}Ax = \lambda^{n-1}\lambda x = \lambda^n x$. By math induction, if $Ax = \lambda x$

for some $x \neq 0$, then $A^n x = \lambda^{n-1} x$ for $x \neq 0$ for all natural numbers n . ■

Thus, λ , the eigenvalue of the matrix A , when squared, becomes the corresponding eigenvalue of the matrix A^2 . Again, the eigenvector of A corresponding to λ is the same as the eigenvector of A^2 corresponding to λ^2 .

THEOREM 2.6 If the matrix A has an eigenvalue λ for some $x \neq 0$, then the matrix $A + kI$ has an eigenvalue $\lambda + k$ with corresponding eigenvector x .

Proof. $(A + kI)x = Ax + kIx = \lambda x + kIx = \lambda x + kx = (\lambda + k)x$. ■

Note that incrementing each diagonal element of the matrix A by the value of k also increments the eigenvalues of A by the value k .

As stated in Chapter I, the spectrum of the matrix A does not reveal the multiplicity of the eigenvalues of A . Following is the delineation between the algebraic multiplicity and the geometric multiplicity of an eigenvalue of the matrix A . The characteristic polynomial of the matrix A can be written as a function of μ ; $f(\mu) = \det(A - \mu I)$ which is an n -degree polynomial of the form

$$(2.7) \quad f(\mu) = (-1)^n (\mu^n + \alpha_{n-1} \mu^{n-1} + \dots + \alpha_0).$$

If $\sigma(A) = \{\lambda_1, \dots, \lambda_k\}$, then f can be represented in the form

$$(2.8) \quad f(\mu) = (-1)^n (\mu - \lambda_1)^{\delta_1} (\mu - \lambda_2)^{\delta_2} \dots (\mu - \lambda_k)^{\delta_k}.$$

The integer δ_1 is called the algebraic multiplicity of the eigenvalue

λ_i . Along with the zero vector, the eigenvectors (not uniquely determined) corresponding with the eigenvalue λ fill the linear subspace of eigenvectors associated with λ . If x and y are eigenvectors belonging to the eigenvalue λ , then so is every linear combination $\alpha x + \gamma y \neq 0$. The maximum number of linearly independent eigenvectors associated with the eigenvalue λ (in other words, the dimensions of the subspace) is the geometric multiplicity of the eigenvalue λ . The geometric multiplicity of λ can also be described as the dimension of the null space of $A - \lambda I$.

When beginning the process of determining the spectrum of the matrix A , we will produce a matrix B whose eigenvalues are the same as A . The matrix B will take one of two forms. One possibility will be a tridiagonal matrix T with $t_{ij} = 0$ if $|i-j| \geq 2$. The alternate form that the matrix B takes is either a lower Hessenberg matrix H with $h_{ij} = 0$ if $j \geq i + 2$ or an upper Hessenberg matrix H with $h_{ij} = 0$ if $i \geq j + 2$. When every subdiagonal element of an upper Hessenberg matrix is nonzero, the matrix is an irreducible Hessenberg matrix.

We can write the n eigenvalue equations of the $n \times n$ matrix A as

$$\begin{aligned}
 (2.9) \quad Ax^{(1)} &= \lambda_1 x^{(1)} \\
 Ax^{(2)} &= \lambda_2 x^{(2)} \\
 &\cdot \\
 &\cdot \\
 &\cdot \\
 Ax^{(n)} &= \lambda_n x^{(n)}.
 \end{aligned}$$

If X is the matrix whose n columns are $x^{(1)}$, $x^{(2)}$, ..., $x^{(n)}$, then (2.9) can be written as the single matrix equation

$$(2.10) \quad AX = X\Lambda,$$

where Λ is the diagonal matrix of the eigenvalues of A ,

$$(2.11) \quad \Lambda = \begin{bmatrix} \lambda_1 & & & & 0 \\ & \lambda_2 & & & \\ & & \cdot & & \\ & & & \cdot & \\ 0 & & & & \lambda_n \end{bmatrix}.$$

If the columns of X in (2.10) form a set of n linearly independent eigenvectors, then X is nonsingular and we can write (2.10) as

$$(2.12) \quad X^{-1}AX = \Lambda.$$

In order to proceed with this discussion, we need two definitions. The matrix B is said to be similar to the matrix A if, and only if, there exists a nonsingular matrix P such that $PAP^{-1} = B$. This is defined as a similarity transformation on A .

Producing a matrix B whose eigenvalues are the same as a given matrix A is accomplished by a finite number of similarity transformations

$$\begin{aligned} \hat{A} &= A_0 \rightarrow A_1 \rightarrow A_2 \rightarrow \dots \rightarrow A_k, \\ (A_i &= P_i A_{i-1} P_i^{-1}, i=1,2,\dots,k) \end{aligned}$$

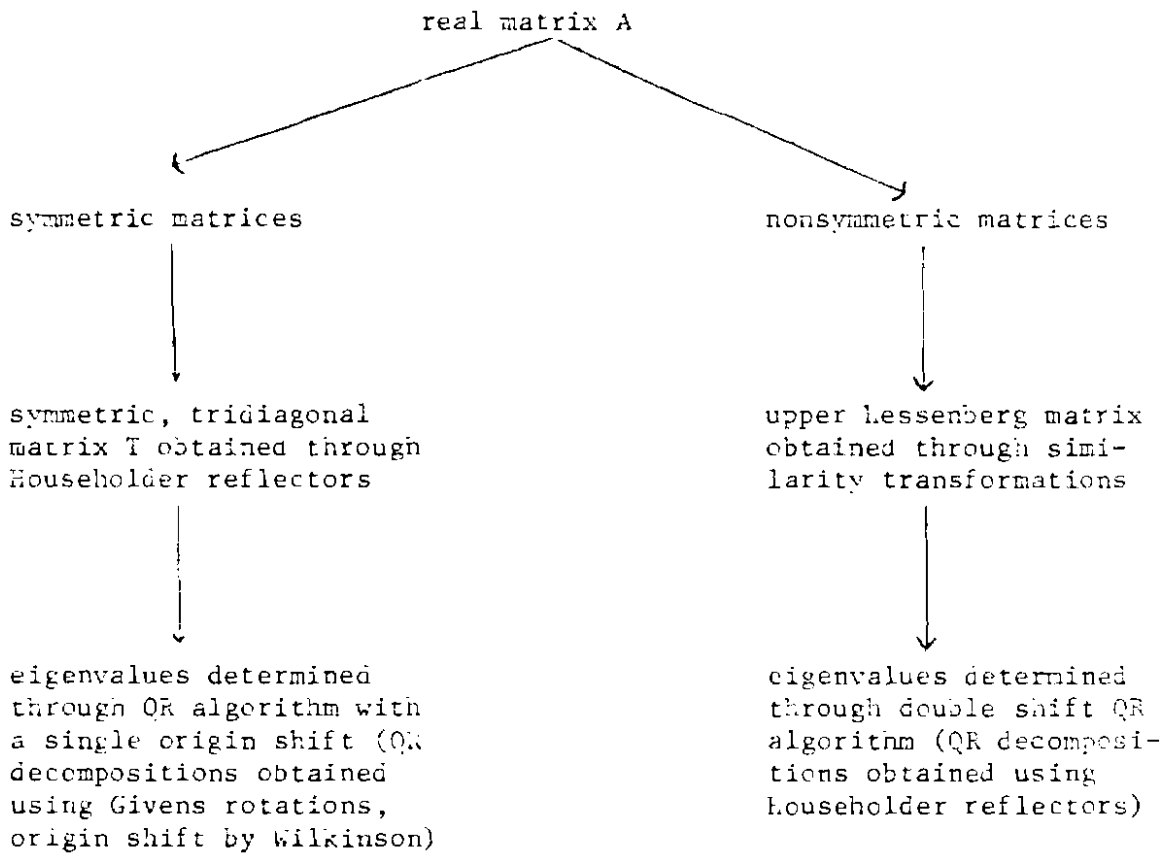
where $B = A_k = PAP^{-1}$, $P = P_k P_{k-1} \dots P_2 P_1$. The spectrum of B is, in fact, the same as the spectrum of A .

THEOREM 2.13 If A and B are both $n \times n$ matrices with real entries and there exists a real, $n \times n$ nonsingular matrix P such that $PAP^{-1} = B$, then A and B have the same set of eigenvalues.

Proof. Let λ be an eigenvalue of A and x be an associated eigenvector so that $Ax = \lambda x$. Let $y = Px$ which means $x = P^{-1}y$. If we substitute for x , we obtain $AP^{-1}y = \lambda P^{-1}y$ which may be written $PAP^{-1}y = P\lambda P^{-1}y = \lambda y$. Since $PAP^{-1} = B$, $By = \lambda y$. Thus, λ is an eigenvalue of B . Similarly, let λ be an eigenvalue of B and let y be an associated eigenvector so that $By = \lambda y$. Let $x = P^{-1}y$ which means $y = Px$. If we substitute for y , we obtain $BPx = \lambda Px$ which may be written $P^{-1}BPx = P^{-1}\lambda Px = \lambda x$. Since $A = P^{-1}BP$, $Ax = \lambda x$. Thus, λ is an eigenvalue of A . ■

It will be our goal in the next three chapters to show how to choose a matrix B whose eigenvalues are the same as a given dense (relatively few zeros) matrix A . The matrix B shall be selected in such a way that 1) the structure of the matrix B is "simpler" than the structure of the matrix A (i.e., has a greater number of zero entries); 2) the determination of the eigenvalues of the matrix B is as "simple" as possible (i.e., requires as few operations as possible) and 3) the eigenvalue problem for the matrix B is not substantially worse conditioned than that for A (i.e., small changes in the matrix B do not perturb the eigenvalues of B sub-

stantially more than small changes in the matrix A). Chapter III presents methods for producing the all important similar matrix B . The outline describing the two-case approach to obtaining the eigenvalues for a square matrix, whose presentations are included in Chapters III, IV and V, may be illustrated by the following diagram.



CHAPTER III

Because of the structure of the eigenvalue problem, it might appear that a good method for finding the eigenvalues of a matrix A would be to compute the zeros of the characteristic polynomial

$$(3.1) \quad \det(A - \lambda I) = (-1)^n |\lambda^n - a_{n-1}\lambda^{n-1} - \dots - a_1\lambda - a_0|.$$

However, if the polynomial is ill-conditioned with respect to the computation of its zeros, the results can be extremely poor. Consider the polynomial

$$(3.2) \quad P_{20}(x) = (x-1)(x-2)(x-3)\dots(x-20)$$

whose zeros are $x_1 = 1, x_2 = 2, \dots, x_{20} = 20$. In comparison, the slightly perturbed polynomial $Q_{20}(x)$ defined by

$$(3.3) \quad Q_{20}(x) = P_{20}(x) - 2^{-23}x^{19}$$

has only ten real zeros. The remaining ten are five complex conjugate pairs, four of which lie in the complex plane between 1.6 and 2.9 units away from the real axis [5, Chapter 2, Section 7].

It is possible for rounding errors to occur during the computation of the coefficients a_0, a_1, \dots, a_{n-1} in (3.1). These computations might introduce perturbations in the characteristic polynomial which can, as seen in Wilkinson's example, drastically alter the results. Therefore, the procedure for finding the eigenvalues of a square matrix by

first determining the characteristic polynomial and, subsequently, determining its zeros is not a viable option.

As stated in Chapters I and II, the usual initial step for determining the spectrum of a real, square matrix A is to construct (through similarity transformations) a matrix B that is similar to A . A natural way to categorize matrices for the purpose of finding eigenvalues is to group matrices as symmetric or nonsymmetric. Constructing algorithms for computing eigenvalues for symmetric matrices is a simpler process than for nonsymmetric matrices because every symmetric matrix is diagonalizable under a real orthogonal ($A^T = A$) similarity transformation. That is, for every real symmetric matrix A there exists a real orthogonal matrix R such that

$$(3.4) \quad R^{-1}AR = \Lambda = \begin{bmatrix} \lambda_1 & & & & 0 \\ & \lambda_2 & & & \\ & & \cdot & & \\ & & & \cdot & \\ 0 & & & & \lambda_n \end{bmatrix}$$

where the eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$ are real. In addition, real symmetric matrices are well-conditioned with respect to computing eigenvalues. In other words, small perturbations in the matrix elements produce only small perturbations in the eigenvalues. Neither of these facts holds for an arbitrary nonsymmetric matrix which we will consider later.

I_n shall denote the identity matrix of order n .

In the process of studying real symmetric matrices, we define a Householder matrix H . For each vector u we will construct H such that

$$(3.5) \quad H = I - \frac{2}{u^T u} uu^T.$$

Given that $x = (x_1, x_2, \dots, x_n)^T$, u shall be defined as the vector $u = x \pm \|x\|e_1$ where $e_1 = (1, 0, \dots, 0)^T$. It is valuable to consider the result when the vector x is multiplied on the left (transformed) by H_u (the matrix defined in 3.5 as a function of u):

$$\begin{aligned} (3.6) \quad H_u x &= \left(I - \left(\frac{2}{u^T u} \right) uu^T \right) x \\ &= x - \frac{2(x \pm \|x\|e_1)(x \pm \|x\|e_1)^T x}{(x \pm \|x\|e_1)^T (x \pm \|x\|e_1)} \\ &= x - \frac{2(x \pm \|x\|e_1)(x^T x \pm x_1 \|x\|)}{x^T x \pm 2x_1 \|x\| + \|x\|^2} \\ &= x - \frac{2(x \pm \|x\|e_1)(\|x\|^2 \pm x_1 \|x\|)}{2\|x\|^2 \pm 2x_1 \|x\|} \\ &= x - \frac{2(x \pm \|x\|e_1)(\|x\|^2 \pm x_1 \|x\|)}{2(\|x\|^2 \pm x_1 \|x\|)} \\ &= x - (x \pm \|x\|e_1) \\ &= \pm \|x\|e_1 \end{aligned}$$

That is, H_u maps x into a vector all of whose components, except the

first, are zero. Since H requires a division by $u^T u = \|u\|^2$, the sign is chosen so that $\|u\|$ is maximum, which maximizes numerical stability.

Using Householder matrices to transform a real symmetric matrix A to a similar matrix B appears to be useful. However, stability or the lack of stability must be considered. If a transformation by a Householder matrix results in a well-conditioned matrix, then we have a method to be reckoned with.

THEOREM 3.7 If H is defined as above, then i) $H = H^T$ and ii) $H = H^{-1}$.

Proof. i) By definition, $H^T = (I - (\frac{2}{u^T u})uu^T)^T = I^T - (\frac{2}{u^T u})(uu^T)^T = I - (\frac{2}{u^T u})uu^T = H$.

$$\begin{aligned} \text{ii) } HH &= (I - (\frac{2}{u^T u})uu^T)(I - (\frac{2}{u^T u})uu^T) \\ &= I - (\frac{4}{u^T u})uu^T + \frac{4}{(u^T u)^2}u(u^T u)u^T \\ &= I - (\frac{4}{u^T u})uu^T + (\frac{4}{u^T u})uu^T \\ &= I. \end{aligned}$$

Hence, $H = H^{-1}$. Therefore, $H = H^T = H^{-1}$ and H is symmetric and orthogonal. ■

As established in Chapter II, pre- and post-multiplication of a matrix A by a matrix H and its inverse, respectively, (HAH^{-1}) result in a matrix whose spectrum is identical to the spectrum of A . Because of the symmetry of the matrix A , whatever zeros are introduced in the first

column of A_1 ($A = A_0 \rightarrow A_1 \rightarrow A_2 \rightarrow \dots \rightarrow A_k = B$) will be introduced in the first row of A_1 by the same Householder transformation. By constructing matrices with the correct dimensions, using the identity matrix, the zero matrix, and a Householder matrix constructed from the appropriate vector, we obtain an orthogonal similarity transformation (a most stable procedure) that introduces $n-k-1$ zeros in the k th row and $n-k-1$ zeros in the k th column of a symmetric matrix A (i.e., in the off-tridiagonal positions). Tridiagonalization of the matrix A is completed after $n-2$ Householder transformations. This procedure is strongly endorsed by Wilkinson [4].

Given an $n \times n$ real symmetric matrix $A = [a_{ij}]$, Householder transformations to tridiagonalize A are constructed in the following manner. Remembering the symmetry of A , let $x_1 = (a_{12}, a_{13}, a_{14}, \dots, a_{1n})^T$. Then $u_1 = (a_{12} \mp x_1, a_{13}, a_{14}, \dots, a_{1n})^T$. H_1 is constructed as $H_1 = I - \frac{2}{u_1^T u_1} u_1 u_1^T$. The first of the transformations will be

$$\begin{bmatrix} I_1 & 0 \\ 0 & H_1 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} & \dots & a_{1n} \\ a_{12} & a_{22} & a_{23} & a_{24} & \dots & a_{2n} \\ a_{13} & a_{23} & a_{33} & a_{34} & \dots & a_{3n} \\ a_{14} & a_{24} & a_{34} & a_{44} & \dots & a_{4n} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ a_{1n} & a_{2n} & a_{3n} & a_{4n} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} I_1 & 0 \\ 0 & H_1 \end{bmatrix}$$

$$= \begin{bmatrix} a_{11} & b_{12} & 0 & 0 & \dots & 0 \\ b_{12} & b_{22} & b_{23} & b_{24} & \dots & b_{2n} \\ 0 & b_{23} & b_{33} & b_{34} & \dots & b_{3n} \\ 0 & b_{24} & b_{34} & b_{44} & \dots & b_{4n} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & b_{2n} & b_{3n} & b_{4n} & \dots & b_{nn} \end{bmatrix}.$$

Next, $x_2 = (b_{23}, b_{24}, \dots, b_{2n})^T$ and $u_2 = (b_{23} \pm \|x_2\|, b_{24}, \dots, b_{2n})^T$. H_2 will be $I - \left(\frac{2}{u_2^T u_2}\right) u_2 u_2^T$. The second transformation will be

$$\begin{bmatrix} I_2 & 0 \\ 0 & H_2 \end{bmatrix} \begin{bmatrix} a_{11} & b_{12} & 0 & 0 & \dots & 0 \\ b_{12} & b_{22} & b_{23} & b_{24} & \dots & b_{2n} \\ 0 & b_{23} & b_{33} & b_{34} & \dots & b_{3n} \\ 0 & b_{24} & b_{34} & b_{44} & \dots & b_{4n} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & b_{2n} & b_{3n} & b_{4n} & \dots & b_{nn} \end{bmatrix} \begin{bmatrix} I_2 & 0 \\ 0 & H_2 \end{bmatrix}$$

$$= \begin{bmatrix} a_{11} & b_{12} & 0 & 0 & \dots & 0 \\ b_{12} & b_{22} & c_{23} & 0 & \dots & 0 \\ 0 & c_{23} & c_{33} & c_{34} & \dots & 0 \\ 0 & 0 & c_{34} & c_{44} & \dots & c_{4n} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & c_{3n} & c_{4n} & \dots & c_{nn} \end{bmatrix}.$$

In like manner we continue until tridiagonalization is completed after $n-2$ Householder transformations. Consider the 4×4 real symmetric matrix

$$A = \begin{bmatrix} 2 & 2 & 6 & 3 \\ 2 & 1 & 2 & 1 \\ 6 & 2 & 1 & 1 \\ 3 & 1 & 1 & 3 \end{bmatrix}.$$

We will employ Householder reflectors to transform A to a tridiagonal matrix T . To obtain zeros in the last two positions of the first row and the first column, let $x = (2, 6, 3)^T$. Then $u = (9, 6, 3)^T$ and the Householder reflector is

$$H_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -\frac{2}{7} & -\frac{6}{7} & -\frac{3}{7} \\ 0 & -\frac{6}{7} & \frac{3}{7} & -\frac{2}{7} \\ 0 & -\frac{3}{7} & -\frac{2}{7} & -\frac{6}{7} \end{bmatrix}.$$

Thus,

$$H_1 A H_1 = \begin{bmatrix} 2 & -7 & 0 & 0 \\ -7 & \frac{163}{49} & \frac{97}{49} & -\frac{25}{49} \\ 0 & \frac{97}{49} & -\frac{3}{49} & -\frac{26}{49} \\ 0 & -\frac{25}{49} & -\frac{26}{49} & \frac{65}{49} \end{bmatrix}.$$

For the next iteration, let $x = \left(\frac{97}{49}, \frac{-25}{49} \right)^T$. Then $u = (4.02387, -0.51020)^T$ and

$$H_2 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -0.96835 & 0.24957 \\ 0 & 0 & 0.24957 & 0.96836 \end{bmatrix} .$$

Thus, the symmetric, tridiagonal matrix transformed from A is

$$H_2 H_1 A H_1 H_2 = \begin{bmatrix} 2 & -7 & 0 & 0 \\ -7 & 3.32653 & -2.04427 & -0.0001 \\ 0 & -2.04427 & .30711 & .89854 \\ 0 & -0.0001 & .89844 & 1.36637 \end{bmatrix} .$$

Again, it is the symmetry which permits a symmetric matrix A to be transformed to a tridiagonal matrix by an orthogonal similarity transformation. Householder transformations can also be applied to nonsymmetric matrices. However, rather than obtaining a tridiagonal matrix, one obtains an upper Hessenberg matrix. But, the required number of multiplications for placing a nonsymmetric matrix in upper Hessenberg form using Householder transformations is $5n^3/3$, as opposed to $5n^3/6$ multiplications to achieve the same form using elementary similarity transformations. The trade-off, though, is that elementary similarity transformations are not always stable; pivotal growth is a possibility (although not a high probability).

The choice between the two methods is similar to the choice between partial and complete pivoting in Gaussian elimination. The higher rate of stability comes with complete pivoting, but most choose partial pivoting because the stability factor is satisfactory and the number of calculations is much less. Concerning elementary similarity transformations, when pivotal growth does not exist and double precision arithmetic is used, elementary similarity transformations result in a better rate of accuracy [8, p. 924] than do Householder transformations. With that in mind, we now describe the use of elementary similarity transformations to reduce a nonsymmetric matrix to upper Hessenberg form.

We can illustrate the process for $n = 4$ and $A_1 = [a_{ij}]$. We shall assume that row and column interchanges are required at each stage of the reduction. Thus, suppose $|a_{41}| > |a_{31}|$ and $|a_{41}| > |a_{21}|$. In this case we interchange rows 2 and 4 and columns 2 and 4 by the similarity transformation $A_1' = I_{24} A_1 I_{24} =$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} a_{11} & a_{14} & a_{13} & a_{12} \\ a_{41} & a_{44} & a_{43} & a_{42} \\ a_{31} & a_{34} & a_{33} & a_{32} \\ a_{21} & a_{24} & a_{23} & a_{22} \end{bmatrix}$$

$= [a'_{ij}]$. Next we annihilate a'_{31} and a'_{41} by the similarity transformation $A_2 = M_2 A_1 M_2^{-1} =$

$$\begin{bmatrix} 1 & & & \\ 0 & 1 & & \\ 0 & m_{32} & 1 & \\ 0 & m_{42} & 0 & 1 \end{bmatrix} \begin{bmatrix} a'_{11} & a'_{12} & a'_{13} & a'_{14} \\ a'_{21} & a'_{22} & a'_{23} & a'_{24} \\ a'_{31} & a'_{32} & a'_{33} & a'_{34} \\ a'_{41} & a'_{42} & a'_{43} & a'_{44} \end{bmatrix} = \begin{bmatrix} 1 & & & \\ 0 & 1 & & \\ 0 & -m_{32} & 1 & \\ 0 & -m_{42} & 0 & 1 \end{bmatrix} =$$

$$\begin{bmatrix} a''_{11} & a''_{12} & a''_{13} & a''_{14} \\ a''_{21} & a''_{22} & a''_{23} & a''_{24} \\ 0 & a''_{32} & a''_{33} & a''_{34} \\ 0 & a''_{42} & a''_{43} & a''_{44} \end{bmatrix} = \begin{bmatrix} b_{11} & b_{12} & b_{13} & b_{14} \\ b_{21} & b_{22} & b_{23} & b_{24} \\ 0 & b_{32} & b_{33} & b_{34} \\ 0 & b_{42} & b_{43} & b_{44} \end{bmatrix},$$

where $m_{32} = -a'_{31}/a'_{21}$.
 $m_{42} = -a'_{41}/a'_{21}$

Suppose $|b_{42}| > |b_{32}|$. Then we interchange the last two rows and the last two columns by the similarity transformation $A'_2 = I_{34} A_2 I_{34}$. Finally, we reduce A'_2 to Hessenberg form by the similarity transformation $A_3 = M_3 A'_2 M_3^{-1} =$

$$\begin{bmatrix} 1 & & & \\ 0 & 1 & & \\ 0 & 0 & 1 & \\ 0 & 0 & m_{43} & 1 \end{bmatrix} \begin{bmatrix} b'_{11} & b'_{12} & b'_{13} & b'_{14} \\ b'_{21} & b'_{22} & b'_{23} & b'_{24} \\ 0 & b'_{32} & b'_{33} & b'_{34} \\ 0 & b'_{42} & b'_{43} & b'_{44} \end{bmatrix} \begin{bmatrix} 1 & & & \\ 0 & 1 & & \\ 0 & 0 & 1 & \\ 0 & 0 & -m_{43} & 1 \end{bmatrix}$$

$$= \begin{bmatrix} b_{11}'' & b_{12}'' & b_{13}'' & b_{14}'' \\ b_{21}'' & b_{22}'' & b_{23}'' & b_{24}'' \\ 0 & b_{32}'' & b_{33}'' & b_{34}'' \\ 0 & 0 & b_{43}'' & b_{44}'' \end{bmatrix}, \text{ where } m_{43} = -b_{42}'/b_{32}'.$$

To carry out the reduction, in general, let $A_1 = [a_{ij}]$ and examine the magnitudes of the elements $a_{21}, a_{31}, \dots, a_{i_1 1}, \dots, a_{n1}$. Let $a_{i_1 1}$ be the element with largest magnitude (the pivot). This means we must interchange row 2 with row i_1 and column 2 with column i_1 by the similarity transformation

$$A_1' = I_{2i_1} A_1 I_{2i_1}.$$

Next, we annihilate $a_{31}', a_{41}', \dots, a_{n1}'$ with the transformation

$$A_2 = M_2 A_1' M_2^{-1},$$

where

$$M_2 = \begin{bmatrix} 1 & & & & & & \\ 0 & 1 & & & & & \\ 0 & m_{32} & 1 & & & & \\ 0 & m_{42} & 0 & 1 & & & \\ \cdot & \cdot & \cdot & \cdot & \cdot & & \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \\ 0 & m_{n2} & 0 & 0 & \dots & 1 \end{bmatrix}$$

and $m_{t2} = -a_{t1}'/a_{21}'$, ($t = 3, 4, \dots, n$). This completes the first step.

We begin the k th step ($k \leq n-2$) with the matrix

$$A_k = \left[\begin{array}{ccc|ccc} f_{11} & f_{12} & \cdots & f_{1k} & \cdots & f_{1n} \\ f_{21} & f_{22} & \cdots & f_{2k} & \cdots & f_{2n} \\ 0 & f_{32} & \cdots & f_{3k} & \cdots & f_{3n} \\ \cdot & \cdot & & \cdot & & \cdot \\ \cdot & \cdot & & \cdot & & \cdot \\ \cdot & \cdot & & \cdot & & \cdot \\ 0 & 0 & \cdots & f_{kk} & \cdots & f_{kn} \\ \hline 0 & 0 & \cdots & f_{k+1,k} & \cdots & f_{k+1,n} \\ 0 & 0 & \cdots & f_{k+2,k} & \cdots & f_{k+2,n} \\ \cdot & \cdot & & \cdot & & \cdot \\ \cdot & \cdot & & \cdot & & \cdot \\ \cdot & \cdot & & \cdot & & \cdot \\ 0 & 0 & \cdots & f_{nk} & & f_{nn} \end{array} \right]$$

We select the element with greatest magnitude (the pivot) among the elements $f_{k+1,k}, f_{k+2,k}, \dots, f_{nk}$. This means that we interchange row i_k with row $k+1$ and column i_k with column $k+1$ with the similarity transformation

$$A'_k = I_{k+1, i_k} A_k I_{k+1, i_k}^{-1}$$

Next, we annihilate $f'_{k+2,k}, f'_{k+3,k}, \dots, f'_{nk}$ with the transformation

$$A_{k+1} = M_{k+1} A'_k M_{k+1}^{-1}$$

obtain

$$A_1' = \begin{bmatrix} 1 & 3 & 1 & 1 \\ 4 & 1 & 2 & 1 \\ 2 & 1 & 2 & 2 \\ 1 & 1 & 1 & 1 \end{bmatrix} .$$

Then

$$M_2 A_1' M_2^{-1} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{bmatrix} \begin{bmatrix} \\ \\ \\ \end{bmatrix} A_1' \begin{bmatrix} \\ \\ \\ \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}$$

which results in

$$A_2 = \begin{bmatrix} 1 & \frac{15}{4} & 1 & 1 \\ 4 & \frac{9}{4} & 2 & 1 \\ 0 & \frac{11}{8} & 1 & \frac{3}{2} \\ 0 & \frac{19}{16} & \frac{1}{2} & \frac{3}{4} \end{bmatrix} .$$

Because $11/8 > 19/16$, we will not interchange any rows or columns. Then the final step is

$$M_3 A_2 M_3^{-1} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -\frac{19}{22} & 1 \end{bmatrix} \begin{bmatrix} \\ \\ \\ A_2 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & \frac{19}{22} & 1 \end{bmatrix}$$

to obtain the upper Hessenberg matrix

$$\begin{bmatrix} 1 & \frac{15}{4} & \frac{41}{22} & 1 \\ 4 & \frac{9}{4} & \frac{30}{11} & 1 \\ 0 & \frac{11}{8} & \frac{101}{44} & \frac{3}{2} \\ 0 & 0 & -\frac{101}{121} & \frac{-6}{11} \end{bmatrix}$$

When one or more of the sub-diagonal elements of an upper Hessenberg matrix H are zero, it is called a reducible upper Hessenberg matrix. By partitioning the matrix H with respect to the zero subdiagonal elements, we obtain a block upper triangular structure where each diagonal block is an irreducible Hessenberg matrix. The QR transformation (to be discussed for Hessenberg matrices in Chapter V) acts independently on each diagonal block.

To reiterate, a symmetric matrix A is transformed into a tridiagonal matrix T through similarity transformations constructed with Householder reflectors. An arbitrary nonsymmetric matrix B is transformed into an upper Hessenberg matrix H through elementary similarity transformations. Chapters IV and V present methods for determining the eigenvalues of symmetric matrices and nonsymmetric matrices, respectively.

CHAPTER IV

In this chapter we shall describe the procedure for determining the eigenvalues for a real, symmetric matrix. The procedure will incorporate the QR method, using the Wilkinson origin shift. Through similarity transformations constructed with Householder matrices, a real, symmetric matrix A has been transformed to a symmetric, tridiagonal matrix T . The QR algorithm, a numerically stable procedure [4], is defined as follows for the matrix T .

$$\begin{aligned}
 (4.1) \quad T &= T_1 = Q_1 R_1 \\
 &T_2 = R_1 Q_1 \\
 &T_2 = Q_2 R_2 \\
 &T_3 = R_2 Q_2 \\
 &\quad \cdot \\
 &\quad \cdot \\
 &\quad \cdot \\
 &T_{k-1} = Q_{k-1} R_{k-1} \\
 &T_k = R_{k-1} Q_{k-1} \\
 &\quad \cdot \\
 &\quad \cdot \\
 &\quad \cdot
 \end{aligned}$$

The product $Q_i R_i = T_i$ is determined by constructing a real orthogonal matrix Q_i and a real upper triangular matrix R_i . This is known as a QR decomposition of T_i . Note that T_{i+1} is simply the product $R_i Q_i$. It can be shown [6, pp. 516-519] that the sequence of matrices $\{T_i\}$ converges to a diagonal

matrix and that all the matrices T_i are similar to T . Therefore, the sequence $\{T_i\}$ can be employed to determine the eigenvalues of T . Constructing QR decompositions for the sequence of matrices $\{T_i\}$ is accomplished through the use of Givens rotations.

As stated above, it is imperative that the spectrums of the matrices T_{i+1} and T_i are identical. If $T_i = Q_i R_i$ and $Q_i^T = Q_i^{-1}$, then $Q_i^{-1} T_i = R_i$. Substituting into $T_{i+1} = R_i Q_i$ results in

$$(4.2) \quad T_{i+1} = Q_i^{-1} R_i Q_i.$$

Hence, T_{i+1} and T_i are similar matrices. The import of this process is that the eigenvalues of the matrices T_i are, in fact, the eigenvalues of the symmetric, tridiagonal matrix T .

To accelerate the rate of convergence of the sequence $\{T_i\}$ to a diagonal matrix, we utilize the technique of shifting the origin. As before, the symmetric, tridiagonal matrix is T_1 , the first matrix in the sequence. The matrix $\hat{T}_1 = T_1 - \sigma_1 I$ is built by shifting the origin the amount σ_1 . After determining a QR decomposition of $\hat{T}_1 = Q_1 R_1$, we construct the matrix S_1 to be the product $R_1 Q_1$. The second matrix in the sequence $\{T_i\}$ is constructed by shifting the origin back to form the matrix $T_2 = S_1 + \sigma_1 I$. In general, the QR algorithm with origin shifts is defined as follows:

$$\begin{aligned}
 (4.3) \quad T &= T_1 \\
 \hat{T}_1 &= T_1 - \sigma_1 I \\
 \hat{T}_1 &= Q_1 R_1 \\
 S_1 &= R_1 Q_1 \\
 T_2 &= S_1 + \sigma_1 I \\
 \hat{T}_2 &= T_2 - \sigma_2 I \\
 \hat{T}_2 &= Q_2 R_2 \\
 S_2 &= R_2 Q_2 \\
 T_3 &= S_2 + \sigma_2 I \\
 &\cdot \\
 &\cdot \\
 &\cdot \\
 \hat{T}_{j-1} &= T_{j-1} - \sigma_{j-1} I \\
 \hat{T}_{j-1} &= Q_{j-1} R_{j-1} \\
 S_{j-1} &= R_{j-1} Q_{j-1} \\
 T_j &= S_{j-1} + \sigma_{j-1} I \\
 &\cdot \\
 &\cdot \\
 &\cdot
 \end{aligned}$$

Again, it is necessary that the matrix $T = T_1$ and each matrix in the sequence $\{T_j\}$ are similar. Theorem 2.6 establishes that if $\sigma(T_1) = \{\lambda_1, \lambda_2, \dots, \lambda_n\}$, then $\sigma(\hat{T}_1) = \{\lambda_1 - \sigma_1, \lambda_2 - \sigma_2, \dots, \lambda_n - \sigma_n\}$. Recall from (4.2) that the spectrum of S_1 is identical to the spectrum of \hat{T}_1 . Because the origin is shifted to construct matrix T_2 from the matrix S_1 , Theorem 2.6 establishes that $\sigma(T_2) = \{(\lambda_1 - \sigma_1) + \sigma_1, (\lambda_2 - \sigma_2) + \sigma_2, \dots, (\lambda_n - \sigma_n) + \sigma_n\} = \sigma(T_1)$. In like manner, it can be shown that the eigenvalues

of the matrix T_1 are identical to the eigenvalues of each matrix in the sequence $\{T_j\}$.

Since equivalent spectrums are assured for the matrices in the sequence $\{T_j\}$ developed through the QR algorithm with origin shifts, a method for determining the amount of the shift is the next step in the process. Consider the first matrix in the sequence, the symmetric, tri-diagonal matrix

$$T = \begin{bmatrix} \alpha_1 & \beta_1 & & & 0 \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \beta_2 & \alpha_3 & & \\ & & & \ddots & \\ & & & & \beta_{n-1} & \alpha_n \end{bmatrix}.$$

$$\text{Let } W = \begin{bmatrix} \alpha & \beta \\ \beta & \tau \end{bmatrix} = \begin{bmatrix} \alpha_{n-1} & \beta_{n-1} \\ \beta_{n-1} & \alpha_n \end{bmatrix}. \quad \text{Check the size of } \beta.$$

$$\text{If } \beta \text{ is "small", let } W = \begin{bmatrix} \alpha & \beta \\ \beta & \tau \end{bmatrix} = \begin{bmatrix} \alpha_{n-2} & \beta_{n-2} \\ \beta_{n-2} & \alpha_{n-1} \end{bmatrix}.$$

(Note: If β is "small", then one of the eigenvalues of the matrix T is apparent. For example, if $\beta = \beta_{n-1}$ and $|\beta_{n-1}|$ is less than or equal to 10^{-12} , then α_n is an eigenvalue of the matrix T .) Again, check the size of β . If β is not "small", then consider $T - \sigma I$ where σ is computed to be the eigenvalue of the matrix W lying closest to τ . Determine σ as follows:

- 1) If $\alpha = \tau$, then $\sigma = \alpha - |\beta|$.
- 2) If $\alpha \neq \tau$, then $\phi = (\alpha - \tau)/2$ and

$$\sigma = \frac{\tau - \text{sign}(\phi) \cdot \beta^2}{|\phi| + \sqrt{\phi^2 + \beta^2}}.$$

This choice for an origin shift is attributed to Wilkinson [6, pp. 507-512].

Recall that Givens rotations are to be used to construct QR decompositions for the sequence of matrices that converges to a diagonal matrix. After the introduction of Wilkinson's origin shift σ_j to accelerate convergence, QR decompositions are determined for the sequence of matrices $\{\hat{T}_j\}$ where $\hat{T}_j = T_j - \sigma_j I$.

Consider the symmetric, tridiagonal matrix

$$\hat{T}_1 = \begin{bmatrix} \epsilon_1 & \beta_1 & & & 0 \\ \beta_1 & \epsilon_2 & \beta_2 & & \\ & \beta_2 & \epsilon_3 & & \\ & & & \ddots & \\ & & & & \epsilon_{n-1} \\ 0 & & & & \beta_{n-1} & \epsilon_n \end{bmatrix}.$$

The Givens matrix G_1 is constructed using the value $\omega_1 = \sqrt{\epsilon_1^2 + \beta_1^2}$. Then the product of G_1 and \hat{T}_1 results in the matrix R_1 whose first subdiagonal element is zero.

$$\begin{array}{c}
 G_1 \\
 \left[\begin{array}{cc|c}
 \frac{\epsilon_1}{\epsilon_1} & \frac{\beta_1}{\epsilon_1} & \\
 \frac{\beta_1}{\epsilon_1} & \frac{\epsilon_1}{\epsilon_1} & \\
 \hline
 0 & & \\
 \hline
 0 & & I_{n-2} \\
 \hline
 0 & & \\
 \hline
 \end{array} \right]
 \end{array}
 \begin{array}{c}
 T_1 \\
 \left[\begin{array}{cc|cccc}
 \epsilon_1 & \beta_1 & 0 & 0 & \dots & 0 & 0 \\
 \epsilon_1 & \epsilon_2 & \beta_2 & 0 & \dots & 0 & 0 \\
 \hline
 0 & \beta_2 & \epsilon_3 & \beta_3 & \dots & 0 & 0 \\
 0 & 0 & \beta_3 & \epsilon_4 & \dots & 0 & 0 \\
 \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\
 \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\
 0 & 0 & 0 & 0 & \dots & \epsilon_{n-1} & \beta_{n-1} \\
 0 & 0 & 0 & 0 & \dots & \beta_{n-1} & \epsilon_n
 \end{array} \right]
 \end{array}$$

$$= \begin{array}{c}
 R_1 \\
 \left[\begin{array}{cccc|cc}
 \epsilon_1 & x & x & 0 & \dots & 0 & 0 \\
 0 & \beta_2 & x & x & \dots & 0 & 0 \\
 0 & \beta_2 & \epsilon_3 & \beta_3 & \dots & 0 & 0 \\
 0 & 0 & \beta_3 & \epsilon_4 & \dots & 0 & 0 \\
 \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\
 \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\
 \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\
 0 & 0 & 0 & 0 & \dots & \epsilon_{n-1} & \beta_{n-1} \\
 0 & 0 & 0 & 0 & \dots & \beta_{n-1} & \epsilon_n
 \end{array} \right]
 \end{array}$$

Using the value $\omega_2 = \sqrt{\ell_2^2 + \beta_2^2}$, the Givens matrix G_2 is built to zero out the next sub-diagonal element in R_1 .

$$\begin{array}{c}
 G_2 \\
 \left[\begin{array}{ccc|c}
 1 & 0 & 0 & \\
 \hline
 0 & \frac{\ell_2}{\omega_2} & \frac{\beta_2}{\omega_2} & 0 \\
 0 & -\frac{\beta_2}{\omega_2} & \frac{\ell_2}{\omega_2} & \\
 \hline
 & & & I_{n-3} \\
 & 0 & &
 \end{array} \right]
 \end{array}
 \begin{array}{c}
 R_1 \\
 \left[\begin{array}{ccc|cccc}
 \omega_1 & x & x & 0 & \dots & 0 & 0 \\
 \hline
 0 & \ell_2 & x & 0 & \dots & 0 & 0 \\
 0 & \beta_2 & \epsilon_3 & \beta_3 & \dots & 0 & 0 \\
 \hline
 0 & 0 & \beta_3 & \epsilon_4 & \dots & 0 & 0 \\
 \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot \\
 0 & 0 & 0 & 0 & \dots & \epsilon_{n-1} & \beta_{n-1} \\
 0 & 0 & 0 & 0 & \dots & \epsilon_{n-1} & \epsilon_n
 \end{array} \right]
 \end{array}$$

 R_2

$$= \left[\begin{array}{cccccccc}
 \omega_1 & x & x & 0 & \dots & 0 & 0 \\
 0 & \omega_2 & x & x & \dots & 0 & 0 \\
 0 & 0 & \ell_3 & x & \dots & 0 & 0 \\
 0 & 0 & \beta_3 & \epsilon_4 & \dots & 0 & 0 \\
 \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot \\
 0 & 0 & 0 & 0 & \dots & \epsilon_{n-1} & \beta_{n-1} \\
 0 & 0 & 0 & 0 & \dots & \beta_{n-1} & \epsilon_n
 \end{array} \right] .$$

We continue to construct Givens matrices until the final step when, using

$$\text{the value } \omega_{n-1} = \sqrt{\lambda_{n-1}^2 + \beta_{n-1}^2},$$

$$\begin{array}{c}
 G_{n-1} \qquad \qquad \qquad R_{n-2} \\
 \left[\begin{array}{cc|cc}
 & & & \\
 & & & \\
 I_{n-2} & & & \\
 & & 0 & \\
 \hline
 & & \frac{\lambda_{n-1}}{\omega_{n-1}} & \frac{\beta_{n-1}}{\omega_{n-1}} \\
 & & -\frac{\beta_{n-1}}{\omega_{n-1}} & \frac{\lambda_{n-1}}{\omega_{n-1}}
 \end{array} \right]
 \left[\begin{array}{cccc|cc}
 \omega_1 & x & x & 0 & \dots & 0 & 0 \\
 0 & \omega_2 & x & x & \dots & 0 & 0 \\
 0 & 0 & \omega_3 & x & \dots & 0 & 0 \\
 0 & 0 & 0 & \omega_4 & \dots & 0 & 0 \\
 \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\
 \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\
 \hline
 0 & 0 & 0 & 0 & \dots & \lambda_{n-1} & x \\
 0 & 0 & 0 & 0 & \dots & \beta_{n-1} & \alpha_n
 \end{array} \right]
 \end{array}$$

$$= \left[\begin{array}{ccccccc}
 \omega_1 & x & x & 0 & \dots & 0 & 0 \\
 0 & \omega_2 & x & x & \dots & 0 & 0 \\
 0 & 0 & \omega_3 & x & \dots & 0 & 0 \\
 0 & 0 & 0 & \omega_4 & \dots & 0 & 0 \\
 \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\
 \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\
 0 & 0 & 0 & 0 & \dots & \omega_{n-1} & x \\
 0 & 0 & 0 & 0 & \dots & 0 & x
 \end{array} \right] = R_{n-1}.$$

Note that this process results in an upper triangular matrix R_{n-1} . Also note that the matrix $G = G_{n-1} \dots G_2 G_1$ is orthogonal since it is the pro-

duct of orthogonal matrices. Finally, note that the matrix G is lower Hessenberg by observing the following.

$$\begin{array}{c} G_{n-1} \end{array}
 \begin{bmatrix} 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots & \vdots \\ \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 & 0 \\ 0 & 0 & \dots & 0 & \frac{\ell_{n-1}}{\omega_{n-1}} & \frac{\delta_{n-1}}{\omega_{n-1}} \\ 0 & 0 & \dots & 0 & -\frac{\beta_{n-1}}{\omega_{n-1}} & \frac{\ell_{n-1}}{\omega_{n-1}} \end{bmatrix}
 \begin{array}{c} G_{n-2} \end{array}
 \begin{bmatrix} 1 & 0 & \dots & 0 & 0 & 0 \\ 1 & 1 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots & \vdots \\ \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & \frac{\ell_{n-2}}{\omega_{n-2}} & \frac{\beta_{n-2}}{\omega_{n-2}} & 0 \\ 0 & 0 & \dots & -\frac{\beta_{n-2}}{\omega_{n-2}} & \frac{\ell_{n-2}}{\omega_{n-2}} & 0 \\ 0 & 0 & \dots & 0 & 0 & 1 \end{bmatrix}$$

$$G_{n-1}G_{n-2}$$

$$\begin{bmatrix} 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots & \vdots \\ \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & \dots & x & x & 0 \\ 0 & 0 & \dots & x & x & x \\ 0 & 0 & \dots & x & x & x \end{bmatrix}$$

$G_{n-1}G_{n-2}$ G_{n-3}

$$\begin{bmatrix}
 1 & 0 & \dots & 0 & 0 & 0 & 0 \\
 0 & 1 & \dots & 0 & 0 & 0 & 0 \\
 \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots \\
 0 & 0 & \dots & 1 & 0 & 0 & 0 \\
 0 & 0 & \dots & 0 & x & x & 0 \\
 0 & 0 & \dots & 0 & x & x & x \\
 0 & 0 & \dots & 0 & x & x & x
 \end{bmatrix}
 \begin{bmatrix}
 1 & 0 & \dots & 0 & 0 & 0 & 0 \\
 0 & 1 & \dots & 0 & 0 & 0 & 0 \\
 \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots \\
 0 & 0 & & \frac{\lambda_{n-3}}{\omega_{n-3}} & \frac{\beta_{n-3}}{\omega_{n-3}} & 0 & 0 \\
 0 & 0 & \dots & -\frac{\beta_{n-3}}{\omega_{n-3}} & \frac{\lambda_{n-3}}{\omega_{n-3}} & 0 & 0 \\
 0 & 0 & \dots & 0 & 0 & 1 & 0 \\
 0 & 0 & \dots & 0 & 0 & 0 & 1
 \end{bmatrix}$$

 $G_{n-1}G_{n-2}G_{n-3}$

$$\begin{bmatrix}
 1 & 0 & \dots & 0 & 0 & 0 & 0 \\
 0 & 1 & \dots & 0 & 0 & 0 & 0 \\
 \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots \\
 0 & 0 & \dots & x & x & 0 & 0 \\
 0 & 0 & \dots & x & x & x & 0 \\
 0 & 0 & \dots & x & x & x & x \\
 0 & 0 & \dots & x & x & x & x
 \end{bmatrix}$$

The final product to produce the matrix G is

$$\begin{matrix}
 G_{n-1}G_{n-2}G_{n-3}\dots G_2 & & G_1 \\
 \left[\begin{array}{ccccccc}
 1 & 0 & 0 & \dots & 0 & 0 & 0 \\
 0 & x & x & \dots & 0 & 0 & 0 \\
 0 & x & x & \dots & 0 & 0 & 0 \\
 \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot \\
 0 & 0 & 0 & \dots & x & x & 0 \\
 0 & 0 & 0 & \dots & x & x & 0 \\
 0 & 0 & 0 & \dots & x & x & x
 \end{array} \right] & \left[\begin{array}{ccccccc}
 \frac{\epsilon_1}{\epsilon_1} & \frac{\beta_1}{\epsilon_1} & 0 & \dots & 0 & 0 & 0 \\
 -\frac{\beta_1}{\epsilon_1} & \frac{\epsilon_1}{\epsilon_1} & 0 & \dots & 0 & 0 & 0 \\
 0 & 0 & 1 & \dots & 0 & 0 & 0 \\
 \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot \\
 0 & 0 & 0 & \dots & 1 & 0 & 0 \\
 0 & 0 & 0 & \dots & 0 & 1 & 0 \\
 0 & 0 & 0 & \dots & 0 & 0 & 1
 \end{array} \right]
 \end{matrix}$$

G

$$H = \left[\begin{array}{ccccccc}
 x & x & 0 & 0 & \dots & 0 & 0 \\
 x & x & x & 0 & \dots & 0 & 0 \\
 x & x & x & x & \dots & 0 & 0 \\
 \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot \\
 x & x & x & x & \dots & x & 0 \\
 x & x & x & x & \dots & x & x \\
 x & x & x & x & \dots & x & x
 \end{array} \right]$$

The result of these observations is that a QR decomposition for the matrix \hat{T} can be defined. Because the matrix G is orthogonal and lower Hessenberg, we choose $Q = G^T$. Consequently, Q is orthogonal and upper Hessenberg. We define $R = R_{n-1}$, the upper triangular matrix.

Earlier it was established that if $\hat{T}_j = Q_j R_j$ and $S_j = R_j Q_j$, then \hat{T}_j and S_j are similar matrices. Therefore, the sequence $\{T_j\}$ can be employed to determine the eigenvalues of T . However, the processes of utilizing Givens rotations to determine a QR decomposition for \hat{T}_j and of utilizing Wilkinson's origin shift to accelerate the rate of convergence of the sequence $\{T_j\}$ also require that the matrix $R_j Q_j$ be symmetric and tridiagonal.

THEOREM 4.4 If the symmetric matrix $T = QR$, where Q is orthogonal, then the product RQ is symmetric.

Proof. Because T is symmetric, $T = QR = (QR)^T = R^T Q^T$. Since $Q^T = Q^{-1}$, $TQ = (R^T Q^T)Q = R^T (Q^T Q) = R^T$. Then $(RQ)^T = Q^T R^T = Q^T (TQ) = Q^T (T)Q = Q^T (QR)Q = (Q^T Q)(RQ) = RQ$. Hence, the matrix RQ is symmetric. ■

THEOREM 4.5 If the matrix R is upper triangular and the matrix Q is upper Hessenberg, then RQ is tridiagonal.

Proof. Multiplying R and Q results in (for 5x5 matrices)

$$\begin{array}{ccc}
 R & Q & RQ
 \end{array}$$

$$\begin{bmatrix}
 x & x & x & x & x \\
 0 & x & x & x & x \\
 0 & 0 & x & x & x \\
 0 & 0 & 0 & x & x \\
 0 & 0 & 0 & 0 & x
 \end{bmatrix}
 \begin{bmatrix}
 x & x & x & x & x \\
 x & x & x & x & x \\
 0 & x & x & x & x \\
 0 & 0 & x & x & x \\
 0 & 0 & 0 & x & x
 \end{bmatrix}
 =
 \begin{bmatrix}
 x & x & z & z & z \\
 x & x & x & z & z \\
 0 & x & x & x & z \\
 0 & 0 & x & x & x \\
 0 & 0 & 0 & x & x
 \end{bmatrix}
 .$$

By Theorem 4.4 the matrix RQ is symmetric. Consequently, the triangular block of zeros in the lower left-hand corner of RQ has a corresponding triangular block of zeros in the upper right-hand corner of RQ . Thus, RQ is tridiagonal. ■

We now consider a 4×4 real, symmetric matrix

$$A = \begin{bmatrix} 5 & 4 & 1 & 1 \\ 4 & 5 & 1 & 1 \\ 1 & 1 & 4 & 2 \\ 1 & 1 & 2 & 4 \end{bmatrix} .$$

The QR algorithm with an origin shift is employed to determine the spectrum of A . The QR decompositions are built using Givens rotations and the origin shifts are chosen according to Wilkinson.

After A is transformed using Householder reflectors, we have

$$T = T_1 =$$

$$\begin{bmatrix} 0.500000D 01 & -0.424264D 01 & 0.0 & 0.0 \\ -0.424264D 01 & 0.600000D 01 & 0.141421D 01 & 0.0 \\ 0.0 & 0.141421D 01 & 0.500000D 01 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.200000D 01 \end{bmatrix} .$$

Note that $t_{4,3} = t_{3,4} = 0$. Therefore, $t_{4,4} = \lambda = 2$ is an eigenvalue of A . Wilkinson's choice for the first shift $\sigma_1 = 4$. A QR decomposition

for $T_1 - \sigma_1 I = Q_1 R_1$ is built using Givens rotations.

Then

$$T_2 = R_1 Q_1 + \sigma_1 I =$$

$$\begin{bmatrix} 0.784211D 01 & -0.382874D 01 & 0.0 & 0.0 \\ -0.382874D 01 & 0.317830D 01 & -0.377414D 00 & 0.0 \\ 0.0 & -0.377414D 00 & 0.497959D 01 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.200000D 01 \end{bmatrix} .$$

From the matrix T_2 , σ_2 is defined as $0.505547E 01$. Again, a QR decomposition is constructed for $T_2 - \sigma_2 I = Q_2 R_2$. Then

$$T_3 = R_2 Q_2 + \sigma_2 I =$$

$$\begin{bmatrix} 0.843664D 01 & -0.340972D 01 & 0.0 & 0.0 \\ -0.340972D 01 & 0.256337D 01 & -0.498482D-02 & 0.0 \\ 0.0 & -0.498482D-02 & 0.500000D-01 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.200000D 01 \end{bmatrix} .$$

For appearance sake, the following iterations have zeros inserted in positions when the entries become "small".

$$\sigma_3 = 0.500001E 01, T_4 =$$

$$\begin{bmatrix} 0.893270D 01 & -0.290974D 01 & 0.0 & 0.0 \\ -0.290974D 01 & 0.206730D 01 & -0.690428D-08 & 0.0 \\ 0.0 & -0.690428D-08 & 0.500000D 01 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.200000D 01 \end{bmatrix}$$

$$\sigma_4 = 0.500000E 01, T_5 =$$

$$\begin{bmatrix} 0.928647D 01 & -0.243160D 01 & 0.0 & 0.0 \\ -0.243160D 01 & 0.171353D 01 & 0.163513D-14 & 0.0 \\ 0.0 & 0.161059D-14 & 0.500000D 01 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.200000D 01 \end{bmatrix}$$

$$\sigma_5 = 0.100000E 01, T_6 =$$

$$\begin{bmatrix} 0.100000D 02 & -0.174905D-07 & 0.0 & 0.0 \\ 0.174905D-07 & 0.100000D 01 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.500000D 01 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.200000D 01 \end{bmatrix}$$

$$\sigma_6 = 0.100000E 01, T_7 =$$

$$\begin{bmatrix} 0.100000D 02 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.100000D 01 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.500000D 01 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.200000D 01 \end{bmatrix}$$

Thus, $\sigma(A) = \{10, 1, 5, 2\}$. Note that the four eigenvalues of A were determined with six iterations of the QR algorithm with an origin shift applied to the symmetric, tridiagonal T_1 . The QR algorithm takes less than two iterations per eigenvalue for a tridiagonal matrix [7, p. 230].

CHAPTER V

In Chapter III an arbitrary nonsymmetric matrix B was transformed into an upper Hessenberg matrix H through elementary similarity transformations. In this chapter we shall describe the procedure for determining the eigenvalues of the upper Hessenberg matrix H . The QR algorithm utilized in producing the eigenvalues of a real, symmetric matrix will again be used. When applied to an upper Hessenberg matrix H , the unmodified QR algorithm has two possible results. One is convergence to a block upper triangular matrix whose diagonal blocks are at most of order two. The other possible result is that convergence does not occur. With the modification of a single origin shift as described in Chapter IV, the QR algorithm applied to H requires complex arithmetic because the eigenvalues of an upper Hessenberg matrix can be either real or complex. The procedure used is the double shift QR algorithm which avoids complex arithmetic, guarantees convergence with "proper" strategy, and accelerates the rate of convergence.

Before confronting the situation of real or complex arithmetic, the convergence or nonconvergence of the QR algorithm for a Hessenberg matrix must be discussed. The QR algorithm is said to converge for $n \times n$ Hessenberg matrix $H_1 = [h_1^{(1)}]$ if the sequence $\{H_i\}$, generated by (4.1) and there referred to as T_i , satisfies $h_{j+1,j}^{(i)} \cdot h_{j,j-1}^{(i)} \rightarrow 0$ as $i \rightarrow \infty$, for $j = 2, 3, \dots, n-1$. In other words, the QR algorithm converges if, for each pair of adjacent subdiagonal elements of H_1 , at least one of the entries converges to zero.

Note that convergence does not require (but may result in) a triangular matrix whose eigenvalues are displayed on the diagonal. This form results when all of the eigenvalues are real. However, when some of the eigenvalues are complex, it is sufficient for the sequence of matrices to

converge to upper block triangular form with 1×1 or 2×2 blocks on the diagonal. We now state necessary and sufficient conditions for convergence.

THEOREM 5.1 The QR algorithm applied to an irreducible Hessenberg matrix H converges if, and only if, among each set of eigenvalues of H with equal modulus, there are at most two of even algebraic multiplicity and two of odd algebraic multiplicity.

Proof. See Parlett (1968).

Consequently, given a matrix H with more than two distinct eigenvalues of equal modulus, the sequence of matrices $\{H_1^k\}$ generated by the QR algorithm does not converge. An example of this condition is the matrix

$$(5.2) \quad M = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

whose eigenvalues are 1 , w , and w^2 where $w = \exp(2\pi i/3)$. In other words, the spectrum of M is $\{1, -\frac{1}{2} + \sqrt{3}/2i, -\frac{1}{2} - \sqrt{3}/2i\}$, each of whose members has algebraic multiplicity one. Because more than two eigenvalues of equal modulus have odd algebraic multiplicity, the sequence of matrices $\{M_1^k\}$ defined by the QR algorithm does not converge.

The importance of the theorem can be realized when the QR algorithm is applied to real, symmetric matrices. Since the eigenvalues of real, symmetric matrices are always real, there can be at most two distinct eigenvalues of equal modulus, resulting in compliance with the conditions

for convergence of Theorem 5.1.

Returning to consideration of Hessenberg matrices, we examine an irreducible, complex, Hessenberg matrix H with four distinct eigenvalues of equal modulus $|\lambda_1| = |\lambda_2| = |\lambda_3| = |\lambda_4|$ with multiplicities 4, 3, 2 and 1, respectively. Since λ_1 and λ_3 have even algebraic multiplicity and λ_2 and λ_4 have odd algebraic multiplicity, the QR algorithm will converge when applied to the matrix H . In fact, the QR algorithm has strong convergence properties when applied to Hessenberg matrices. If the basic QR algorithm fails to produce the eigenvalues of an irreducible Hessenberg matrix the situation can easily be remedied by the introduction of the technique of shifting the origin. The matrix H might have a spectrum that does not fulfill the conditions of Theorem 5.1. However, the matrix $H - qI$ would have a spectrum for which convergence occurs.

Consider the first two steps of the QR algorithm with an origin shift for an upper Hessenberg matrix H .

$$\begin{aligned}
 (5.3) \quad H &= H_1 \\
 \hat{H}_1 &= H_1 - q_1 I \\
 \hat{H}_1 &= Q_1 R_1 \\
 H_2 &= R_1 Q_1 + q_1 I \\
 \hat{H}_2 &= H_2 - q_2 I \\
 \hat{H}_2 &= Q_2 R_2 \\
 H_3 &= R_2 Q_2 + q_2 I
 \end{aligned}$$

From (4.2) we know that

$$\begin{aligned}
 (5.4) \quad H_3 &= Q_2^T H_2 Q_2 \\
 &= Q_2^T (Q_1^T H_1 Q_1) Q_2 \\
 &= (Q_1 Q_2)^T H_1 (Q_1 Q_2).
 \end{aligned}$$

The result is that H_3 can be computed from H_1 and the product $Q_1 Q_2$. However, we would like to be able to determine H_3 without constructing the QR decompositions for \hat{H}_1 and \hat{H}_2 . In order to accomplish this, we need the following discussion.

Substituting from (5.3) we observe that

$$\begin{aligned}
 (5.5) \quad Q_1 Q_2 R_2 R_1 &= Q_1 (H_2 - q_2 I) R_1 \\
 &= Q_1 H_2 R_1 - q_2 Q_1 R_1 \\
 &= Q_1 (R_1 Q_1 + q_1 I) R_1 - q_2 Q_1 R_1 \\
 &= Q_1 R_1 Q_1 R_1 + q_1 Q_1 R_1 - q_2 Q_1 R_1 \\
 &= (Q_1 R_1 + q_1 I) Q_1 R_1 - q_2 Q_1 R_1 \\
 &= H_1 Q_1 R_1 - q_2 Q_1 R_1 \\
 &= (H_1 - q_2 I) Q_1 R_1 \\
 &= (H_1 - q_2 I) (H_1 - q_1 I).
 \end{aligned}$$

Specific choices for the origin shifts q_1 and q_2 will be made later. At this point note that if q_2 is chosen to be \bar{q}_1 or if q_1 and q_2 are both real, then the product $(H_1 - q_2 I)(H_1 - q_1 I)$ is real. This implies that the matrices $Q_1 Q_2$ and $R_2 R_1$ are real. Thus, from (5.4) H_3 is real. Realizing that H_{2t+1} can be determined by H_{2t-1} as H_3 is by H_1 , then the sequence H_1, H_3, H_5, \dots is real. Observe that if q_1 is complex, then the matrix

$H_2 = R_1 Q_1 + q_1 I$ is complex. Thus, the sequence H_2, H_4, H_6, \dots may be complex.

We want to avoid constructing the matrices H_2, H_4, H_6, \dots (i.e., avoid determining the QR decompositions for $\hat{H}_2, \hat{H}_4, \hat{H}_6, \dots$) because of the complex values they possibly contain. Consider the following theorem.

THEOREM 5.6 If the matrix A is real and nonsingular, then there exists a decomposition $A = QR$ for which Q is orthogonal and R is upper triangular. Furthermore, if the diagonal elements of R are real and positive, the decomposition is unique.

Proof. See Young-Gragory (1973), pp. 921-922.

Thus, to bypass the composition of $Q_1 R_1$ and $Q_2 R_2$ and to build $Q_1 Q_2$ directly, we determine the product $M = (H_1 - q_2 I)(H_1 - q_1 I)$. If q_1, q_2 are not eigenvalues of H_1 , then M is nonsingular. Find the QR decomposition

$$(5.7) \quad M = (H_1 - q_2 I)(H_1 - q_1 I) = \tilde{Q}_1 \tilde{R}_1$$

where the diagonal elements of \tilde{R}_1 are real and positive and $q_2 = \bar{q}_1$ or q_1, q_2 are real. Thus, Theorem 5.6 states that $\tilde{Q}_1 = Q_1 Q_2$. The result is that we can avoid forming H_2 . The matrix H_3 is determined from H_1 and all computations are accomplished with real arithmetic.

In general, the double shift QR algorithm applied to an upper Hessenberg matrix H is as follows.

$$\begin{aligned}
 H &= H_1 \\
 H_3 &= \tilde{Q}_1^T H_1 \tilde{Q}_1 \\
 H_5 &= \tilde{Q}_3^T H_3 \tilde{Q}_3 \\
 &\vdots \\
 &\vdots \\
 H_{2t+1} &= \tilde{Q}_{2t-1}^T H_{2t-1} \tilde{Q}_{2t-1} \\
 &\vdots \\
 &\vdots
 \end{aligned}$$

where $(H_{2t-1}^{-q_{t+1}} I) (H_{2t-1}^{-q_t} I) = \tilde{Q}_t^T \tilde{R}_t$.

The unique decomposition theorem (5.6) provides the basis for constructing the matrix H_3 in one step of the double shift QR algorithm rather than two steps of the QR algorithm with a single origin shift. Theoretically, then, we are concerned that $M = (H_1 - q_2 I)(H_1 - q_1 I)$ is non-singular and that the diagonal elements of the upper triangular K are real and positive. However, empirically it has been established that checking M for its singularity or nonsingularity is not a concern. In fact, a matrix like (5.2) whose eigenvalues cannot be produced by the QR algorithm is a rare situation. In other words, this algorithm is more powerful than Theorem 5.6 leads us to believe. Therefore, in practice we can apply the double shift QR algorithm to upper Hessenberg matrices and, in most cases, successfully obtain the eigenvalues.

We initiate the process of determining eigenvalues of an upper Hessenberg matrix H^* by considering its subdiagonal elements. A negligible entry on the subdiagonal allows us to decompose H^* into two upper Hessenberg matrices which can be operated on independently. After all of the eigenvalues of the matrix in the lower right-hand corner are deter-

mined, we can then continue the process by performing iterations on the upper matrix. Thus, the matrix H^* can be decomposed into

$$H^* = \begin{bmatrix} H^{(1)} & & & & \\ & H^{(2)} & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & H^{(k)} \end{bmatrix}$$

where $H^{(i)}$ is an irreducible, upper Hessenberg matrix. Let $H^{(k)} = H_1^{(k)} = H_1 = (h_{ij})$. Then the matrix

$$H_1 = \begin{bmatrix} W & & & \\ \hline & h_{n-1,n-1} & h_{n-1,n} & \\ & h_{n,n-1} & h_{n,n} & \\ \hline & & & Y \end{bmatrix} = \begin{bmatrix} W & & \\ \hline & & \\ \hline & & Y \end{bmatrix}.$$

To choose the origin shifts for the first step of the double shift QR algorithm, find $\sigma(Y) = \{\alpha_1, \alpha_2\}$. Then find the product

$$(H_1 - \alpha_1 I)(H_1 - \alpha_2 I) =$$

$$\begin{bmatrix} h_{11}^{-\alpha_1} & h_{12} & \dots & h_{1n} \\ h_{21} & h_{22}^{-\alpha_1} & \dots & h_{2n} \\ 0 & h_{32} & \dots & h_{3n} \\ \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & h_{nn}^{-\alpha_1} \end{bmatrix} \begin{bmatrix} h_{11}^{-\alpha_2} & h_{12} & \dots & h_{1n} \\ h_{21} & h_{22}^{-\alpha_2} & \dots & h_{2n} \\ 0 & h_{32} & \dots & h_{3n} \\ \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & h_{nn}^{-\alpha_2} \end{bmatrix}$$

$$= \begin{bmatrix} x_1 & v & v & \dots & v \\ y_1 & v & v & \dots & v \\ z_1 & v & v & \dots & v \\ 0 & v & v & \dots & v \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & & & & \end{bmatrix}$$

where

$$x_1 = h_{11}^2 - h_{11}(\alpha_1 + \alpha_2) + \alpha_1\alpha_2 + n_{12}h_{21}$$

$$y_1 = h_{21}(h_{11} + n_{22} - \alpha_1 - \alpha_2)$$

$$z_1 = h_{32}h_{21}.$$

Note that the product is not a Hessenberg matrix. Consequently, Givens rotations that were utilized in constructing the QR decomposition of a symmetric, tridiagonal matrix are not useful, because the number of multiplications would be too great. Instead, we will determine an orthogonal Q using Householder transformations. Furthermore, we will pre- and post-multiply h_1 , rather than $(H_1 - \alpha_1 I)(H_1 - \alpha_2 I)$, by Householder matrices

to build an orthogonal Q . When $AQ = QH$ where A is nonsingular, Q is orthogonal and H is irreducible upper Hessenberg, then Q is determined by its first column [5, p. 178]. Because the first Householder matrix will be built on x_1, y_1, z_1 , the nonzero elements of the first column of $(H_1 - \alpha_1 I)(H_1 - \alpha_2 I)$, the Q we determine will produce the appropriate Hessenberg matrix for the next iteration.

Therefore, in practice, we calculate only the first column of the product $(H_1 - \alpha_1 I)(H_1 - \alpha_2 I)$. Let $s_1^T = (x_1, y_1, z_1)^T$ with $\|s_1\| = c_1$. Build the first Householder matrix

$$U_1 = \begin{bmatrix} R_1 & & \\ & & \\ & & I_{n-3} \end{bmatrix}$$

where $R_1 = I - (2/u_1^T u_1)u_1 u_1^T$ and $u_1 = (x_1 \pm c_1, y_1, z_1)^T$.

Recall that a Householder matrix is both orthogonal and symmetric; therefore, pre- and post-multiply H_1 by U_1 to obtain

$$U_1 H_1 U_1 = \begin{bmatrix} R_1 & & 0 \\ & & \\ & & \\ 0 & & I_{n-3} \end{bmatrix} \begin{bmatrix} x & x & x & & \\ x & x & x & & \\ 0 & x & x & & \\ 0 & 0 & x & x & \\ \cdot & \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \cdot & \\ 0 & 0 & 0 & & x \end{bmatrix} \begin{bmatrix} R_1 & & 0 \\ & & \\ & & \\ 0 & & I_{n-3} \end{bmatrix}$$

$$= \begin{bmatrix} x & x & x & x & x & \dots & x & x & x \\ x & x & x & x & x & \dots & x & x & x \\ x & x & x & x & x & \dots & x & x & x \\ x & x & x & x & x & \dots & x & x & x \\ 0 & 0 & 0 & x & x & \dots & x & x & x \\ 0 & 0 & 0 & 0 & x & \dots & x & x & x \\ \cdot & \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 & \dots & 0 & x & x \end{bmatrix} = H_2 = ({}_2h_{ij}).$$

The next Householder matrix is

$$U_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & R_2 & 0 \\ 0 & 0 & 1_{n-4} \end{bmatrix}$$

where R_2 is based on $s_2 = \begin{bmatrix} 2^h_{21} \\ 2^h_{31} \\ 2^h_{41} \end{bmatrix}$ with $\|s_2\| = c_2$. Then

$$U_2 H_2 U_2 = \begin{bmatrix} x & x & x & x & x & x & \dots & x & x & x \\ x & x & x & x & x & x & \dots & x & x & x \\ 0 & x & x & x & x & x & \dots & x & x & x \\ 0 & x & x & x & x & x & \dots & x & x & x \\ 0 & x & x & x & x & x & \dots & x & x & x \\ 0 & 0 & 0 & 0 & x & x & \dots & x & x & x \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & x & x \end{bmatrix} = H_3 = (h_{ij}).$$

Next let $s_3 = \begin{bmatrix} 3^{h_{32}} \\ 3^{h_{42}} \\ 3^{h_{52}} \end{bmatrix}$ with $\|s_3\| = c_3$. Then build a Householder matrix

U_3 based on s_3 .

$$U_3 = \left[\begin{array}{c|c|c} I_2 & 0 & 0 \\ \hline 0 & R_3 & 0 \\ \hline 0 & 0 & I_{n-5} \end{array} \right].$$

Pre- and post-multiplication by U_3 produces

$$U_3 U_3 U_3 = \begin{bmatrix} x & x & x & x & x & x & \dots & x & x & x \\ x & x & x & x & x & x & \dots & x & x & x \\ 0 & x & x & x & x & x & \dots & x & x & x \\ 0 & 0 & x & x & x & x & \dots & x & x & x \\ 0 & 0 & x & x & x & x & \dots & x & x & x \\ 0 & 0 & x & x & x & x & \dots & x & x & x \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & x & x \end{bmatrix} = H_4 = (h_{ij}).$$

The next to last Householder matrix produces

$$U_{n-2} H_{n-2} U_{n-2} = \begin{bmatrix} x & & & & & & & & & & \\ & x & & & & & & & & & \\ & & x & & & & & & & & \\ & & & x & & & & & & & \\ & & & & x & & & & & & \\ & & & & & \cdot & & & & & \\ & & & & & & \cdot & & & & \\ & & & & & & & \cdot & & & \\ & & & & & & & & x & & \\ & & & & & & & & x & x & x & x \\ 0 & 0 & 0 & 0 & \dots & 0 & x & x & x & & \\ 0 & 0 & 0 & 0 & \dots & 0 & x & x & x & & \end{bmatrix} = H_{n-1} = (h_{ij}).$$

The final step is to build

$$U_{n-1} = \left[\begin{array}{c|c} I_{n-2} & \\ \hline & R_{n-1} \end{array} \right]$$

where R_{n-1} is based on $s_{n-1} = \begin{bmatrix} h_{n-1,n-2} \\ h_{n,n-2} \end{bmatrix}$ with $\|s_{n-1}\| = c_{n-1}$. Thus

$U_{n-1} H_{n-1} U_{n-1} = H_2^{(k)}$, the next upper Hessenberg matrix in the sequence for $H^{(k)}$.

At this point we check the subdiagonal elements of $H_2^{(k)}$. If $h_{n,n-1}$ is approximately zero (acceptably small or negligible), $h_{n,n}$ is an eigenvalue of $H_2^{(k)}$ (hence, an eigenvalue of H^*). Thus, we "deflate" $H_2^{(k)}$ by deleting its last row and column and then continue. If $h_{n-1,n-2}$ is approximately zero, then the eigenvalues of the 2x2 matrix in the lower right-hand corner are a complex conjugate pair of eigenvalues of H^* . We deflate $H_2^{(k)}$ by deleting its last two rows and columns and then continue. If any other subdiagonal elements of $H_2^{(k)}$ are negligible, we decompose $H_2^{(k)}$ and continue with the upper Hessenberg matrix in the lower right-hand corner.

One complete step of the double shift QR algorithm and corresponding "checks" have been delineated. If after ten QR steps, no eigenvalue has been determined, then the shifts α_1, α_2 are defined by [7, p.362].

$$(5.9) \quad \begin{aligned} \alpha_1 + \alpha_2 &= 1.5(|h_{n,n-1}| + |h_{n-1,n-2}|), \\ \alpha_1 \alpha_2 &= (|h_{n,n-1}| + |h_{n-1,n-2}|)^2 \end{aligned}$$

instead of being defined as eigenvalues of the lower right-hand 2x2 matrix. If after twenty iterations, we are still unsuccessful in determining an

eigenvalue, then the definition of (5.9) is again used. After thirty unsuccessful iterations, we admit failure of convergence.

In Chapter III we obtain, through elementary similarity transformations, an upper Hessenberg matrix H from a nonsymmetric matrix B . Now we can determine the spectrum of H using the double shift QR algorithm with the QR decompositions constructed using Householder reflectors.

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