Error bounds in the isometric Arnoldi process

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Abstract

Error bounds for the eigenvalues computed in the isometric Arnoldi method are derived. The Arnoldi method applied to a unitary matrix U successively computes a sequence of unitary upper Hessenberg matrices $H_k, k = 1, 2, \ldots$. The eigenvalues of the H_k's are increasingly better approximations to eigenvalues of U. An upper bound for the distance of the spectrum of H_k from the spectrum of U, and an upper bound for the distance between each individual eigenvalue of H_k and one of U are given. Between two eigenvalues of H_k on the unit circle, there is guaranteed to lie an eigenvalue of U. The results are applied to a problem in signal processing.

Key words. unitary eigenvalue problem, Arnoldi process, error bounds, signal processing
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1 Introduction

A number of signal processing problems can be seen to require the numerical solution of unitary eigenvalue problems. The task of estimating dominant harmonics of a time series for instances arises in many applications, such as geology, astronomy and speech processing. The problem is to approximate frequencies and amplitudes of a discrete time signal $\{s_k\}_{k=-\infty}^{\infty}$. One may for instance consider the signal as a superposition of exponentials corrupted by small sized white noise, i.e.

$$s_k \approx \sum_{\ell=1}^{n} \rho_\ell e^{\imath(k\theta_\ell+\phi_\ell)} \tag{1}$$

for some (unknown) n, amplitudes $\rho_\ell > 0$, distinct frequencies $\theta_\ell \in]-\pi, \pi]$, and phases $\phi_\ell \in]-\pi, \pi]$, $\imath = \sqrt{-1}$. Given a finite subsequence $\{s_k\}_{k=1}^{N}$ the aim is to retrieve the frequencies $\theta_1, \ldots, \theta_n$ and the amplitudes $\rho_1, \ldots, \rho_n$. Typically N is very large and n is very small.

It is a common approach to determine the unknown quantities such that the first n autocorrelation lags of the signal s (or approximations of them) are matched. It can be shown and will be developed in detail in Section 4 that this task leads to an eigenvalue problem for the unitary $N \times N$ circular shift matrix J of the following more generally formulated kind: Given a vector $s \in \mathbb{C}^N$ and a unitary $N \times N$ matrix U, where the dimension N is very large and U is sparse, find approximations to the (typically very few) eigenvalues of U which are dominant in s, i.e. if $s = \sum_{k=1}^{N} \beta_k z_k$ is an expansion of s in terms of the eigenvectors

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$z_1, \ldots, z_N$ of U, corresponding to the eigenvalues $e^{\imath\theta_1}, \ldots, e^{\imath\theta_N}$, then the approximations to those eigenvalues $e^{\imath\theta_k}$ are sought for which the weights β_k of the corresponding eigenvectors are much larger in magnitude than the remaining weights.

The Arnoldi method is a well known iterative method for approximating eigenvalues of large and sparse matrices. For a given matrix A and a given vector q_1 with $||q_1||_2 = 1$ it computes the columns $q_1, q_2, \ldots$ of a unitary matrix Q which transforms A into an upper Hessenberg matrix $H = Q^H AQ$. It only requires matrix-vector multiplications, the sparse matrix itself is never modified. Using properties of polynomials that are orthogonal with respect to an inner product on the unit circle (Szegö polynomials) Gragg [14] showed that the Arnoldi method is very special if applied to an isometric operator and he developed an efficient isometric Arnoldi process. Jagels and Reichel presented in [22, 21, 23] an elementary derivation of the isometric Arnoldi process that does not require knowledge of orthogonal polynomials. In [22, 21] the application of the isometric Arnoldi process to the computation of a few eigenvalues and eigenvectors of a large unitary matrix is discussed.

After k steps of the Arnoldi method applied to U and s we get

$$UQ_k = Q_k H_k + (\sigma_k q_{k+1} + (\gamma_k - \gamma_k/|\gamma_k|)\widetilde{q}_k)e_k^T \tag{2}$$

where $Q_k = [q_1, q_2, \ldots, q_k]$ is a rectangular matrix with orthonormal columns and $q_1 = s/\|s\|$. $H_k = H(\gamma_1, \ldots, \gamma_{k-1}, \gamma_k/|\gamma_k|)$ is a unitary upper Hessenberg matrix, given in parameterized form with $|\gamma_j| < 1$ for $j = 1, \ldots k$ (see [15] and also Section 2 and 3). The $\gamma_1, \ldots, \gamma_k$ are called reflection coefficients or Schur parameters and the $\sigma_j \in \mathbb{R}, \sigma_j \geq 0$ are the complementary parameters for γ_j satisfying $|\gamma_j|^2 + |\sigma_j|^2 = 1$.
If $|\gamma_k|$ is close to 1 and therefore $\gamma_k - \gamma_k/|\gamma_k|$ is very small, and $\sigma_k \approx 0$, then the eigenvalues of H_k are in general good approximations to some of the eigenvalues of U which are dominant in s, and it would be desirable to have explicit bounds for the error.

The general question is: Given a unitary matrix U and the sequence of unitary Hessenberg matrices H_k, $k = 0, 1, \ldots$ derived in the isometric Arnoldi process for U. How far are the eigenvalues of an H_k from the eigenvalues of U? The main purpose of this paper is to derive bounds for the corresponding errors.

Note that in order to solve (1) via the isometric Arnoldi method, one has to compute eigenvalues of unitary upper Hessenberg matrices. Special fast and efficient $O(n^2)$ methods exist which make use of the special structure of unitary matrices, see [15, 16, 17, 7, 18, 19].

The paper is organized as follows. Section 2 briefly reviews some well-known properties of unitary (upper Hessenberg) matrices. The isometric Arnoldi method is described in Section 3. Applied to a unitary matrix U it successively computes unitary upper Hessenberg matrices H_k. The eigenvalues of the H_k are increasingly better approximations to eigenvalues of U. An upper bound for the distance of the spectrum of H_k to that of U is given. Furthermore we prove that if the last component of an eigenvector of H_k is small, the corresponding eigenvalue is a good approximation to an eigenvalue of U. An upper bound for the distance between each eigenvalue of H_k and one of U is given. As a consequence we will see that between two eigenvalues of H_k on the unit circle, there lies an eigenvalue of U. Section 4 discusses the signal processing application. The results of Section 3 are applied. Section 5 presents some numerical examples to elucidate the statements of Section 3 and Section 4.

2 Some properties of unitary matrices

Unitary matrices have a rich mathematical structure that is closely analogous to Hermitian matrices. For unitary matrices we can therefore often develop analogues for the good numerical methods and for the theoretical results that exist for the symmetric/Hermitian

eigenvalue problem, which has intensively been studied see, e.g. [28, 13, 20, 26]. In some cases the Cayley transformation helps to develop such analogues.

The one-dimensional Cayley transformation with respect to ρ $x = \imath(\rho+\lambda)^{-1}(\rho-\lambda), |\lambda| = 1$ maps the unit circle one-to-one onto the extended real line. For simplicity let $\rho = 1$. Defining $\theta = arctan[\imath(1+\lambda)^{-1}(1-\lambda)]$ each λ on the unit circle corresponds to an angle $\theta, \theta \in [-\frac{\pi}{2}, \frac{\pi}{2}]$. Hence it is reasonable to define for $\lambda_i, \lambda_j \in \mathbb{C}, |\lambda_i| = |\lambda_j| = 1$

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

This gives a complete ordering of the points on the unit circle with respect to the cutting point $\rho = -1$. 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).

It is well known that any (unitary) $n \times n$ matrix A can be transformed to an upper Hessenberg matrix H by a similarity transformation with a unitary matrix Q. If the first column of Q is fixed and H is an unreduced upper Hessenberg matrix with positive subdiagonal elements, then the transformation is unique. If A is unitary, then the resulting upper Hessenberg matrix H has to be unitary as well. 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, 7, 9, 11, 15, 16, 17, 18, 19, 31] to develop fast algorithms for the solution of 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 $H = H(\gamma_1, \gamma_2, \ldots, \gamma_n) := G_1(\gamma_1)G_2(\gamma_2)\cdots G_{n-1}(\gamma_{n-1})\widetilde{G}_n(\gamma_n) =$

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

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 $\widetilde{G}_n^H G_{n-1}^H \cdots G_2^H G_1^H H = I$. Thus H has a unique factorization of the form

$$H = H(\gamma_1, \gamma_2, ..., \gamma_n) = G_1(\gamma_1)G_2(\gamma_2)\cdots G_{n-1}(\gamma_{n-1})\widetilde{G}_n(\gamma_n). \tag{3}$$

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 [15]. In statistics the Schur parameters are referred to as *partial correlation coefficients* and in signal processing as *reflection coefficients* [2, 9, 10, 25, 29, 30, 32].

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) is used to solve a unitary eigenvalue problem. If λ is an eigenvalue of such an unreduced Hessenberg matrix, then its geometric multiplicity is one [13, 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.

The Arnoldi method for unitary matrices discussed in the next section computes the reflection coefficients directly. After k steps the first k reflection coefficients and a corresponding upper Hessenberg matrix $H'_k = H'_k(\gamma_1, \ldots, \gamma_k)$ are known. These upper Hessenberg matrices H'_k are principal submatrices of the desired $n \times n$ unitary upper Hessenberg matrix $H = H(\gamma_1, \ldots, \gamma_n)$ which is unitarily similar to the given unitary matrix U. Unfortunately principal submatrices of a unitary matrix are in general not unitary. As we will see, it is useful to consider the unitary $k \times k$ Hessenberg matrix $H_k = H_k(\gamma_1, \ldots, \gamma_{k-1}, \zeta_k)$ with $|\zeta_k| = 1$ instead of H'_k. The following theorem relates the eigenvalues of H to those of the unitary Hessenberg matrix H_k, called the *modified kth leading principal submatrix* H_k [12].

Theorem 2.1 *[6, Corollary 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 $\zeta \in \mathbb{C}, |\zeta| = 1$ let*

$$H_k = H_k(\gamma_1, \ldots, \gamma_{k-1}, \zeta) \in \mathbb{C}^{k\times k}, k \in \{2, \ldots, n\}.$$

Then every arc on the unit circle formed by two eigenvalues of H_k contains an eigenvalue of H.

In particular, the above theorem says 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.

Finally we state some results on the dependence of the eigenvalues on the last reflection parameter, for a proof see [6]. To measure the distance between two spectra $\lambda_1, \ldots, \lambda_n$ and $\mu_1, \ldots, \mu_n$ of matrices A and B we use the *eigenvalue variation* $\nu(A, B)$ defined by

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

Theorem 2.2 *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. *$\nu(H_a, H_b) \le |\zeta_a - \zeta_b|$*
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*

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

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

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

Arnoldi method for unitary matrices

input : $U \in \mathbb{C}^{n\times n}$ unitary, $q_1 \in \mathbb{C}^n$ with $||q_1||_2 = 1$
output : $\{\gamma_j\}_{j=1}^{n}, \{\sigma_j\}_{j=0}^{n-1}, Q = [q_1, q_2, \ldots, q_n]$
let $\widetilde{q}_1 = q_1$
for $j = 1, 2, \ldots, n-1$
$\gamma_j = -\widetilde{q}_j^H U q_j$
$\sigma_j = ||Uq_j + \gamma_j \widetilde{q}_j||_2$
$q_{j+1} = \frac{1}{\sigma_j}(Uq_j + \gamma_j \widetilde{q}_j)$
$\widetilde{q}_{j+1} = \sigma_j \widetilde{q}_j + \overline{\gamma_j} q_{j+1}$
end for
$\gamma_n = -\widetilde{q}_n^H U q_n$

Figure 1:

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

3 The Arnoldi Method for unitary matrices

The Arnoldi method is a well known technique for approximating eigenvalues of large and sparse matrices or for building sparse linear equation solvers. Basically it is one of several methods to transform a matrix U into an upper Hessenberg matrix H by a similarity transformation with a unitary matrix Q. The matrices Q and H are built up columnwise from the equation $UQ = QH$ such that after k steps, the factorization

$$UQ_k = Q_k H'_k + f_k e_k^T$$

is computed where $Q_k^H Q_k = I_k$ and $H'_k \in \mathbb{C}^{k\times k}$ is an upper Hessenberg matrix. The vector f_k is the residual vector and is orthogonal to the columns of Q_k. If the norm of f_k is small, the k eigenvalues of H'_k are approximations to k eigenvalues of U. But even if the norm of f_k is not small, some of the eigenvalues of H'_k are typically good approximations to eigenvalues of U. Gragg develops an Arnoldi method for isometric operators in [14]. Here we take a different approach for the development similar to the one of Jagels and Reichel in [22, 21].

If U is unitary then the resulting upper Hessenberg matrix $H = Q^H U Q$ has to be unitary as well. Hence H can be parameterized as $H = H(\gamma_1, ..., \gamma_n)$. Making use of this fact, one can derive an Arnoldi method for unitary matrices which computes the n reflection coefficients γ_k instead of the upper Hessenberg matrix H. This Arnoldi method builds up Q and H from the equation

$$UQe_j = QG_1(\gamma_1)G_2(\gamma_2)\cdots G_{n-1}(\gamma_{n-1})\widetilde{G}_n(\gamma_n)e_j \qquad j = 1, 2, \ldots, n. \tag{4}$$

Let $Qe_1 = q_1$ be given; then we obtain the algorithm given in Figure 1. For a more detailed derivation see, e.g., [22].

After k steps we obtain

$$U[q_1, q_2, \ldots, q_k] = [q_1, q_2, \ldots, q_k]G_1(\gamma_1)\cdots G_{k-1}(\gamma_{k-1})\widetilde{G}_k(\gamma_k) + \sigma_k q_{k+1} e_k^T \tag{5}$$

where $G_j(\gamma_j) \in \mathbb{C}^{k\times k}$ for $j = 1,\ldots,k$, $Q_k^H Q_k = I_k$ ($Q_k = [q_1, q_2, \ldots, q_k]$) and $q_{k+1}^H Q_k = 0$. The auxilary vectors $\widetilde{q}_2, \widetilde{q}_3, \ldots$ can be shown to satisfy

$$\widetilde{q}_k = Q_k G_1 \cdots G_{k-1} e_k \qquad k = 2,\ldots,n \tag{6}$$

and thus

$$\widetilde{q}_k^T q_j = 0 \qquad \text{for all} \quad j > k.$$

In exact arithmetic, the process stops after n steps with $\sigma_n = 0$. In case $\sigma_k = 0$ for $k < n$, an invariant subspace of U is found. Moreover, we know:

Theorem 3.1 *[33, Theorem 2.9] Let*

$$U[q_1, q_2, \ldots, q_k] - [q_1, q_2, \ldots, q_k] G_1(\gamma_1) \cdots G_{k-1}(\gamma_{k-1}) \widetilde{G}_k(\gamma_k) = \sigma_k q_{k+1} e_k^T$$

be a k-step Arnoldi factorization of U with $G_1(\gamma_1) \cdots G_{k-1}(\gamma_{k-1}) \widetilde{G}_k(\gamma_k) \in \mathbb{C}^{k\times k}$ unreduced. Then $\sigma_k = 0$ if and only if $q_1 = Vy$ where $UV = VR$ with $V^H V = I_k$ and R upper triangular of order k.

As pointed out before, if the norm of the residual $f_k = \sigma_k q_{k+1}$ is small, then the k eigenvalues of the $k \times k$ matrix $H_k' = G_1(\gamma_1) \cdots G_{k-1}(\gamma_{k-1}) \widetilde{G}_k(\gamma_k)$ are good approximations to eigenvalues of U. But even if σ_k is not small, typically some eigenvalues of H_k' are good approximations to eigenvalues of U. Unfortunately, H_k' is usually not unitary and therefore its eigenvalues are not on the unit circle. As U is unitary, it seems natural to force the approximating spectrum to lie on the unit circle. This can be done by working with $H_k = G_1(\gamma_1) \cdots G_{k-1}(\gamma_{k-1}) \widetilde{G}_k(\zeta)$ where $|\zeta| = 1$ which can be viewed as a rank one modification of $H_k' = G_1(\gamma_1) \cdots G_{k-1}(\gamma_{k-1}) \widetilde{G}_k(\gamma_k)$. This was already noted by Gragg in [14]. Incorporating H_k into (5) yields

$$UQ_k = Q_k H_k + (\sigma_k q_{k+1} + (\zeta - \gamma_k)\widetilde{q}_k) e_k^T \tag{7}$$

since we see with (6)

$$\begin{aligned} Q_k H_k' &= Q_k H_k + Q_k (H_k' - H_k) \\ &= Q_k H_k + Q_k G_1 \cdots G_{k-1} (\widetilde{G}_k(\gamma_k) - \widetilde{G}_k(\zeta)) \\ &= Q_k H_k + (\zeta - \gamma_k) Q_k G_1 \cdots G_{k-1} e_k e_k^T \\ &= Q_k H_k + (\zeta - \gamma_k) \widetilde{q}_k e_k^T. \end{aligned}$$

Please note :

- While $H_k' = Q_k^H U Q_k$ is the orthogonal projection of U onto the range of Q_k, $H_k = Q_k^H U Q_k \widetilde{G}_k(\frac{\zeta}{\gamma_k})$ in general is not a projection anymore.
- While the residual $\sigma_k q_{k+1}$ in (5) is orthogonal to the columns of Q_k, this is in general no longer true for the residual $\sigma_k q_{k+1} + (\zeta - \gamma_k)\widetilde{q}_k$ in (7).
- While H_k' minimizes the norm of the residual $R(M) = UQ_k - Q_k M$ (where $U \in \mathbb{C}^{n\times n}$ unitary, $Q_k \in \mathbb{C}^{n\times k}$ with $Q_k^H Q_k = I_k$ and $M \in \mathbb{C}^{k\times k}$) (see, e.g., Theorem IV.1.15 in [34]), this is no longer true for H_k.

But we can derive bounds for the distance between the eigenvalues of H_k and suitable eigenvalues of U.

Theorem 3.2 *Let $U \in \mathbb{C}^{n\times n}$ be unitary with eigenvalues $\lambda_1, \ldots, \lambda_n$ and $q_1 \in \mathbb{C}^n$ with $||q_1||_2 = 1$. Assume that k steps of the Arnoldi method for unitary matrices are performed such that*

$$UQ_k = Q_k H_k + (\sigma_k q_{k+1} + (\zeta - \gamma_k)\widetilde{q}_k)e_k^T$$

where $H_k = G_1(\gamma_1)\cdots G_{k-1}(\gamma_{k-1})\widetilde{G}_k(\zeta)$, with $|\zeta| = 1$. Let $\mu_1, \ldots, \mu_k$ be the eigenvalues of H_k and $R(H_k) = UQ_k - Q_k H_k$. Then

$$||R(H_k)||_2 = \sqrt{\sigma_k^2 + |\zeta - \gamma_k|^2},$$

and furthermore,

$$\min_{j\in\{1,\ldots,n\}} |\mu_i - \lambda_j| \leq \sqrt{\sigma_k^2 + |\zeta - \gamma_k|^2} \quad \textit{for} \quad i = 1, \ldots, k.$$

For a suitable permutation Π of $i = 1, \ldots, k$

$$|\mu_i - \lambda_{\Pi(i)}| \leq \sqrt{\sigma_k^2 + |\zeta - \gamma_k|^2}.$$

Proof :

$$\begin{aligned} ||R(H_k)||_2^2 &= ||(\sigma_k q_{k+1} + (\zeta - \gamma_k)\widetilde{q}_k)e_k^T||_2^2 \\ &= (\sigma_k^2 + |\zeta - \gamma_k|^2) \end{aligned}$$

since $\widetilde{q}_k^T q_{k+1} = 0$ and $||q_{k+1}||_2 = ||\widetilde{q}_k||_2 = 1$.

Let $\widetilde{U} = U - R(H_k)Q_k^H$. Then $\|U - \widetilde{U}\|_2 = \|R(H_k)\|_2$ and $\widetilde{U}Q_k = Q_k H_k$, such that $\mu_1, \ldots, \mu_k$ are eigenvalues of $\widetilde{U}$. Therefore by the Bauer-Fike Theorem (see, e.g., [13, Theorem 7.2.2])we obtain for $i = 1, \ldots, k$

$$\min_{j\in\{1,\ldots,n\}} |\mu_i - \lambda_j| \leq \|R(H_k)\|_2 = \sqrt{\sigma_k^2 + |\zeta - \gamma_k|^2}.$$

Define $H(\zeta) = H(\gamma_1, \ldots, \gamma_{k-1}, \zeta, \gamma_{k+1}, \ldots, \gamma_n) \in \mathbb{C}^{n\times n}$ where $|\zeta| = 1$ as before. Let $F = H(\gamma_1, \ldots, \gamma_{k-1}, \gamma_k, \gamma_{k+1}, \ldots, \gamma_n) - H(\zeta)$. Then

$$\begin{aligned} ||F||_2 &= ||G(\gamma_1)\cdots G_{k-1}(\gamma_{k-1})[G_k(\gamma_k) - G_k(\zeta)]G_{k+1}(\gamma_{k+1})\cdots\widetilde{G}_n(\gamma_n)||_2 \\ &= ||G_k(\gamma_k) - G_k(\zeta)||_2 \\ &= \sqrt{\sigma_k^2 + |\zeta - \gamma_k|^2}. \end{aligned}$$

The last statement of the theorem now follows using the following result of Bhatia/Davis [4] :

> *For all constant multiplies $U = \alpha Q$ and $B = \beta V$ of two unitary matrices Q and V we have*
>
> $$\nu(U, B) \leq ||U - B||_2.$$

(When U and B are Hermitian, the above inequality is a classical result of Weyl). This yields

$$\nu(H, H(\zeta)) \leq ||F||_2 = \sqrt{\sigma_k^2 + |\zeta - \gamma_k|^2}.$$

$\surd$

Hence, $\sqrt{\sigma_k^2 + |\zeta - \gamma_k|^2}$ is an upper bound for the distance of the spectrum of H_k to that of U.

Remark 3.3 *The bound for the eigenvalue variation is minimal for* $\zeta = \frac{\gamma_k}{|\gamma_k|}$. *Then*

$$\nu(H, H(\zeta)) \leq \sqrt{2(1 - |\gamma_k|)}.$$

In addition, we can give individual bounds for each eigenvalue of H_k.

Theorem 3.4 *The assumptions are the same as in Theorem 3.2. Let*

$$S_k^H H_k S_k = diag(\mu_1, \ldots, \mu_k)$$

be the Schur decomposition of H_k *and* $Y_k = [y_1, \ldots, y_k] = Q_k S_k \in \mathbb{C}^{n \times k}$. *Then for* $i = 1, \ldots, k$

$$\begin{aligned} \min_{j \in \{1,\ldots,n\}} |\mu_i - \lambda_j| &\leq ||Uy_i - \mu_i y_i||_2 \\ &\leq |s_{ki}| \sqrt{\sigma_k^2 + |\zeta - \gamma_k|^2} \end{aligned}$$

where $S_k = [s_{ij}]_{i,j=1}^k$.

Proof:

Let $r_i = Uy_i - \mu_i y_i$. Then μ_i is an eigenvalue of $(U - r_i y_i^H)$, because $y_i^H y_i = 1$. Therefore from the Bauer-Fike Theorem we obtain

$$\min_{j \in \{1,\ldots,n\}} |\mu_i - \lambda_j| \leq \|r_i y_i^H\|_2 = ||Uy_i - \mu_i y_i||_2 \qquad i = 1, \ldots, k.$$

Now let $S_k = [s_1, \ldots, s_k]$, then $y_j = Q_k s_j$ for $j = 1, \ldots, k$. Since $H_k s_i = \mu_i s_i$ we get

$$\begin{aligned} ||Uy_i - \mu_i y_i||_2 &= ||(UQ_k - Q_k H_k) s_i||_2 \\ &= ||(\sigma_k q_{k+1} + (\zeta - \gamma_k)\widetilde{q}_k) e_k^T s_i||_2 \\ &= |s_{ki}| \; ||\sigma_k q_{k+1} + (\zeta - \gamma_k)\widetilde{q}_k||_2 \\ &= |s_{ki}| \; \sqrt{\sigma_k^2 + |\zeta - \gamma_k|^2}. \end{aligned}$$

$\surd$

The first part of the theorem assures that in each circle around μ_i with radius $||Uy_i - \mu_i y_i||_2$ there is at least one eigenvalue of U. If these circle do not intersect, the eigenvalues of H_k approximate different eigenvalues of U. If two circles intersect, then the corresponding μ might approximate the same eigenvalue of U. The second part of the theorem shows that if the last component of an eigenvector s_i for H_k is small, the eigenpair (μ_i, y_i) is a good approximation to an eigenpair of U.

Analogues of Theorem 3.2 and 3.4 can be given for the unmodified version of the Arnoldi method which compare the eigenvalues of U and H_k'. The bounds are slightly tighter than the ones given here.

A direct consequence of Theorem 2.1 is

Theorem 3.5 *The assumptions are the same as in Theorem 3.2. Then, between two eigenvalues of H_k on the unit circle, there lies an eigenvalue of U.*

Hence, if k steps of the Arnoldi method for unitary matrices are performed and if the last reflection coefficient computed is modified to lie on the unit circle, then we can specify arcs on the unit circle, on which eigenvalues of U must lie. Furthermore, the eigenvalues of H_k and H_{k+1} interlace on the unit circle.

We have seen (Theorem 2.2) that those eigenvalues of H_k whose eigenvectors have a small last component are not sensitive against changes of the last reflection coefficient. These are the eigenvalues which are good approximations to eigenvalues of U (Theorem 3.4). Hence, the choice of the parameter ζ_k is not important for the approximating properties of the eigenvalues. But the parameter ζ_k does influence the distance to an invariant subspace (Theorem 3.2).

Remark 3.6 *The entire discussion given here does not consider rounding errors. In pratice, of course, one has to deal with rounding errors. For example a loss of orthogonality of the computed vectors q_j in the Arnoldi method has to be expected. We believe that the analysis of Paige [27] for these problems in the symmetric case can be carried over to the unitary case.*

4 Computing dominant frequencies of a periodic signal

Consider the problem (1) of finding frequencies $\theta_1, \ldots, \theta_n$ and amplitudes $\rho_1, \ldots, \rho_n$ for a given signal $\{s_k\}_{k=-\infty}^{\infty}$ such that

$$s_k \approx \sum_{\ell=1}^{n} \rho_\ell e^{\imath(k\theta_\ell + \phi_\ell)} \qquad \text{for all } k. \tag{8}$$

The finite subsequence $\{s_k\}_{k=1}^{N}$, $N \gg n$ is explicitly known (measured) and we assume here that the signal is periodic with period N, i.e.

$$s_k = s_{jN+k} \qquad k = 1, \ldots, N, \quad j = \pm 1, \pm 2, \ldots$$

This implies that all frequencies are multiples of $2\pi/N$. We denote by s the signal vector $s = [s_1, \ldots, s_N]^T$.

A simple way to solve the problem is to perform a discrete Fourier transformation of s

$$y = \frac{1}{N} F s, \qquad \text{where} \qquad F = [e^{-\imath(\frac{2\pi k}{N}\ell)}]_{k,\ell=0,\ldots,N-1}. \tag{9}$$

Then

$$s_k = \sum_{\ell=1}^{N} y_\ell e^{\imath(\frac{2\pi k}{N}\ell)} \qquad \text{for all } k, \tag{10}$$

and we could just neglect the terms with very small coefficients y_k in this sum. In order to illustrate the results of the previous chapters, here we will consider methods that determine the unknown quantities via approximating the autocorrelation lags. This may be a useful alternative to the use of the fast Fourier transformation in case $n \ll N$. But it should be noted that there is no guarantee that the approach presented here approximated all n of the desired frequencies.

As the k-th autocorrelation lag of the signal one considers the quantity

$$r_{ss}(k) = \sum_{j=1}^{N} \overline{s_j} s_{j+k}.$$

With the signal s we associate the *n-th order autocorrelation matrix* $T_n(s) = [t_{j-k}]_{j,k=0}^{n-1}$ where

$$t_j := r_{ss}(j) \qquad j = 0, \pm 1, \ldots, \pm(n-1). \tag{11}$$

$T_n(s)$ is a Hermitian positive semidefinite Toeplitz matrix.

It is a common approach to determine n such that $T_{n+1}(s)$ is the smallest dimensional autocorrelation matrix which is almost singular and $\theta_1, \ldots, \theta_n$ and $\rho_1, \ldots, \rho_n$ such that for the signal $\{z_k\}_{k=-\infty}^{\infty}$ with

$$z_k = \sum_{\ell=1}^{n} \rho_\ell e^{\imath(k\theta_\ell)} \qquad \text{for all } k \tag{12}$$

the first n autocorrelation lags match those of the original signal s (see e.g. [9, 10, 24, 25, 29, 32]). This approach assumes that the noise level is small. In the following we show how this problem is related to a large sparse unitary eigenvalue problem.

$T_n(s)$ can obviously be expressed as

$$T_n(s) = [s, Js, \ldots, J^{n-1}s]^H [s, Js, \ldots, J^{n-1}s] \tag{13}$$

where J is the $N \times N$ circular shift matrix

$$J = [e_2, e_3, \ldots, e_N, e_1].$$

Thus T_{n+1} is almost singular if $[s, Js, \ldots, J^n s]$ is almost singular. That is, s lies almost in an n-dimensional invariant subspace of J.

The result of n steps of the isometric Arnoldi method applied to J starting with the initial vector $q_1 = \frac{1}{\|s\|_2} s$ yields (see (7))

$$JQ_n = Q_n H_n + (\sigma_n q_{n+1} + (\zeta - \gamma_n)\widetilde{q}_n)e_n^T, \qquad s = \|s\|_2 Q_n e_1, \tag{14}$$

where $H_n = G_1(\gamma_1) \ldots G(\gamma_{n-1})\widetilde{G}_n(\zeta)$ is a unitary $n \times n$ upper Hessenberg matrix. With (14) we can easily prove that

$$J^k s = \|s\|_2 J^k Q_n e_1 = \|s\|_2 Q_n H_n^k e_1 \qquad \text{for } k < n. \tag{15}$$

Note that because of the special form of $G(\gamma_j)$ and $\widetilde{G}_n(\zeta)$ we have for $k < n$

$$(G_1(\gamma_1) \ldots G(\gamma_{n-1})\widetilde{G}_n(\zeta))^k e_1 = (G_1(\gamma_1) \ldots G(\gamma_{n-1}))^k e_1$$

such that the expressions in (15) do not depend on ζ at all.

Because $Q_n^H Q_n = I$ we see from (14) and (15) that $T_n(s)$ can be written as

$$T_n(s) = \|s\|_2^2 [e_1, H_n e_1, \ldots, H_n^{n-1} e_1]^H [e_1, H_n e_1, \ldots, H_n^{n-1} e_1]. \tag{16}$$

Consider the spectral decomposition of H_n

$$S_n^H H_n S_n = \Lambda = diag(e^{\imath\theta_1}, \ldots, e^{\imath\theta_n}), \qquad S_n^H e_1 = w = [\omega_1, \ldots, \omega_n]^T, \qquad \rho_j > 0,$$

where S_n is unitary. From (16) we get with this eigenvalue information a representation of $T_n(s)$ as

$$T_n(s) = \|s\|_2^2 [w, \Lambda w, \ldots, \Lambda^{n-1} w]^H [w, \Lambda w, \ldots, \Lambda^{n-1} w] \tag{17}$$

and therefore for $j = 0, \ldots, n$

$$t_j = \|s\|_2^2 \sum_{\ell=1}^{n} \omega_\ell^2 e^{\imath(\theta_\ell j)}$$

which is the j-th autocorrelation lag of (12) (up to scaling).

Note that while $T_n(s)$ does not depend on the choice of ζ at all, the quantities $\theta_1, \ldots, \theta_n$ and $\omega_1, \ldots, \omega_n$ do.

Computing the dominant frequencies such that the first autocorrelation lags are matched can thus be interpreted as approximating the eigenvalues of the circular shift J which are dominant in the signal s by the Arnoldi method.

In [30] Reichel and Ammar already propose to compute the dominant frequencies via the eigenproblem for unitary Hessenberg matrices in the following way: Subsequently compute the reflection coefficients $\gamma_1, \gamma_2, \ldots$, (which are all inside the unit circle) associated with the autocorrelation matrices $T_1(s), T_2(s), \ldots$ until you reach a γ_n with magnitude close to 1. Then $\sigma_n \approx 0$ and with $\zeta = \frac{\gamma_n}{|\gamma_n|}$ we get from (14) $JQ_n \approx Q_n H_n$. But then

$$T_{n+1}(s) \approx \|s\|_2^2 [e_1, H_n e_1, \ldots, H_n^n e_1]^H [e_1, H_n e_1, \ldots, H_n^n e_1]$$

and T_{n+1} is almost singular. In fact the latter matrix differs from T_{n+1} only in the position of the n -th autocorrelation lag t_n. Compute the eigenvalues and the first components of the normalized eigenvectors of H_n to achieve the desired frequencies and amplitudes. This is one way of computing the signal approximation in the CSM method [32].

The results of Section 3 can be used to give an estimate for the correctness of the approximation. From Theorem 3.2 we obtain for $H_n = G_1(\gamma_1) \ldots G(\gamma_{n-1}) \widetilde{G}_n(\zeta)$

$$||JQ_n - Q_n H_n(\zeta)||_2 = \sqrt{\sigma_n^2 + |\zeta - \gamma_n|^2}$$

and

$$\min_{j \in \{1,\ldots,N\}} |\theta_k - e^{\imath 2\pi j/N}| \leq \sqrt{\sigma_n^2 + |\zeta - \gamma_n|^2}, \qquad k = 1, \ldots, n.$$

The bounds are minimal for $\zeta = \frac{\gamma_n}{|\gamma_n|}$. If σ_n is small, then for this choice

$$\sqrt{\sigma_n^2 + |\zeta - \gamma_n|^2} = \sqrt{2(1 - |\gamma_n|)}$$

is almost zero, indicating a good approximation. Choosing, e.g., $\zeta = -\gamma_n$, we obtain

$$\sqrt{\sigma_n^2 + |\zeta - \gamma_n|^2} = \sqrt{2(1 + |\gamma_n|)}$$

which is almost 2 if σ_n is small. Thus the way γ_n is modified to lie on the unit circle does influence the quality of the approximation.

From Theorem 2.2 we obtain, that those eigenvalues of H_n whose eigenvectors have a small last component, are not sensitive to changes of the last reflection coefficient. By Theorem 3.4, these are the eigenvalues that are good approximations to eigenvalues of J.

Let $e^{\imath\theta_j}$, $j = 1, \ldots, n$ be the eigenvalues of H_n, then the θ_j are used as approximations to the dominant frequencies of s. The bounds in Theorem 2.2 and 3.4 also give bounds for the errors. A simple calculation yields

Corollary 4.1 *Assume that n steps of the Arnoldi method are applied to J and s such that*

$$JQ_n = Q_n H_n(\zeta) + (\sigma_n q_{n+1} + (\zeta - \gamma_n)\widetilde{q}_n)e_n^T$$

where $H_n(\zeta) = G_1(\gamma_1)\cdots G_{n-1}(\gamma_{n-1})\widetilde{G}_n(\zeta)$, $\zeta \in \mathbb{C}, |\zeta| = 1$. The eigenvalues of J are $e^{\imath 2\pi j/N}, j = 1,\ldots,N$. Let $\zeta_a, \zeta_b \in \mathbb{C}, |\zeta_a| = |\zeta_b| = 1$. Let $e^{\imath\lambda_j}$ be the eigenvalues of $H_n(\zeta_a)$ and $e^{\imath\delta_j}$ be those of $H_n(\zeta_b)$, $j = 1,\ldots,n$. Let

$$S_n^H H_n(\zeta_a) S_n = diag(e^{\imath\lambda_1},\ldots,e^{\imath\lambda_n})$$

be the Schur decomposition of $H_n(\zeta_a)$, $S_n = [s_{ij}]_{i,j=1}^n$. Then for $i = 1,\ldots,n$

$$\min_{j\in\{1,\ldots,k\}} |\lambda_i - \delta_j| \leq arccos(\frac{2 - |\zeta_a - \zeta_b|^2\ |s_{ni}|^2}{2}).$$

Furthermore,

$$\min_{j\in\{1,\ldots,N\}} |\lambda_i - 2\pi j/N| \leq arccos(\frac{2 - \sigma_n^2 + |\zeta_a - \zeta_b|^2}{2})$$

and

$$\min_{j\in\{1,\ldots,N\}} |\lambda_i - 2\pi j/N| \leq arccos(\frac{2 - |s_{ni}|^2(\sigma_n^2 + |\zeta_a - \zeta_b|^2)}{2}).$$

5 Numerical Examples

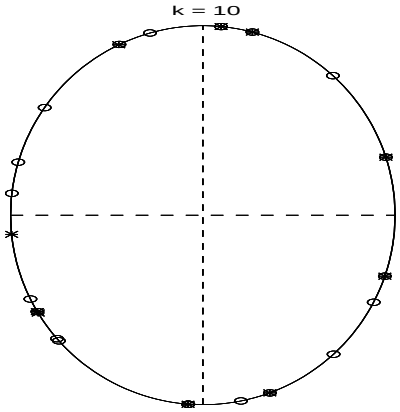
In this section numerical experiments are presented to demonstrate the statements of Section 3 and Section 4. First the eigenvalues of a unitary upper Hessenberg matrix H are compared with the eigenvalues of modified kth leading principal submatrices H_k. All statements of Section 3 can be observed clearly :

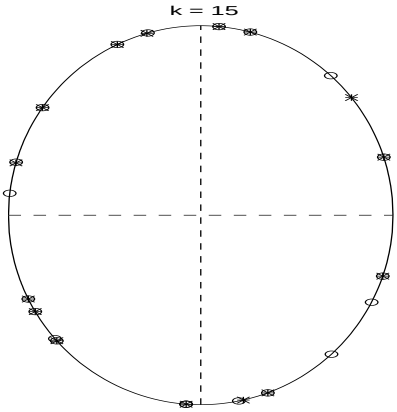
- Between two eigenvalues of H_k on the unit circle there lies an eigenvalue of H (Theorem 2.1).
- If the last component of an eigenvector of H_k is small, then the corresponding eigenvalue is a good approximation to an eigenvalue of H (Theorem 3.4).
- The approximating properties of the eigenvalues of H_k vary only slightly with the choice of the modified reflection coefficient (Theorem 2.2).

In the second part of this section, two examples illustrate the discussion in Section 4. All computations were done using MATLAB on a SUN SparcStation 10 with machine precision $\epsilon \approx 2.2204e-16$.

The first set of tests was performed to demonstrate the statements of Section 3. 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 eigenvalues 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 each eigenvalue μ_j the minimal distance to an eigenvalue of H and the error bound given in Theorem 3.4 was computed.

For the first example $\zeta_k = \frac{\gamma_k}{|\gamma_k|}$ was chosen as the bound for the eigenvalue variation is minimal for this choice of ζ_k (see Remark 3.3). The eigenvalues of H and H_k are plotted for $k = 10$ and $k = 15$ in the following figure. The eigenvalues of H are marked by 'o', the eigenvalues of H_k by '*'.





Although $\sigma_{10} = 0.58940774002982$ and $\sigma_{15} = 0.87680954800405$ are not small, some of the eigenvalues of H_{10} and H_{15} are good approximations to eigenvalues of H. In Theorem 3.4 it was proven that if the last component of an eigenvector of H_k is small, then the corresponding eigenvalue is a good approximation to an eigenvalue of H. Individual bounds for the minimal distance of each eigenvalue of H_k to the eigenvalues λ_j of H can be given

$$\min_{j\in\{1,\ldots,n\}} |\mu_i - \lambda_j| \leq |s_{ki}| \ \sqrt{\sigma_n^2 + |\zeta - \gamma_n|^2} =: ub_i$$

where $s_{\ell i}, \ell \in \{1,\ldots,k\}$ is the ℓth component of the eigenvector to the ith eigenvalue of H_k. The following tables report the minimal distance between each eigenvalue of H_k and the eigenvalues λ_j of H as well as the above error bounds for $k = 10$ and $k = 15$.

$k = 10, \sqrt{\sigma_k^2 + |\zeta - \gamma_k|^2} \approx 0.6199$

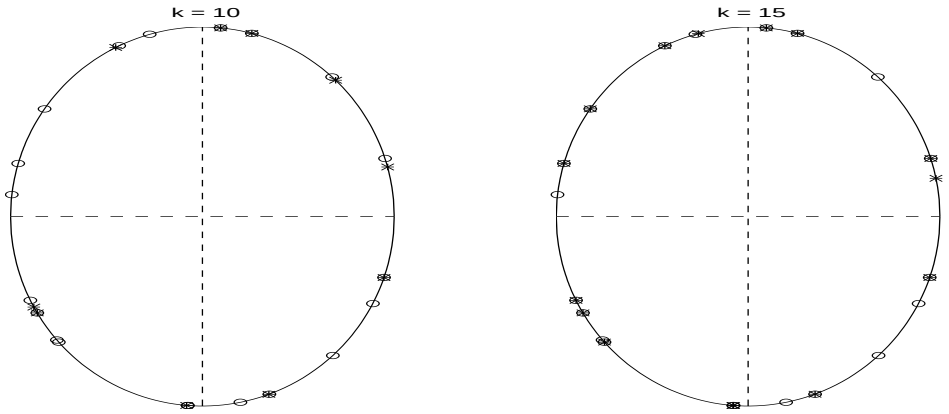
	$min\|\mu_i - \lambda_j\|$	ub_i
μ_1	1.0071e-07	4.1381e-04
μ_2	2.7263e-06	2.3746e-03
μ_3	2.4649e-04	4.8555e-02
μ_4	2.9825e-06	6.3154e-03
μ_5	3.9244e-03	5.6481e-02
μ_6	2.0610e-04	2.3190e-02
μ_7	3.5094e-04	4.0212e-02
μ_8	8.2207e-05	1.8990e-02
μ_9	8.4617e-03	1.9755e-01
μ_{10}	2.1661e-01	5.8068e-01

$k = 15, \sqrt{\sigma_k^2 + |\zeta - \gamma_k|^2} \approx 1.0189$

	$min\|\mu_i - \lambda_j\|$	ub_i
μ_1	4.2658e-10	2.1653e-05
μ_2	7.4752e-07	4.4540e-04
μ_3	5.5443e-08	4.2885e-04
μ_4	5.9287e-04	3.6914e-03
μ_5	3.5522e-09	3.0701e-05
μ_6	1.6636e-05	2.5023e-03
μ_7	2.3986e-02	5.7894e-01
μ_8	4.2465e-08	3.9597e-04
μ_9	1.4195e-12	9.4849e-06
μ_{10}	7.6101e-11	3.9866e-05
μ_{11}	3.7732e-03	7.7117e-02
μ_{12}	2.6922e-04	2.5062e-02
μ_{13}	4.9946e-06	5.0100e-03
μ_{14}	5.3077e-03	1.9032e-01
μ_{15}	1.5772e-01	8.1260e-01

Comparing the actual minimal distance with the error bound one observes that the approximations are much better than the error bound predicts. Another observation is that a small last component and hence a small individual error bound for the eigenvalues indicates good eigenvalue approximations.

For the second example a random complex number $\zeta_k, |\zeta_k| = 1$ was chosen; hence the bound for the eigenvalue variation is not minimal (see Remark 3.3). The following figure and tables display the same information as before.



$k = 10, \sqrt{\sigma_k^2 + |\zeta - \gamma_k|^2} \approx 1.8211$

	$min\|\mu_i - \lambda_j\|$	ub_i
μ_1	1.9902e-06	2.7057e-03
μ_2	8.9514e-05	2.1656e-02
μ_3	4.6934e-02	5.5107e-01
μ_4	3.8414e-04	3.5758e-02
μ_5	1.9734e-02	1.6406e-01
μ_6	2.6689e-03	6.2874e-02
μ_7	5.0207e-03	7.8979e-02
μ_8	1.2924e-05	2.9484e-03
μ_9	3.5443e-02	1.2436e-01
μ_{10}	2.4899e-02	1.7200e+00

$k = 15, \sqrt{\sigma_k^2 + |\zeta - \gamma_k|^2} \approx 1.1519$

	$min\|\mu_i - \lambda_j\|$	ub_i
μ_1	9.3659e-10	3.5684e-05
μ_2	1.1929e-05	4.3049e-02
μ_3	3.1109e-09	1.8487e-04
μ_4	6.0705e-04	5.8196e-03
μ_5	2.6543e-09	4.4310e-05
μ_6	1.0846e-05	3.5051e-03
μ_7	1.5657e-02	1.6624e-01
μ_8	3.0403e-07	1.3257e-03
μ_9	4.4982e-11	7.4116e-06
μ_{10}	7.9706e-10	2.7398e-05
μ_{11}	6.5638e-04	8.6970e-02
μ_{12}	1.6478e-04	2.6234e-02
μ_{13}	8.6488e-06	4.1257e-03
μ_{14}	2.5703e-03	7.6717e-01
μ_{15}	1.0814e-01	8.3703e-01

Although the choice of ζ_k is not optimal, we essentially obtain the same results as before. The eigenvalue approximation is much better than the error bound predicts.

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. If the last component of an eigenvector is small, then the approximation is good no matter how ζ_k is chosen. The best results are obtained for $\zeta_k = \frac{\gamma_k}{|\gamma_k|}$. We omitted an example to demonstrate that if the last component of an eigenvector is not small, then the quality of the eigenvalue approximation depends on the choice of ζ_k. Further it can be seen that between two eigenvalues of H_k on the unit circle there lies an eigenvalues of H (due to the poor resolution, this is very hard to see in the figures presented here).

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. Also, some eigenvalues of the unmodified leading principal submatrices are good approximations to eigenvalues of H.

The following two examples illustrate the discussion given in Section 4. In both examples, the length N of the signal is 1000 and the s_k have the form

$$s_k = \sum_{\ell=1}^{5} \rho_\ell e^{ik\theta_\ell} + \alpha v_k$$

where v_k is a random number (uniformly distributed in $(0,1)$) which represents noise, $\alpha \in \mathbb{R}$ is a scalar and $\theta_\ell = 2\pi m_\ell / N$ where $m_\ell \in \{1,\ldots,N\}, m_\ell \neq m_j$ for $\ell \neq j, \ell, j \in \{1,\ldots,5\}$. In each example, the signal vector $s = [s_1,\ldots,s_N]^T$ is formed and 5 steps of the Arnoldi method are applied to J and s. This yields a unitary upper Hessenberg matrix $H_5 = H_5(\gamma_1,\ldots,\gamma_4,\gamma_5/|\gamma_5|)$. In case $\alpha = 0$ (that is, no noise), we know from Theorem 3.1 that the eigenvalues of H_5 have to be $\theta_1,\theta_2,\ldots,\theta_5$. Hence for small noise, we expect that the eigenvalues of H_5 are good approximations to the desired $\theta_j, j = 1,\ldots,5$. Therefore the eigendecomposition of H_5 is computed. Estimates $\widetilde{\theta}_\ell$ and $\widetilde{\rho}_\ell$ for the frequencies and amplitudes are obtained from the eigenvalues and the first components of the eigenvectors, respectively. Corollary 4.1 gives an upper bound for the distance of $\widetilde{\theta}_\ell$ to $2\pi j/N$:

$$\min_{j\in\{1,\ldots,N\}} |\widetilde{\theta}_i - 2\pi j/N| \leq arccos(\frac{2-|s_{5i}|^2(\sigma_5^2+|\zeta-\gamma_5|^2)}{2}) =: acos_i$$

where s_{5i} denotes the last entry of the ith eigenvector. For each example the actual minimal distance of $\widetilde{\theta}_\ell$ to $\theta_j, j = 1,\ldots,5$ is computed as well as $acos_\ell$ for $\ell = 1,\ldots,5$. As we do not know of an error bound for the amplitudes, we just compute the distance between $\widetilde{\rho}_\ell$ and ρ_ℓ.

For the first example

$$s_k = 1.2e^{2\pi\imath 5k/N} + 3.5e^{2\pi\imath 37k/N} + 5.7e^{2\pi\imath 271k/N} + 0.3e^{2\pi\imath 400k/N} + 2.1e^{2\pi\imath 979k/N} + \alpha * v_k$$

for different $\alpha \in \mathbb{R}$ was chosen. The frequencies are well separated. Table 1 lists the results for this example. Not surprisingly, the smaller the perturbation (αv_k), the better are the approximations. The approximations of the frequencies are much better than the upper bounds indicate. For small perturbations the upper bounds $acos_i$ overestimate the approximation error by several powers of 10. The method seems to approximate the amplitudes with about the same accuracy as the frequencies.

In praxis, of course, we would not know the exact value of n, the number of frequencies and amplitudes needed to express the signal as a sum of exponentials. The above results indicate that a rule of thumb could be to let the Arnoldi method run until a σ_j is obtained which is smaller than some given tolerance. The quality of the approximation depends on σ_j, the biggest perturbations observed are of about the same size as σ_j.

For the second example we modified the signal of the first example a little bit. The second frequency was chosen to be as close as possibly to the first one, the second amplitude to be the same as the first one

$$s_k = 1.2e^{2\pi\imath 5k/N} + 1.2e^{2\pi\imath 6k/N} + 5.7e^{2\pi\imath 271k/N} + 0.3e^{2\pi\imath 400k/N} + 2.1e^{2\pi\imath 979k/N} + \alpha * v_k.$$

Table 2 displays the same information as the table for the last example.

	$min\|\widetilde{\theta}_i - \theta_j\|$	$acos_i$	$\|\widetilde{\rho}_i - \rho_i\|$	
θ_1, ρ_1	5.3429e-16	2.9802e-08	3.1919e-15	
θ_2, ρ_2	4.4409e-16	7.3000e-08	4.4964e-15	
θ_3, ρ_3	4.4409e-16	1.1921e-07	2.2204e-16	α =1e-12, σ_5 = 1.9029e-13
θ_4, ρ_4	2.2204e-15	4.1215e-07	6.3838e-16	
θ_5, ρ_5	2.9976e-15	$< \epsilon$[1]	8.2157e-15	
θ_1, ρ_1	3.9862e-09	8.7236e-06	7.4678e-09	
θ_2, ρ_2	9.3195e-11	2.2166e-05	4.8939e-10	
θ_3, ρ_3	2.0961e-13	3.5988e-05	5.7692e-09	α =1e-06, σ_5 = 1.7417e-08
θ_4, ρ_4	4.5526e-11	1.2471e-04	1.0905e-08	
θ_5, ρ_5	4.1067e-10	9.6880e-07	1.3765e-08	
θ_1, ρ_1	3.9882e-03	8.7095e-03	8.8594e-04	
θ_2, ρ_2	9.1643e-05	2.1697e-02	3.4548e-04	
θ_3, ρ_3	2.0874e-07	3.6867e-02	5.7266e-06	α =1e-03, σ_5 = 1.7218e-02
θ_4, ρ_4	4.5350e-05	1.2412e-01	8.9389e-06	
θ_5, ρ_5	4.2181e-04	9.6624e-04	1.1025e-03	
θ_1, ρ_1	8.9834e-03	8.6531e-02	1.2463e-01	
θ_2, ρ_2	6.9043e-03	1.2295e-01	1.4979e-02	
θ_3, ρ_3	2.0030e-05	3.4552e-01	5.8261e-04	α =1e-01, σ_5 = 4.4414e-01
θ_4, ρ_4	5.8260e-02	6.1589e-01	2.8760e-02	
θ_5, ρ_5	1.8972e-02	2.4824e-01	2.2939e-02	

Table 1

	$min\|\widetilde{\theta}_i - \theta_j\|$	$acos_i$	$\|\widetilde{\rho}_i - \rho_i\|$	
θ_1, ρ_1	9.0206e-16	$< \epsilon$[1]	2.4231e-14	
θ_2, ρ_2	9.5063e-16	$< \epsilon$[1]	2.5424e-14	
θ_3, ρ_3	6.6613e-16	1.7881e-07	2.2204e-16	α= 1e-12, σ_5 = 6.6169e-14
θ_4, ρ_4	3.1086e-15	1.8492e-07	4.9960e-16	
θ_5, ρ_5	1.6653e-15	$< \epsilon$[1]	5.4401e-15	
θ_1, ρ_1	3.3104e-06	7.6164e-06	9.6212e-05	
θ_2, ρ_2	3.0650e-06	6.9887e-05	9.6170e-05	
θ_3, ρ_3	1.4011e-13	3.4954e-03	2.9009e-09	α=1e-06, σ_5 = 2.5320e-05
θ_4, ρ_4	3.4072e-11	3.6190e-03	9.6212e-05	
θ_5, ρ_5	1.5243e-09	7.9760e-07	4.9885e-09	
θ_1, ρ_1	3.4452e-05	4.2054e-03	1.4254e-01	
θ_2, ρ_2	3.0314e-03	3.3297e-03	7.8585e-02	
θ_3, ρ_3	1.3990e-08	4.2764e-03	3.0402e-06	α=1e-03, σ_5 = 4.7117e-01
θ_4, ρ_4	3.4482e-06	7.5652e-01	4.7361e-02	
θ_5, ρ_5	1.8417e-03	2.7975e-02	1.1769e-04	
θ_1, ρ_1	1.6441e-02	2.3596e-01	1.4217e-01	
θ_2, ρ_2	1.2527e-02	2.2402e-01	1.1270e-01	
θ_3, ρ_3	2.2631e-05	2.7498e-01	1.7099e-03	α =1e-01, σ_5= 4.0455e-01
θ_4, ρ_4	4.0867e-02	5.3145e-01	3.3385e-02	
θ_5, ρ_5	1.9591e-01	1.7553e-01	2.5918e-02	

Table 2

[1] $\epsilon \approx 2.2204e-16$

The method has difficulties to approximate the first two frequencies and amplitudes. The results for these approximations have been better in the previous example, where the first two frequencies and amplitudes were much better separated. The actual approximation error for the first two frequencies are only of the order of the error estimate.

6 Concluding Remarks

Some properties of the isometric Arnoldi method have been discussed. The Arnoldi method applied to a unitary matrix U yields after k steps

$$UQ_k = Q_k H'_k + \sigma_k q_{k+1} e_k^T$$

where $H'_k = G_1(\gamma_1) \cdots G_{k-1}(\gamma_{k-1}) \widetilde{G}_k(\gamma_k)$, $Q_k^H Q_k = I_k$, and $q_{k+1}^H Q_k = 0$. If γ_k is modified to lie on the unit circle, one obtains

$$UQ_k = Q_k H_k + (\sigma_k q_{k+1} + (\zeta - \gamma_k)\widetilde{q}_k) e_k^T$$

where $H_k = G_1(\gamma_1) \cdots G_{k-1}(\gamma_{k-1}) \widetilde{G}_k(\zeta)$, $|\zeta| = 1$ is a unitary upper Hessenberg matrix. The distance of the approximation to an invariant subspace of U given by H_k was determined. (Individual) error bounds for the eigenvalues of H_k were derived.

In [1] it was noted that there is a simple equivalence transformation which transforms $H = G_1 \cdots G_{n-1} \widetilde{G}_n$ to $G_o G_e^H$ where G_o and G_e are block diagonal unitary matrices with block size at most two, G_o is the product of all the odd numbered reflectors and G_e is the product of all the even numbered reflectors. Bohnhorst makes use of this fact in [5] to derive a Lanczos-like algorithm to transform a unitary matrix U to $G_o G_e^H$. She gives eigenvalue bounds similar to the ones presented here.

A problem in signal processing and its connection to the isometric Arnoldi method was discussed in detail.

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