ON THE PERTURBATION THEORY FOR UNITARY EIGENVALUE PROBLEMS

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Abstract. Some aspects of the perturbation theory for eigenvalues of unitary matrices are considered. Making use of the close relation between unitary and Hermitian eigenvalue problems a Courant-Fischer-type theorem for unitary matrices is derived and an inclusion theorem analogue to the Kahan theorem for Hermitian matrices is presented. Implications for the special case of unitary Hessenberg matrices are discussed.

Key words. unitary eigenvalue problem, perturbation theory
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1. Introduction. New numerical methods to compute eigenvalues of unitary matrices have been developed during the last ten years. Unitary QR-type methods [19, 9], a divide-and-conquer method [20, 21], a bisection method [10], and some special methods for the real orthogonal eigenvalue problem [1, 2] have been presented. Interest in this task arose from problems in signal processing [11, 29, 33], in Gaussian quadrature on the unit circle [18], and in trigonometric approximations [31, 16] which can be stated as eigenvalue problems for unitary matrices, often in Hessenberg form. As those numerical methods exploit the rich mathematical structure of unitary matrices, which is closely analogous to the structure of Hermitian matrices, the methods are efficient and deliver very good approximations to the desired eigenvalues.

There exist, however, only a few perturbation results for the unitary eigenvalue problem, which can be used to derive error bounds for the computed eigenvalue approximations. A thorough and complete treatment of the perturbation aspects associated with the numerical methods for unitary eigenvalue problems is still missing.

The following perturbation results have been obtained so far. If U and $\widetilde{U}$ are unitary matrices with spectra $\sigma(U) = \{\lambda_j\}$, and $\sigma(\widetilde{U}) = \{\widetilde{\lambda}_j\}$, respectively, we can arrange the eigenvalues in diagonal matrices Λ and $\widetilde{\Lambda}$, respectively, and consider as a measure for the distance of the spectra

$$d_\mu(\sigma(U), \sigma(\widetilde{U})) := \min_P ||\Lambda - P^T \widetilde{\Lambda} P||_\mu, \qquad \mu = 2, F \tag{1.1}$$

where the minimum is taken over all permutation matrices P and the norm is either the spectral or the Frobenius norm. By the Hoffman-Wielandt theorem (see, e.g.,[34]) we get

$$d_F(\sigma(U), \sigma(\widetilde{U})) \leq ||U - \widetilde{U}||_F.$$

Bhatia and Davis [5] proved the corresponding result for the spectral norm

$$d_2(\sigma(U), \sigma(\widetilde{U})) \leq ||U - \widetilde{U}||_2.$$

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Elsner and He consider a relative error in [15]. They use the measure

$$\widetilde{d}_\mu(\sigma(U),\sigma(\widetilde{U})) := \min_P ||(\Lambda + P^T\widetilde{\Lambda}P)^{-1}(\Lambda - P^T\widetilde{\Lambda}P)||_\mu, \tag{1.2}$$

where again $\mu = 2$ or $\mu = F$. They prove that

$$\widetilde{d}_\mu(\sigma(U),\sigma(\widetilde{U})) \leq ||C(U^H\widetilde{U})||_\mu$$

where $C(U) = i(I+U)^{-1}(I-U)$ is the Cayley transformation of U (assuming here that $-1 \notin \sigma(U)$).

To each eigenvalue λ of U, where $-1 \notin \sigma(U)$, we can associate an angle θ_λ by defining

$$\theta_\lambda = arctan[\sqrt{-1}(1+\lambda)^{-1}(1-\lambda)]$$

with $-\pi/2 \leq \theta_\lambda < \pi/2$. It is the angle formed by the line from -1 through λ and the real axis (see also Section 2). With respect to their angles the eigenvalues of U and $\widetilde{U}$ have a natural ordering on the unit circle. Elsner and He give *sine*- and *tangent*-interpretations of the above inequality in terms of these angles. Furthermore they show that with respect to a certain cutting point ζ on the unit circle the eigenvalues of U and $\widetilde{U}$ have a natural ordering $\{\lambda_j(\zeta)\}$ and $\{\widetilde{\lambda}_j(\zeta)\}$ on the unit circle such that

$$\max_j |\lambda_j(\zeta) - \widetilde{\lambda}_j(\zeta)| \leq ||U - \widetilde{U}||_2.$$

An interlacing theorem for unitary matrices is also presented in [15], showing that the eigenvalues of suitably modified principal submatrices of a unitary matrix interlace those of the complete matrix on the unit circle (see Section 2).

In this paper we consider further aspects of the perturbation problem for the eigenvalues of a unitary matrix U. In Section 2 we show how the angles ζ are related to the eigenvalues of the Cayley transform of U. With the aid of this relation we can give a min-max-characterization for the angles of U's eigenvalues in analogy to the Courant-Fischer theorem for Hermitian matrices. We also show that tangents of these angles can be characterized by usual Rayleigh quotients corresponding to the generalized eigenvalue problem

$$\sqrt{-1}(I+U^H)(I-U)x = \mu(I+U^H)(I+U)x.$$

Furthermore we prove a Kahan-like inclusion theorem showing that the eigenvalues of a certain modified leading principal submatrix of U determine arcs on the unit circle such that each arc contains an eigenvalue of U. In applications unitary matrices are often of Hessenberg form. In Section 3 we recall that a unitary unreduced Hessenberg matrix H has a unique parameterization $H = H(\gamma_1,\ldots,\gamma_n)$, where the reflection parameters $\gamma_1,\ldots,\gamma_n \in \mathbb{C}$, with $|\gamma_i| < 1$ for $i = 1,\ldots,n-1$ and $|\gamma_n| = 1$, determine H completely. We show the implications of the results in Section 2 for the special case of unitary Hessenberg matrices. In particular it will be seen that the modified kth leading principal submatrix in this special case is just $H(\gamma_1,\ldots,\gamma_{k-1},\zeta)$ where $|\zeta| = 1$. We discuss the dependence of the eigenvalues on this last reflection parameter ζ. Finally Section 4 will give numerical examples which elucidate the statements proved in Section 3.

2. Perturbation Results for unitary Matrices.

Unitary matrices have a rich mathematical structure that is closely analogous to that of Hermitian matrices. In this section we first discuss the intimate relationship between unitary and Hermitian matrices which indicates that one can hope to find unitary analogues for the good numerical methods and for the theoretical results that exist for the symmetric/Hermitian eigenvalue problem. We will adapt some eigenvalue bounds for Hermitian matrices to the unitary case.

Let ρ be a complex unimodular number. The Cayley transformation with respect to ρ maps the unitary matrices whose spectrum does not include ρ, onto the Hermitian matrices. The *Cayley transformation with respect to* ρ for a unitary matrix $U \in \mathbb{C}^{n\times n}$ is defined as

$$C(U) = \imath(\rho I_n - U)^{-1}(\rho I_n + U)$$

where ρ is not an eigenvalue of U and $\imath = \sqrt{-1}$. I_n denotes the $n \times n$ identity matrix. A simple calculation shows that $C(U)$ is Hermitian. The mapping is one-to-one and the *inverse Cayley transformation with respect to* ρ for a Hermitian matrix X is given by

$$C^{-1}(X) = \rho(X + \imath I_n)^{-1}(X - \imath I_n).$$

The symmetric/Hermitian eigenproblem has been extensively studied, see, e.g. [28, 17, 24, 26]. Due to this relation between Hermitian and unitary matrices, one can hope to get similar results for unitary matrices.

With the aid of the Cayley transformation we can order the eigenvalues conveniently. Let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of U numbered starting at ρ moving counterclockwise along the unit circle. Let $\mu_1 \leq \mu_2 \leq \ldots \leq \mu_n$ be the eigenvalues of $X = C(U)$. Then for $k = 1, \ldots, n$

$$\mu_k = \imath\frac{\rho + \lambda_k}{\rho - \lambda_k}. \tag{2.1}$$

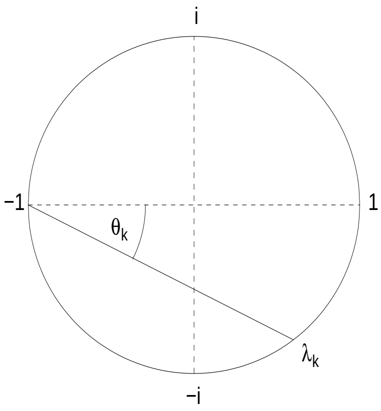
For simplicity assume that $\rho = -1$. Then

$$\begin{aligned}\mu_k &= \imath\frac{1 - \lambda_k}{1 + \lambda_k}\\ &= \frac{Im(\lambda_k)}{1 + Re(\lambda_k)}\\ &= tan(\theta_k)\end{aligned}$$

where $\theta_k = arg(1+\lambda_k)$. For $z \in \mathbb{C}\backslash\{0\}$ the argument of z, $arg(z) \in (-\pi, \pi]$ is defined by

$$arg(z) = \begin{cases} arctan(\frac{Im(z)}{Re(z)}) + \pi & Re(z) < 0\\ arctan(\frac{Im(z)}{Re(z)}) & Re(z) > 0\\ \frac{\pi}{2} & Re(z) = 0, Im(z) > 0\\ -\frac{\pi}{2} & Re(z) = 0, Im(z) < 0 \end{cases}.$$

The Cayley transformation of λ_k is the tangent of the angle $\theta_k = arg(1 + \lambda_k)$ which is formed by the real axis and the straight line through λ_k and -1:



Hence it is reasonable to define

$$\lambda_i \leq \lambda_j \quad \text{if} \quad \imath\frac{1-\lambda_i}{1+\lambda_i} \leq \imath\frac{1-\lambda_j}{1+\lambda_j}.$$

This also gives a complete ordering of the points on the unit circle with respect to the cutting point -1. Note that the complete ordering excludes the cutting point -1. For a different cutting point the orders of the eigenvalues are only changed cyclically.

If ζ_1, ζ_2 are complex unimodular numbers such that $\zeta_1 < \zeta_2$, then (ζ_1, ζ_2) will denote the *open arc* from the point ζ_1 to the point ζ_2 on the unit circle (moving counterclockwise).

The Courant-Fischer theorem (see, e.g., [17, Theorem 8.1.2]) characterizes the eigenvalues of Hermitian matrices by Rayleigh quotients. A similar characterization can be given for the eigenvalues of unitary matrices. Let $U \in \mathbb{C}^{n\times n}$ be a unitary matrix with eigenvalues $\lambda_1, \ldots, \lambda_n$. Assume that -1 is not an eigenvalue of U and number the eigenvalues starting at -1 moving counterclockwise along the unit circle. Let $v_1, \ldots, v_n$ be an orthonormal basis in $\mathbb{C}^{n\times n}$ of eigenvectors of U. Let $z \in \mathbb{C}^n$ with $||z||_2 = 1$. Then we can expand z as

$$z = \sum_{i=1}^{n} \alpha_i v_i \qquad \alpha_i \in \mathbb{C},\ i = 1, \ldots, n.$$

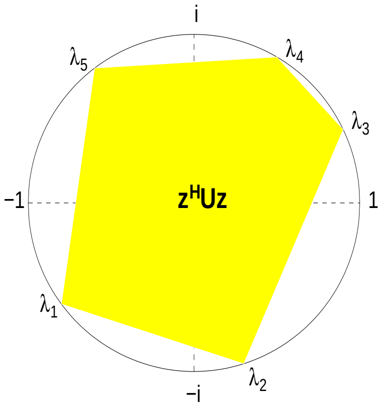
From $||z||_2 = 1$ we obtain

$$\sum_{i=1}^{n} |\alpha_i|^2 = 1.$$

Because of

$$z^H U z = \sum_{i=1}^{n} |\alpha_i|^2 \lambda_i$$

we see that the Rayleigh quotient $z^H U z$ lies in the convex polygon which is spanned by the eigenvalues of U.



THEOREM 2.1. *With the notation given above we obtain for* $\theta_k = arg(1+\lambda_k), k = 1, \ldots, n$

$$\begin{aligned} \theta_k &= \max_{V \in V_{n-k+1}} \min_{z \in V, ||z||_2 = 1} arg(1 + z^H U z) \\ &= \min_{V \in V_k} \max_{z \in V, ||z||_2 = 1} arg(1 + z^H U z) \end{aligned}$$

where V_k *denotes the set of all* k*-dimensional subspaces of* $\mathbb{C}^n$.
In particular,

$$\begin{aligned} \theta_1 &= \min_{z \in \mathbb{C}^n, ||z||_2 = 1} arg(1 + z^H U z) \\ \theta_n &= \max_{z \in \mathbb{C}^n, ||z||_2 = 1} arg(1 + z^H U z) \end{aligned}$$

Proof. Let $v_1, \ldots, v_n$ be an orthonormal basis of eigenvectors of U. Let $V \in V_{n-k+1}$. Then $V \cap \{v_1, \ldots, v_k\} \neq \emptyset$. Let z be a vector in this intersection, $||z||_2 = 1$. Then

$$z = \sum_{i=1}^{k} \alpha_i v_i, \qquad \sum_{i=1}^{k} |\alpha_i|^2 = 1, \qquad \alpha_i \in \mathbb{C}, \; i = 1, \ldots, k.$$

Hence, the Rayleigh quotient $z^H U z$ lies in the convex polygon spanned by the eigenvalues $\lambda_1, \ldots, \lambda_k$. Therefore

$$arg(1 + z^H U z) \leq arg(1 + \lambda_k)$$

and

$$\max_{V \in V_{n-k+1}} \min_{z \in V, ||z||_2 = 1} arg(1 + z^H U z) \leq \theta_k.$$

Now consider the subspace of dimension $n-k+1$ which is spanned by $v_k, \ldots, v_n$. A vector $z, ||z||_2 = 1$ in this subspace can be written as

$$z = \sum_{i=k}^{n} \gamma_i v_i, \qquad \sum_{i=k}^{n} |\gamma_i|^2 = 1, \qquad \gamma_i \in \mathbb{C}, \; i = k, \ldots, n.$$

Hence, the Rayleigh quotient $z^H U z$ lies in the convex polygon spanned by the eigenvalues $\lambda_k, \ldots, \lambda_n$. Therefore

$$arg(1 + z^H U z) \geq arg(1 + \lambda_k)$$

and

$$\max_{V \in V_{n-k+1}} \min_{z \in V, ||z||_2 = 1} arg(1 + z^H U z) = \theta_k.$$

The second equation can be shown analogously. □

Corollary 2.2. *With the notation given above we define for* $z \in \mathbb{C}^n$ *with* $||z||_2 = 1$:

$$R(z) = \frac{z^H [\imath (I_n + U^H)(I_n - U)] z}{z^H [(I_n + U^H)(I_n + U)] z}$$

Then

$$\tan(arg(1 + z^H U z)) = R(z) \tag{2.2}$$

and for $k = 1, \ldots, n$

$$\begin{aligned}\tan(\theta_k) &= \max_{V \in V_{n-k+1}} \min_{z \in V, ||z||_2 = 1} R(z) \\ &= \min_{V \in V_k} \max_{z \in V, ||z||_2 = 1} R(z).\end{aligned}$$

Proof. A simple calculation yields (2.2). The rest of the corollary follows from Theorem 2.1 and the monotonicity of the function tan in $(-\frac{\pi}{2}, \frac{\pi}{2})$. □

The corollary shows that the angles θ_k can be characterized by usual Rayleigh quotients. $R(z)$ can be interpreted as the Rayleigh quotient corresponding to the generalized eigenvalue problem

$$\{\imath (I_n + U^H)(I_n - U) - \mu (I_n + U^H)(I_n + U)\} x = 0. \tag{2.3}$$

Since U is unitary, $\imath (I_n + U^H)(I_n - U)$ is Hermitian and $(I_n + U^H)(I_n + U)$ is Hermitian and positive definite. (2.3) is equivalent to the eigenvalue problem

$$\imath (I_n + U)^{-1} (I_n - U) x = \mu x$$

for the Cayley transformation of U.

Remark 2.3. *For ease of notation the above theorem and corollary are formulated for the case that* $\rho = -1$ *is not an eigenvalue of* U. *This restriction is not necessary, one can proof the corresponding statements for any cutting point* $\rho \in \mathbb{C}, |\rho| = 1, \rho$ *not an eigenvalue of* U.

In [15], the Cauchy interlacing theorem for Hermitian matrices is generalized to the unitary case. The Cauchy interlace theorem shows that the eigenvalues of the $k \times k$ leading principal submatrix of a Hermitian matrix X interlace the eigenvalues of X. Adapting this theorem to the unitary case, one has to deal with the problem that leading principal submatrices of unitary matrices are in general not unitary and that their eigenvalues lie inside the unit circle. In [15] it is shown that certain modified leading principal submatrices of a unitary matrix U have the property that their eigenvalues interlace with those of U.

THEOREM 2.4. *[15, Theorem 5.2 and 5.3] Let*

$$U = \begin{bmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{bmatrix} \tag{2.4}$$

be an $n \times n$ unitary matrix, U_{11} the $k \times k$ leading principal submatrix of U, and

$$U_k = U_{11} - U_{12}(U_{22} - \rho I_{n-k})^{-1} U_{21} \tag{2.5}$$

where $\rho \in \mathbb{C}, |\rho| = 1$ and ρ is not an eigenvalue of U. Then U_k is unitary. Let

$$\lambda_1 \leq \ldots \leq \lambda_n$$

be the eigenvalues of U and

$$\mu_1 \leq \ldots \leq \mu_k$$

be those of U_k ordered with respect to ρ. Then

$$\lambda_i \leq \mu_i \leq \lambda_{i+n-k}.$$

U_k is called the *modified kth leading principal submatrix* of U. Furthermore, analogues of the Hoffman-Wielandt theorem and a Weyl-type theorem are derived in [15].

With the help of Theorem 2.4 one can specify for each eigenvalue of a modified leading principal submatrix U_k an arc on the unit circle which contains that eigenvalue. These bounds are fairly rough, especially if k is much smaller than n. This result is of theoretical nature, because in practice we are more interested in the question, whether the arc (μ_1, μ_2) contains an eigenvalue of U or not.

The same problem arises in the Hermitian case. Lehmann and Kahan derived inclusion theorems which consider this problem (see, e.g., [28] and the references therein). A special case of their results is

THEOREM 2.5. *[28, Theorem on page 196] Let $X \in \mathbb{C}^{n \times n}$ be a Hermitian matrix. Partition X as*

$$X = \begin{bmatrix} X_k & C^H \\ C & V \end{bmatrix} \qquad \text{where } X_k \in \mathbb{C}^{k \times k}.$$

Let μ_i be the eigenvalues of $X_k, i = 1, \ldots, k$, $\mu_1 \leq \ldots \leq \mu_k$. If rank$(C) = 1$, then each interval $[\mu_i, \mu_{i+1}], i = 0, 1, \ldots, k$ contains an eigenvalue of X, where $\mu_0 = -\infty, \mu_{k+1} = \infty$.

The following theorem states the analogous result for unitary matrices.

THEOREM 2.6. *Let $U \in \mathbb{C}^{n \times n}$ be a unitary matrix and let U be partitioned as in (2.4). Let $\rho \in \mathbb{C}, |\rho| = 1$, be not an eigenvalue of U. Define a unitary matrix U_k as in (2.5) with eigenvalues $\mu_1, \ldots, \mu_k$. The eigenvalues are numbered starting at ρ moving counterclockwise along the unit circle. If rank$(U_{21}) = 1$, then each arc*

(μ_i, μ_{i+1}) on the unit circle, $i = 1, \ldots, k$ contains at least one eigenvalue of U, where $\mu_0 = \mu_{k+1} = \rho$.

Proof. Since ρ is not an eigenvalue of U, it is not an eigenvalue of U_{22}: Assume ρ is an eigenvalue of U_{22}. Then there is a normalized eigenvector $x \in \mathbb{C}^{n-k}$ such that $U_{22}x = \rho x$. Therefore

$$U \begin{bmatrix} 0 \\ x \end{bmatrix} = \begin{bmatrix} U_{12}x \\ U_{22}x \end{bmatrix} = \begin{bmatrix} U_{12}x \\ \rho x \end{bmatrix}.$$

As $|\rho| = 1$, $\|x\| = 1$ and U is unitary, $U_{12}x$ has to be zero. But this would imply that ρ is an eigenvalue of U in contradiction to our general assumption. Hence ρ is not an eigenvalue of U_{22}.

U_k is defined as

$$U_k = U_{11} - U_{12}(U_{22} - \rho I_{n-k})^{-1} U_{21}.$$

$U_k - \rho I_k$ can be interpreted as the Schur complement of $U_{22} - \rho I_{n-k}$ in $U - \rho I_n$. We can make use of this fact to construct $(U - \rho I_n)^{-1}$ using the following result of Duncan [13] (see Corollary 2.4 in [27])

Let $A \in \mathbb{C}^{n \times n}$ be partioned as

$$A = \begin{bmatrix} E & F \\ G & H \end{bmatrix} \qquad \textit{where } H \in \mathbb{C}^{n-k \times n-k}.$$

Let A and H be nonsingular, then $T = E - FH^{-1}G \in \mathbb{C}^{k \times k}$ is the Schur complement of H in A, T is nonsingular and

$$A^{-1} = \begin{bmatrix} T^{-1} & -T^{-1}FH^{-1} \\ -H^{-1}GT^{-1} & H^{-1} + H^{-1}GT^{-1}FH^{-1} \end{bmatrix}.$$

We obtain

$$(U - \rho I_n)^{-1} =$$

$$\begin{bmatrix} (U_k - \rho I_k)^{-1} & -(U_k - \rho I_k)^{-1} U_{12} (U_{22} - \rho I_{n-k})^{-1} \\ -(U_{22} - \rho I_{n-k})^{-1} U_{21} (U_k - \rho I_k)^{-1} & (U_{22} - \rho I_{n-k})^{-1} [I + U_{21}(U_k - \rho I_k)^{-1} U_{12} (U_{22} - \rho I_{n-k})^{-1}] \end{bmatrix}.$$

In particular, $(U_k - \rho I_k)^{-1}$ is the $k \times k$ leading principal submatrix of $(U - \rho I_n)^{-1}$.

Now we consider the Cayley transformation with respect to ρ of U

$$\begin{aligned} X = C(U) &= \imath(\rho I_n - U)^{-1}(\rho I_n + U) \\ &= -\imath I_n - 2\imath\rho(U - \rho I_n)^{-1}. \end{aligned}$$

This yields

$$X + \imath I_n = -2\imath\rho(U - \rho I_n)^{-1}. \tag{2.6}$$

We partition X as we did U:

$$X = \begin{bmatrix} X_k & X_{12} \\ X_{21} & X_{22} \end{bmatrix}$$

where X_k is the $k \times k$ leading principal submatrix of X. From (2.6) it follows that

$$X_k + \imath I_k = -2\imath\rho(U_k - \rho I_k)^{-1}.$$

Therefore, X_k is the Cayley transformation of U_k. Further we obtain from (2.6):

$$X_{21} = 2\imath\rho(U_{22} - \rho I_{n-k})^{-1} U_{21} (U_k - \rho I_k)^{-1}.$$

If $rank(U_{21}) = 1$, then $rank(X_{21}) = 1$ as the other two matrices in the product have full rank.

Now we can use Theorem 2.5 to obtain that each interval formed by two eigenvalues of X_k contains at least one eigenvalue of X. We have seen in (2.1) that the eigenvalues of X and X_k can be obtained from those of U and U_k via the Cayley transformation. As the Cayley transformation is monotone, this yields: each arc (μ_i, μ_{i+1}) on the unit circle, $i = 1, \ldots, k-1$ contains at least one eigenvalue of U. For the two outer arcs $(\rho, \mu_1), (\mu_k, \rho)$ the statement follows directly from Theorem 2.4. □

The last result we mention in this section clarifies the question of how the eigenvalues of a unitary matrix change if the matrix is modified by a unitary differing from I only by rank one. For the Hermitian case, the answer is given, e.g., in [17, chapter 12.5.3]. For the unitary case we obtain

Theorem 2.7. *Let $U, S \in \mathbb{C}^{n \times n}$ be unitary matrices and S such that*

$$rank(I_n - S) = 1.$$

Then the eigenvalues of U and US interlace on the unit circle.

Proof. See [4, section 6]. □

3. Unitary upper Hessenberg Matrices.

It is well known that any (unitary) $n \times n$ matrix can be transformed to an upper Hessenberg matrix H by a unitary similarity transformation Q. If the first column of Q is fixed and H is an unreduced upper Hessenberg matrix with positive subdiagonal elements (that is $h_{i+1,i} > 0$), then the transformation is unique. Any $n \times n$ unitary upper Hessenberg matrix with nonnegative subdiagonal elements can be uniquely parameterized by $2n - 1$ real parameters. This compact form is used in [1, 3, 9, 11, 14, 19, 20, 21, 22, 23, 32] to develop fast algorithms for solving the unitary eigenvalue problem.

Let

$$G_k = G_k(\gamma_k) = diag(I_{k-1}, \begin{bmatrix} -\gamma_k & \sigma_k \\ \sigma_k & \overline{\gamma_k} \end{bmatrix}, I_{n-k-1})$$

with $\gamma_k \in \mathbb{C}$, $\sigma_k \in \mathbb{R}^+$ and $|\gamma_k|^2 + \sigma_k^2 = 1$, and

$$\widetilde{G}_n(\gamma_n) = diag(I_{n-1}, -\gamma_n)$$

with $\gamma_n \in \mathbb{C}$, $|\gamma_n| = 1$.

The product $H = H(\gamma_1, \gamma_2, \ldots, \gamma_n) := G_1(\gamma_1) \cdots G_{n-1}(\gamma_{n-1}) \widetilde{G}_n(\gamma_n) =$

$$= \begin{pmatrix} -\gamma_1 & -\sigma_1\gamma_2 & -\sigma_1\sigma_2\gamma_3 & \cdots & -\sigma_1 \ldots \sigma_{n-1}\gamma_n \\ \sigma_1 & -\overline{\gamma_1}\gamma_2 & -\overline{\gamma - 1}\sigma_2\gamma_3 & \cdots & -\overline{\gamma_1}\sigma_2 \ldots \sigma_{n-1}\gamma_n \\ & \sigma_2 & -\overline{\gamma}_2\gamma_3 & \cdots & -\overline{\gamma}_2\sigma_3 \ldots \sigma_{n-1}\gamma_n \\ & & \ddots & \ddots & \vdots \\ & & & \sigma_{n-1} & -\overline{\gamma_{n-1}}\gamma_n \end{pmatrix}$$

is a unitary upper Hessenberg matrix with positive subdiagonal elements. Conversely, if $H \in \mathbb{C}^{n\times n}$ is a unitary upper Hessenberg matrix with positive subdiagonal elements, then it follows from elementary numerical linear algebra that one can determine matrices $G_1, G_2, \ldots, G_{n-1}, \widetilde{G}_n$ such that $\widetilde{G}_n^H G_{n-1}^H \cdots G_2^H G_1^H H = I$. Since H as a unitary matrix has a unique inverse, this has to be $\widetilde{G}_n^H G_{n-1}^H, ... G_2^H G_1^H$. Thus H has a unique factorization of the form

$$H = H(\gamma_1, \gamma_2, ..., \gamma_n) = G_1(\gamma_1)G_2(\gamma_2)\cdots G_{n-1}(\gamma_{n-1})\widetilde{G}_n(\gamma_n). \tag{3.1}$$

The *Schur parameters* $\{\gamma_k\}_{k=1}^n$ and the *complementary Schur parameters* $\{\sigma_k\}_{k=1}^n$ can be computed from the elements of H by a stable $O(n^2)$ algorithm [19]. In statistics the Schur parameters are referred to as partial correlation coefficients and in signal processing as reflection coefficients [2, 11, 12, 25, 29, 30, 33].

If $\sigma_k = 0$, then $|\gamma_k| = 1$, and we have the direct sum decomposition

$$H = H(\gamma_1, ..., \gamma_k) \oplus H(\overline{\gamma}_k\gamma_{k+1}, ..., \overline{\gamma}_k\gamma_n).$$

Hence, in general $\sigma_1\sigma_2...\sigma_{n-1} > 0$ is assumed if the factorization (3.1) is used to solve a unitary eigenvalue problem. Such a unitary upper Hessenberg matrix is called *unreduced.* If λ is an eigenvalue of an unreduced Hessenberg matrix, then its geometric multiplicity is one [17, Theorem 7.4.4]. Since unitary matrices are diagonalizable, no eigenvalue of an unreduced unitary upper Hessenberg matrix is defective, that is, the eigenvalues of an unreduced unitary upper Hessenberg matrix are distinct.

We will adapt the general theorems given in the last section to the more specific case of unitary upper Hessenberg matrices. Let $H \in \mathbb{C}^{n\times n}$ be a unitary upper Hessenberg matrix with positive subdiagonal elements, $H = H(\gamma_1, \ldots, \gamma_n)$. Partition H as

$$H = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} \tag{3.2}$$

where H_{11} is the $k \times k$ leading principal submatrix. From Theorem 2.4 we obtain that the modified kth leading principal submatrix of H, $H_k = H_{11} - H_{12}(H_{22} - \rho I)^{-1}H_{21}$, is unitary (if $\rho \in \mathbb{C}, |\rho| = 1, \rho$ not an eigenvalue of H). As H_k is a unitary upper Hessenberg matrix, we can factor $H_k = G_1(\widehat{\gamma}_1)G_2(\widehat{\gamma}_2)\cdots G_{k-1}(\widehat{\gamma}_{k-1})\widetilde{G}_k(\widehat{\gamma}_k)$. Taking a closer look at H_k reveals that H_k differs from H_{11} only in the last column. Hence the modification of H_{11} to H_k is equivalent to a modification of the reflection coefficient γ_k, i.e.

$$H_k = H_k(\gamma_1, \ldots, \gamma_{k-1}, \zeta_k), \qquad |\zeta_k| = 1.$$

The following theorem by Bunse-Gerstner and He characterizes the correct choice of the parameter ζ_k:

THEOREM 3.1. *Let $H = H(\gamma_1, \ldots, \gamma_n) \in \mathbb{C}^{n\times n}$ be a unitary upper Hessenberg matrix with positive subdiagonal elements. For $k \in \{1, \ldots, n-1\}$ let H be partioned as in (3.2). Let $\rho \in \mathbb{C}, |\rho| = 1$ not be an eigenvalue of H. Define parameters $\zeta_l(\rho), l = 1, \ldots, n$ by*

$$\begin{aligned} \zeta_n(\rho) &= \gamma_n \\ \zeta_l(\rho) &= \frac{\rho\gamma_l + \zeta_{l+1}(\rho)}{\rho + \overline{\gamma_l}\zeta_{l+1}(\rho)} \qquad l = n-1, \ldots, 1. \end{aligned} \tag{3.3}$$

Then

$$H_k(\gamma_1,\ldots,\gamma_{k-1},\zeta_k(\rho)) = H_{11} - H_{12}(H_{22}-\rho I_{n-k})^{-1}H_{21}.$$

Let $\mu_1,\ldots,\mu_k$ *and* $\lambda_1,\ldots,\lambda_n$ *be the eigenvalues of* $H_k(\gamma_1,\ldots,\gamma_{k-1},\zeta_k(\rho))$ *and* H *respectively, where the eigenvalues are numbered starting at* ρ *moving counterclockwise along the unit circle. Then for each* $i = 1,\ldots,k$ *the eigenvalue* μ_i *lies on the arc* $(\lambda_i, \lambda_{i+n-k})$.

Proof. The interlace property follows directly from Theorem 2.4. For the rest of the proof see [10]. □

Using Theorem 2.6 and 3.1 we obtain

THEOREM 3.2. *Let* $H = H(\gamma_1,\ldots,\gamma_n) \in \mathbb{C}^{n\times n}$ *be a unitary upper Hessenberg matrix with positive subdiagonal elements. Let* $\rho \in \mathbb{C}, |\rho| = 1$ *not be an eigenvalue of* H. *For* $k \in \{1,\ldots,n\}$ *let* $H_k = H_k(\gamma_1,\ldots,\gamma_{k-1},\zeta_k(\rho))$ *where* $\zeta_k(\rho)$ *is defined as in (3.3). Let* $\mu_1,\ldots,\mu_k$ *be the eigenvalues of* H_k. *Then for* $i = 0,\ldots,k$ *each arc* (μ_i,μ_{i+1}) *on the unit circle contains at least one eigenvalue of* H, *where* $\mu_0 = \mu_{k+1} = \rho$.

Moreover,we obtain

THEOREM 3.3. *Let* $H = H(\gamma_1,\ldots,\gamma_n) \in \mathbb{C}^{n\times n}$ *be a unitary upper Hessenberg matrix with positive subdiagonal elements. Then for any* $\zeta \in \mathbb{C}, |\zeta| = 1$ *there exists a cutting point* $\rho \in \mathbb{C}, |\rho| = 1$ *such that the eigenvalues of* $H_k = H_k(\gamma_1,\ldots,\gamma_{k-1},\zeta)$ *and* H *have the interlace properties with respect to* ρ *on the unit circle given by Theorem 3.1 and 3.2.*

Proof. We will show that $\rho \mapsto \zeta_k(\rho)$ is an automorphism on the unit circle, this proves the theorem. Note that for unitary upper Hessenberg matrices with positive subdiagonal elements we have $|\gamma_j| < 1, j = 1,\ldots,n-1$.

Obviously

$$\rho \mapsto \zeta_{n-1}(\rho) = \frac{\rho\gamma_{n-1}+\gamma_n}{\rho+\overline{\gamma_{n-1}}\gamma_n}$$

is bijective on the unit circle. The same is true for the mapping

$$\zeta_j(\rho) \mapsto \zeta_{j-1}(\rho) = \frac{\rho\gamma_{j-1}+\zeta_j(\rho)}{\rho+\overline{\gamma_{j-1}}\zeta_j(\rho)} \qquad j = n-1,\ldots,2.$$

Hence $\rho \mapsto \zeta_k(\rho)$ is a one-to-one mapping of the unit circle onto itself. □

The statement of the above theorem can be summarized as follows: Any leading principal submatrix of a unitary upper Hessenberg matrix with positive lower subdiagonal elements can be modified to be unitary by replacing the last reflection coefficient with a parameter on the unit circle. No matter how this parameter is chosen, there is always a cutting point ρ on the unit circle such that the eigenvalues of the modified leading principal submatrix and those of the entire matrix satisfy the interlace properties given by Theorem 3.1 and 3.2.

Disregarding the cutting point ρ and the two arcs formed with it, Theorem 3.3 implies the following corollary.

COROLLARY 3.4. *Let* $H = H(\gamma_1,\ldots,\gamma_n) \in \mathbb{C}^{n\times n}$ *be a unitary upper Hessenberg matrix with positive subdiagonal elements. For* $\zeta \in \mathbb{C}, |\zeta| = 1$ *let* $H_k =$

$H_k(\gamma_1,\ldots,\gamma_{k-1},\zeta) \in \mathbb{C}^{k\times k}, k \in \{1,\ldots,n\}$. Then every arc on the unit circle formed by two eigenvalues of H_k contains an eigenvalue of H.

In particular the above theorems show that the eigenvalues of two consecutive modified leading principal submatrices H_k and H_{k+1} of a unitary upper Hessenberg matrix with positive subdiagonal elements interlace on the unit circle. More specifically, consider the modified leading principal submatrices $H_k = H_k(\gamma_1,\ldots,\gamma_{k-1},\zeta_k)$ and $H_{k+1} = H_{k+1}(\gamma_1,\ldots,\gamma_k,\zeta_{k+1})$ where $|\zeta_k| = |\zeta_{k+1}| = 1$ and $k < n$. The eigenvalues of H_k and H_{k+1} interlace with respect to the cutting point ρ on the unit circle where ρ is given by

$$\rho = \frac{\zeta_{k+1}(1-\overline{\gamma_k}\zeta_k)}{\zeta_k - \gamma_k}.$$

The remaining question is: how strongly do the eigenvalues of $H_k(\gamma_1,\ldots,\gamma_{k-1},\zeta)$ depend of the choice of ζ? We present some results on this dependence on the last reflection parameter.

THEOREM 3.5. *Let $H_a = H(\gamma_1,\ldots,\gamma_{n-1},\zeta_a), H_b = H(\gamma_1,\ldots,\gamma_{n-1},\zeta_b)$ be unitary upper Hessenberg matrices with positive subdiagonal elements, $|\zeta_a| = |\zeta_b| = 1$.*

1. *The eigenvalues of H_a and H_b interlace on the unit circle.*
2. *$\nu(H_a,H_b) \le |\zeta_a - \zeta_b|$ where the eigenvalue variation $\nu(U,B)$ is defined by*

   $$\nu(U,B) = \min\{\max_{i\in\{1,\ldots,n\}} |\lambda_i - \mu_{\Pi(i)}|, \Pi \text{ permutation of } \{1,\ldots,n\}\},$$

   the λ_i's being the eigenvalues of U and the μ_i's those of B.
3. *Let $\lambda_1^a,\ldots,\lambda_n^a$ and $\lambda_1^b,\ldots,\lambda_n^b$ be the eigenvalues of H_a and H_b. Let*

   $$S_k^H H_a S_k = diag(\lambda_1^a,\ldots,\lambda_n^a)$$

   be the Schur decomposition of H_a, $S_k = [s_1,\ldots,s_k] = [s_{ij}]_{i,j=1}^k$. Then for $i = 1,\ldots,k$

   $$\begin{aligned}\min_{j\in\{1,\ldots,k\}} |\lambda_i^a - \lambda_j^b| &\le \|H_b s_i - \lambda_i^a s_i\|_2 \\ &\le |\zeta_a - \zeta_b|\ |s_{ki}|.\end{aligned}$$

Proof.

1. We have

   $$H_b = H_a S \qquad \text{where } S = diag(I_{n-1}, \overline{\zeta_a}\zeta_b)$$

   S is unitary and $rank(I_n - S) = 1$. According to Theorem 2.7, the eigenvalues of H_a and H_b interlace on the unit circle.
2. As the matrices H_a and H_b differ only in the last column we have

   $$\|H_a - H_b\|_2 = \|G_1(\gamma_1)\cdots G_{n-1}(\gamma_{n-1})[\widetilde{G}_n(\zeta_a) - \widetilde{G}_n(\zeta_b)]\|_2 = |\zeta_a - \zeta_b|.$$

   Since H_a and H_b are unitary, the statement 2. follows from the following theorem of Bhatia/Davis [5]:

   > *For all constant multiplies $U = \alpha Q$ and $B = \beta V$ of two unitary matrices Q and V we have*

   $$\nu(U,B) \le \|U - B\|_2.$$

(For a completely different proof and extension of the result to multiples of unitaries see [6]. When U and B are Hermitian, the above inequality is a classical result of Weyl).

3. H_b is unitary and therefore unitarily diagonalizable. The first inequality follows directly from the following easy to prove result [8, Satz 1.8.14]:

   Let $A \in \mathbb{C}^{n\times n}$ *be diagonalizable,* $A = TDT^{-1}$ *where* $D = diag(\lambda_1, \ldots, \lambda_n)$ *and* $T \in \mathbb{C}^{n\times n}$. *Let* $\mu \in \mathbb{C}, x \in \mathbb{C}^n, ||x||_2 = 1$ *and* $r = Ax - \mu x$. *Then*

   $$\min_{i\in\{1,\ldots,n\}} |\lambda_i - \mu| \leq ||T||_2 \; ||T^{-1}||_2 \; ||r||_2.$$

   Furthermore we obtain

   $$\begin{aligned} ||H_b s_i - \lambda_i^a s_i||_2 &= ||(H_b - H_a)s_i||_2 \\ &= ||G_1(\gamma_1)\cdots G_{n-1}(\gamma_{n-1})[\widetilde{G}_n(\zeta_a) - \widetilde{G}_n(\zeta_b)]s_i||_2 \\ &= ||(\zeta_a - \zeta_b)e_k^T s_i||_2 \\ &= |\zeta_a - \zeta_b| \; |s_{ki}|. \end{aligned}$$

□

Hence, eigenvalues of a unitary upper Hessenberg matrix, whose eigenvectors have a small last component, are not sensitive to changes in the last reflection parameter.

4. Numerical Examples. Numerical experiments are presented to elucidate the statements of Section 3. The eigenvalues of a unitary upper Hessenberg matrix H are compared with the eigenvalues of modified kth leading principal submatrices H_k for different dimensions k. The essential statements of Section 3 can be observed clearly:

- Between two eigenvalues of H_k on the unit circle there lies an eigenvalue of H (Corollary 3.4).
- The eigenvalues of unitary upper Hessenberg matrices, whose corresponding eigenvectors have a small last component, are not sensitive against changes of the last reflection coefficient. (Theorem 3.5).

All computations were done using MATLAB[1] on a SUN SparcStation 10.

A unitary upper Hessenberg matrix $H = H(\gamma_1, \ldots, \gamma_{20}) \in \mathbb{C}^{20\times 20}$ was constructed from 20 randomly chosen reflection coefficients $\gamma_1, \ldots, \gamma_{20} \in \mathbb{C}$. The eigenvalues λ_j of H lie randomly on the unit circle. The eigenvalue μ_j of the modified kth leading principal submatrices $H_k = H_k(\gamma_1, \ldots, \gamma_{k-1}, \zeta_k)$ were computed for different dimensions $k < 20$.

For the first example $\zeta_k = \frac{\gamma_k}{|\gamma_k|}$ was chosen. The eigenvalues of H and H_k are plotted for $k = 10$ and $k = 15$ in the following typical figure. The eigenvalues of H are marked by 'o', the eigenvalues of H_k by '*'.

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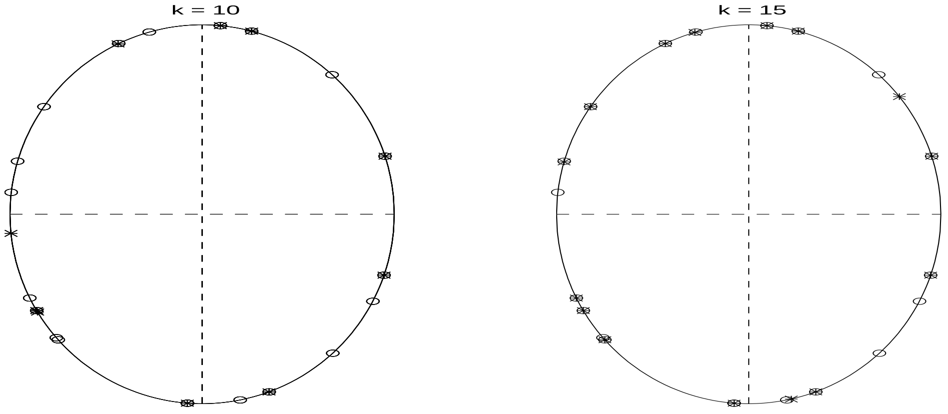
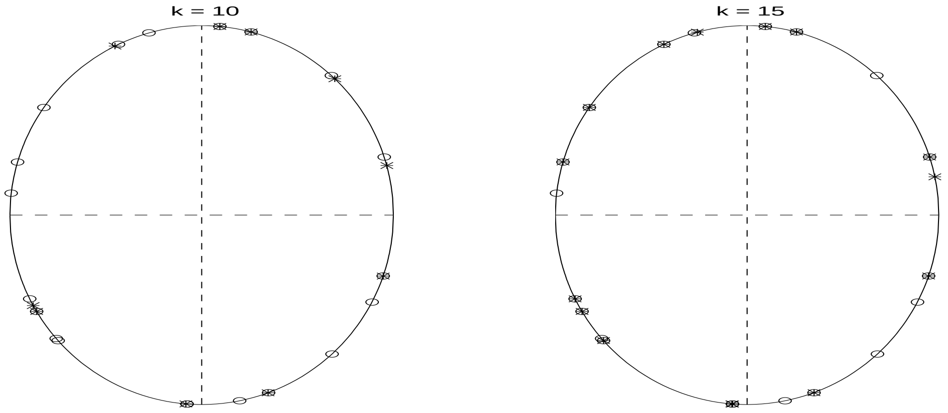
[1] MATLAB is a trademark of The MathWorks, Inc.



For the second example a random complex number $\zeta_k, |\zeta_k| = 1$ was chosen. The following figure displays the same information as before.



Corollary 3.4 states that every arc on the unit circle formed by two eigenvalues of H_k contains an eigenvalue of H. This can be seen in the above figures. Comparing the results of the two examples presented, one observes that independent of the choice of ζ_k the same eigenvalues of H are approximated. In Theorem 3.5 it was proven that if the last component of an eigenvector of a unitary upper Hessenberg matrix is small, then the corresponding eigenvalue is not sensitive against changes in the last reflection coefficient. Individual bounds for the minimal distance of each eigenvalue λ_j^a of $H_a = H_k(\gamma_1, \ldots, \gamma_{k-1}, \zeta_a)$ to the eigenvalues λ_j^b of $H_b = H_k(\gamma_1, \ldots, \gamma_{k-1}, \zeta_b)$ are given

$$\min_{j \in \{1,\ldots,n\}} |\lambda_i^a - \lambda_j^b| \leq |\zeta_a - \zeta_b| \; |s_{ki}|$$

where $s_{\ell i}, \ell \in \{1, \ldots, k\}$ is the ℓth component of the eigenvector for the ith eigenvalue of H_a. This means that if there is an eigenvalue λ_i^a of H_a such that the last component of the corresponding eigenvector is small, then any unitary upper Hessenberg matrix of the form H_b will have an eigenvalue λ_j^b that is close to λ_i^a.

The following table reports the minimal distance between each eigenvalue $\lambda_i^{\gamma_k}$ of $H_k = H_k(\gamma_1, \ldots, \gamma_{k-1}, \gamma_k/|\gamma_k|)$ and the eigenvalues λ_j^{rand} of $H_k = H_k(\gamma_1, \ldots, \gamma_{k-1}, \zeta)$

(where $\zeta \in \mathbb{C}, |\zeta| = 1$ is randomly chosen as above) as well as the error bounds for $k = 10$. The absolute difference between ζ_a and ζ_b was $|\zeta_a - \zeta_b| = 1.9052e + 00$.

	$\min\limits_{j\in\{1,\dots,n\}} \lvert\lambda_i^{\gamma_{10}} - \lambda_j^{rand}\rvert$	$\lvert\zeta_a - \zeta_b\rvert\, \lvert s_{ki}\rvert$
$\lambda_1^{\gamma_{10}}$	1.8894e-06	1.2717e-03
$\lambda_2^{\gamma_{10}}$	8.6787e-05	7.2976e-03
$\lambda_3^{\gamma_{10}}$	4.7180e-02	1.4922e-01
$\lambda_4^{\gamma_{10}}$	3.8116e-04	1.9408e-02
$\lambda_5^{\gamma_{10}}$	1.5810e-02	1.7357e-01
$\lambda_6^{\gamma_{10}}$	2.4628e-03	7.1265e-02
$\lambda_7^{\gamma_{10}}$	5.3716e-03	1.2358e-01
$\lambda_8^{\gamma_{10}}$	9.5131e-05	5.8360e-02
$\lambda_9^{\gamma_{10}}$	8.4488e-03	6.0709e-01
$\lambda_{10}^{\gamma_{10}}$	3.9452e-01	1.7845e+00

Comparing the actual minimal distance with the error bound one observes that the approximations are much better than the error bound predicts.

The same results can be observed for larger unitary upper Hessenberg matrices H. Moreover, one can observe that the eigenvalues of the modified leading principal submatrices H'_{k-1} and H'_k interlace on the unit circle with respect to a cutting point ρ.

5. Concluding Remarks. In this paper, we have proved that the angles θ_k associated with the eigenvalues λ_j of a unitary matrix U can be characterized by Rayleigh quotients. An inclusion theorem for the eigenvalues of symmetric matrices given by Kahan was adapted to the unitary case. We discussed the special case of unitary Hessenberg matrices, which is important for certain applications. We proved that every arc on the unit circle formed by two eigenvalues of a modified kth leading principal submatrix of a unitary upper Hessenberg matrix contains an eigenvalue of the complete matrix. Results on the dependence of the eigenvalues of unitary upper Hessenberg matrices on the last reflection coefficient are given.

Parts of this paper (Section 2 and most of Section 3) first appeared in [7]. Bohnhorst analyses the connection between a unitary matrix U and its Cayley transformation more closely with the help of structure ranks.

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