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**Ritz Values and Arnoldi Convergence for
Nonsymmetric Matrices**

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ABSTRACT

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The restarted Arnoldi method, useful for determining a few desired eigenvalues of a matrix, employs shifts to refine eigenvalue estimates. In the symmetric case, using selected Ritz values as shifts produces convergence due to interlacing. For nonsymmetric matrices the behavior of Ritz values is insufficiently understood, and hence no satisfactory general convergence theory exists. Towards developing such a theory, this work demonstrates that Ritz values of nonsymmetric matrices can obey certain geometric constraints, as illustrated through careful analysis of Jordan blocks. By constructing conditions for localizing the Ritz values of a matrix with one simple normal wanted eigenvalue, this work develops sufficient conditions that guarantee convergence of the restarted Arnoldi method with exact shifts. As Ritz values are the basis for many iterative methods for determining eigenvalues and solving linear systems, an understanding of Ritz value behavior for nonsymmetric matrices has the potential to inform a broad range of analysis.

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Chapter 1

Introduction

This thesis analyzes the behavior of Ritz values and convergence of the restarted Arnoldi method for nonsymmetric matrices. Understanding the behavior of Ritz values is essential to establishing convergence of methods for approximating eigenvalues. In the symmetric case, for which much is known, convergence of the restarted Arnoldi method with exact shifts follows from the interlacing property of Ritz values. In the nonsymmetric case, the restarted Arnoldi method with exact shifts performs well in practice. Researchers have observed typical patterns of behavior for Ritz values, but these are not sufficiently understood to establish criteria for convergence. In this thesis I analyze nonsymmetric matrices for which the Ritz values can be localized. This information will then be used to develop sufficient criteria for convergence of the restarted Arnoldi method with exact shifts for these nonsymmetric matrices. Specifically, the criteria will address constraints on the starting vector and the spectral properties of the original matrix.

1.1 Eigenvalues

The restarted Arnoldi method is an indispensable tool for determining a few selected eigenvalues of a matrix, such as those with the largest real part. Eigenvalues provide insight into the behavior of dynamical systems. They indicate how modeled features will grow, decay or oscillate. An important use of eigenvalues is to deter-

mine the stability of the system $x'(t) = Ax(t)$. No real world system can sustain the constant growth of a modeled feature that correspond to eigenvalues with positive real part. Similarly, undamped oscillations associated with purely imaginary eigenvalues, when coupled with resonant driving forces, can lead to unsustainable behavior. The determination of system stability typically involves the computation of only a few of the eigenvalues. This is fortunate, as it limits the work needed to solve real-world problems; moreover, many of the eigenvalues of the matrix can be spurious approximations to the true eigenvalues of an underlying infinite dimensional operator.

To determine eigenvalues of a matrix A of order n , one must determine x and λ such that

$$Ax = x\lambda$$

where x , the eigenvector, is a nonzero vector of order n and λ , the eigenvalue, is a complex scalar. The vector x and scalar λ are said to be an eigenpair and are denoted (x, λ) . The set of all eigenvalues of a matrix is called the spectrum of the matrix, denoted by $\sigma(A)$. A space spanned by eigenvectors is called an eigenspace. Eigenvalues can be characterized as roots of the characteristic polynomial,

$$p_A(\lambda) = \det(\lambda I - A).$$

The roots of the characteristic polynomial correspond to the values for which $\lambda I - A$ is singular, which means that $\lambda I - A$ has a nontrivial null space. As the roots of polynomials of order greater than five cannot generally be determined in a finite number of steps, eigenvalues must be determined iteratively.

1.2 Krylov Subspaces

The Arnoldi method approximates eigenvalues by orthogonally projecting a matrix onto a subspace. The performance and analysis of many iterative methods for eigenvalues and systems of equations relies on Krylov subspaces. A Krylov subspace is spanned by the iterates of the power method,

$$K_k(A, v) = \text{span}\{v, Av, A^2v, \dots, A^{k-1}v\},$$

where v is the starting vector. The power method itself is an eigenvalue method that approximates the eigenvector associated with a distinct, largest-magnitude eigenvalue, if such an eigenvalue exists. The power method approximates the vector that $A^k v$ approaches (in angle), the desired eigenvector, as k becomes large. A Krylov subspace contains not only all power method iterates, but it contains all shifted power method iterates $(A - \sigma I)^i v$ for any complex σ , $i = 1, \dots, k - 1$. As a Krylov subspace is larger than the span of any single power method iterate, $(A - \sigma I)^i v$, provided that the starting vector v is not an eigenvector, the Krylov subspace should offer a better approximation to desired eigenspaces than any single vector method. Subspaces are particularly useful for eigenvalue estimation when the size of the matrix prohibits dense eigenvalue methods, and also when the number of eigenvalues desired makes single vector iteration/deflation techniques impractical.

1.3 Ritz Values

Eigenvalue approximations from a subspace are known as Ritz values. The set of all possible Ritz values is known as the *numerical range* or *field of values* of a matrix. The numerical range of $A \in \mathbb{C}^{n \times n}$ is

$$W(A) \equiv \{x^*Ax : x \in \mathbb{C}^n, x^*x = 1\}.$$

Hence the numerical range is the set of all possible Rayleigh quotients of a matrix. Methods for sketching the numerical range make use of the following property: the Hermitian part of A , $H(A) \equiv \frac{1}{2}(A + A^*)$, satisfies $W(H(A)) = \text{Re } W(A)$, where Re denotes the real part. Hence the boundary of the numerical range of A can be determined by computing $W(H(e^{i\theta}A))$ for various values of θ . Ritz values have numerous interesting properties. The Ritz value associated with v is the scalar θ such that $Av - \theta v$ is orthogonal to the space spanned by v , i.e., $v^*(Av - \theta v) = 0$. A Ritz value is optimal in the sense that it minimizes the norm of $Av - \theta v$. The Ritz value represents the action of A restricted to the subspace spanned by v . For a Ritz value to be a good approximation to an eigenpair, the residual $Av - \theta v$ should be small. For Ritz values generated from a subspace spanned by the columns of a matrix V , the residual is orthogonal not only to the Ritz vector, but also to any vector in the subspace. Hence

$$V^*(Ax - x\theta) = 0.$$

Since any $x \in \text{Ran}(V)$ can be written as Vy ,

$$V^*(AVy - Vy\theta) = 0,$$

which is written as

$$Hy = V^*Vy\theta,$$

where $H = V^*AV$. Thus the problem of determining Ritz values from a subspace is equivalent to solving the generalized eigenvalue problem $Hy = V^*Vy\theta$. If the columns of V are orthonormal, then $V^*V = I$, and the problem of determining Ritz values from a subspace reduces to an ordinary eigenvalue problem.

1.4 The Arnoldi Method

The Arnoldi method determines Ritz values by generating an orthonormal basis for the Krylov subspace. The Arnoldi method was introduced in the early 1950s by W.E. Arnoldi [1] as a generalization of the Lanczos method for symmetric matrices [12]. Though both Lanczos and Arnoldi recognized that their methods had some iterative potential, at the time they were proposed both methods were seen primarily as ways of reducing a matrix to tridiagonal or upper Hessenberg form by a unitary similarity transformation [16]. In the symmetric case, for which the eigenvalues all fall on the real line, in their most basic form Sturm sequence methods determine eigenvalues by repeatedly evaluating the characteristic polynomial, locating eigenvalues by noting sign changes. The idea of the Arnoldi and Lanczos methods was that the evaluation of the characteristic polynomial is much simpler for such structured matrices. However, numerical instabilities in the methods lead to inaccuracies in the reduced matrices that limit the ability to accurately determine eigenvalues. As result, until the 1970s neither method received much attention as anything other than a procedure for reducing a matrix to tridiagonal or upper Hessenberg form (see, e.g. Wilkinson [26]).

The utility of the Arnoldi and Lanczos methods comes from their ability to generate accurate eigenvalue approximations from a partial rather than full upper Hessenberg factorization of a matrix. Both the Arnoldi and Lanczos methods work by generating an orthonormal basis for the Krylov subspace. Each step of the Arnoldi method generates a new basis vector v_i such that $\|v_i\| = 1$ and $v_i \perp K_j(A, v)$ for $j < i$ and $v_i \in K_i(A, v)$. At the k th step, the columns of the matrix $V_k = [v_1, v_2, \dots, v_{k-1}, v_k]$ span the k th Krylov subspace. Based on these properties, the v_i must satisfy

$$Av_i = \sum_{j=1}^i h_{ji} v_j + h_{i+1,i} v_{i+1}.$$

This recurrence is a consequence of the nesting of Krylov subspaces, $K_k(A, v) \subseteq K_{k+1}(A, v)$. Combining these recurrence equations into a matrix equation, A and V_k must satisfy

$$AV_k = V_k H_k + h_{k+1,k} v_{k+1} e_k^*,$$

where $[H_k]_{ij} = h_{ij}$ is an upper Hessenberg matrix, the orthogonal restriction of A onto the k th Krylov subspace. Similar to the optimality of the Ritz values, H_k is optimal in that it minimizes the norm of $AV_k - V_k H$ over all H [23]. If $h_{k+1,k} = 0$, the columns of V_k span an eigenspace of A . If $h_{k+1,k}$ is small, then the entire k th Krylov subspace approximates well an eigenspace of A . Even if $h_{k+1,k}$ is large, there may be Ritz pairs that are good approximations to eigenvalues. The residual for a Ritz pair, $x = V_k y$ and θ , obeys

$$\begin{aligned} Ax - \theta x &= AV_k y - \theta V_k y \\ &= V_k H_k y + h_{k+1,k} v_{k+1} e_k^* y - \theta V_k y \\ &= \theta V_k y + h_{k+1,k} v_{k+1} e_k^* y - \theta V_k y \\ &= h_{k+1,k} v_{k+1} e_k^* y, \end{aligned}$$

and hence $\|Ax - \theta x\| = |h_{k+1,k}| |e_k^* y|$. Thus if together the product of $|h_{k+1,k}|$ and the k th component of y are small, then x and θ are likely to be a good approximation to an eigenpair. The matter of how small $|h_{k+1,k}|$ must be to ensure that the Ritz values are good approximations to eigenvalues depends on the sensitivity of the spectrum to perturbations. The sensitivity to perturbations can be measured using the pseudospectra of the matrix [25].

The ϵ -pseudospectrum of a matrix for a given $\epsilon > 0$ is the set of λ in the complex plane for which there exists some $E \in \mathbb{C}^{n \times n}$ with $\|E\| < \epsilon$ such that λ is an eigenvalue

of $A + E$, i.e.,

$$\sigma_\epsilon(A) = \{\lambda \in \mathbb{C} : \exists E \text{ with } \|E\| < \epsilon \text{ and } \lambda \in \sigma(A + E)\}.$$

Every Arnoldi Ritz value is in the ϵ -pseudospectrum of A for all $\epsilon > |h_{k+1,k}|$. To see this, take $E = -h_{k+1,k}v_{k+1}v_k^*$. From the perspective of pseudospectra, the bound on how accurate a Ritz pair can be for a given $h_{k+1,k}$ is reflected in how large the ϵ -pseudospectrum of A is relative to the spectrum of A . For a normal matrix, (i.e., $A^*A = AA^*$), the ϵ -pseudospectrum for a given ϵ consists of the union of open disks in the complex plane centered about the eigenvalues. Hence small perturbations to a normal matrix produce small changes to the eigenvalues. In this case the eigenvalues are said to be well conditioned. For a nonnormal matrix the pseudospectra can differ significantly from the spectrum. The condition of the eigenvalues may vary; some may be more sensitive to perturbations than others. Typical applications require approximating well-conditioned eigenvalues, which can be complicated by nonnormality associated with the remaining eigenvalues.

1.5 The Restarted Arnoldi Method

The advantage of both the Arnoldi and Lanczos methods is that the Hessenberg factorization can be updated incrementally with the size of the Krylov subspace. The primary difficulty with these methods is maintaining the orthogonal basis. The cost of doing so increases steadily as the dimension of the subspace increases. The costs of maintaining orthogonality and of storing the basis vectors are the primary reasons why these methods must be restarted. Loss of orthogonality in the symmetric case is particularly acute, as the Lanczos method works on the assumption that basis vectors satisfy a three-term recurrence, a huge advantage, as the method only

stores three basis vectors at any one time. However, the three-term recurrence is only true in exact arithmetic. In floating point arithmetic, more must be done to maintain orthogonality. The problem also worsens when the subspace develops a good approximation of a particular eigenvalue. Without modification, the Lanczos method can lead to dubious eigenvalue estimates. In the 1970s Paige and Parlett determined the necessary modifications to the Lanczos method for addressing the loss of orthogonality due to floating point arithmetic [16, 14]. The knowledge and insight developed for Lanczos set the stage for Saad to introduce the restarted Arnoldi method as a means of calculating a few eigenvalues of a nonsymmetric matrix [17].

The impact of Saad's paper on the restarted Arnoldi method was threefold. First, Saad provided an alternative eigenvalue algorithm. At the time, subspace iteration (then also known as simultaneous iteration) was the prominent iterative method for determining several eigenvalues of a nonsymmetric matrix. Subspace iteration is a generalization of the power method to subspaces. Unlike the original Arnoldi method, which requires ever larger subspaces and hence more memory and computation to improve eigenvalue approximations, the restarted Arnoldi method (like subspace iteration) works to refine an approximate eigenspace.

Second, Saad provided the first *a priori* convergence bounds for the approximation of eigenvectors of nonsymmetric matrices from a Krylov subspace. Assuming that the eigenvalues of A are simple and that the starting vector represented in a normalized eigenvector basis $\{u_j\}$ is $v = \sum_{j=1}^N \alpha_j u_j$, then provided that $\alpha_i \neq 0$, the norm of the residual of the projection of the eigenvector u_i onto the Krylov subspace is bounded as

$$\|(I - V_k V_k^*)u_i\| \leq \delta_i \min_{\substack{p \in P_k \\ p(\lambda_i)=1}} \max_{\substack{j=1,2,\dots,N \\ j \neq i}} |p(\lambda_j)|,$$

where $\delta_i = \sum_{j=1, j \neq i}^N |\alpha_j|/|\alpha_i|$. Though presented in terms of a projection, the bound

gives a measure of the angle between an eigenvector and a Krylov subspace. The bound involves a min-max problem for determining a polynomial that is small on the unwanted eigenvalues.

Last, Saad motivated the need for restarting the Arnoldi method and proposed a technique to do so. To restart the Arnoldi method, one must pick a new starting vector, v^+ , for the Krylov subspace. Saad suggested that this new starting vector be a weighted linear combination of the Ritz vectors, with the weights chosen based on how well the Ritz vectors approximate eigenvectors. As every vector in a Krylov subspace can be represented as a polynomial in the matrix times the starting vector, Saad's approach to restarting is equivalent to selecting the roots, μ_i , of a polynomial,

$$\psi(z) = \prod_{i=1}^p (z - \mu_i).$$

Hence the new starting vector is

$$v^+ = \psi(A)v.$$

In the years following his introduction of the restarted Arnoldi method, Saad used the polynomial representation of vectors in a Krylov subspace to suggest that the restart polynomial, $\psi(z)$, should be small on the unwanted portion of the spectrum. Such a choice will amplify the components of the starting vector in the direction of desired eigenvectors. In the case that the spectrum is real, if one can determine an interval containing only the unwanted eigenvalues, then a Chebyshev polynomial can be constructed to be uniformly small on the interval and large everywhere else [19]. Chebyshev polynomials are optimal for intervals; i.e., any other polynomial on the same interval would not be as uniformly small on the interval. For complex spectra, if there exists an ellipse containing only the unwanted eigenvalues, then a Chebyshev

polynomial can be constructed to be small on the ellipse. In this case the Chebyshev polynomial is asymptotically optimal for the ellipse: as the polynomial degree increases, the Chebyshev polynomial will improve asymptotically at the same rate as the optimal polynomials for the ellipse. In practice there may not exist an ellipse that contains only the unwanted eigenvalues. In this case the problem of constructing a polynomial that is small on a region containing the unwanted eigenvalues becomes difficult; one could use another method such as conformal mapping to construct the restart polynomial [22, 9]. The main difficulty in this approach to constructing restart polynomials is estimating the location of the unwanted eigenvalues. The goal of the Arnoldi method is to compute solely the wanted eigenvalues, but in following the recipe above one has to determine estimates of the unwanted eigenvalues as well. This problem remains relevant in analysis and application of the Arnoldi method. My work is partly focused on clarifying how reliably Ritz values can be used to approximate the unwanted portion of the spectrum.

1.6 Implicitly Restarted Arnoldi with Exact Shifts

Nearly a decade after Saad introduced the Arnoldi method, Sorensen [21] formulated the implicitly restarted Arnoldi method. Explicit restarting of the method involves directly applying the restart polynomial to the starting vector to generate the starting vector for the next iteration. The new starting vector is then used to generate a basis for the new Krylov subspace, as well as the projection of the matrix onto that subspace. In floating point arithmetic, explicit restarting is numerically unstable. The direct application of the matrix polynomial to a vector can lead to rounding errors. By interpreting the Arnoldi method as a truncated version of the QR eigenvalue iteration, Sorensen developed a numerically stable method of implicitly applying the

restart polynomial using the tools and concepts from the QR eigenvalue iteration, including implicit shifting and deflation. In addition to putting the restarted Arnoldi method into a reliable numerical form, Sorensen proposed a method for picking the roots of the restart polynomial and showed that this approach under mild assumptions gives a convergent algorithm for symmetric matrices.

To determine a restart polynomial, one must have some knowledge of the location of wanted and unwanted eigenvalues. Unless one has some prior knowledge of the system, this information has to be determined adaptively as the algorithm proceeds. With prior knowledge one can construct a fixed restart polynomial. In this case the Arnoldi method is similar to applying the power method with the fixed polynomial. Not surprisingly, Sorensen showed that the convergence criteria for Arnoldi with a fixed restart polynomial is similar to the convergence criteria for the power method. Fixed restart polynomials are rarely used in practice, but they are useful in theory for establishing convergence bounds. For a more potent practical algorithm, Sorensen proposed using some of the Ritz values as the roots of the restart polynomial. Depending upon the type of eigenvalue desired (largest/smallest magnitude, real part or imaginary part), the Ritz values are sorted and a fixed number of the least desirable Ritz values at each iteration are used as roots for the restart polynomial. These Ritz values are referred to as *exact shifts*. Using properties of symmetric matrices that localize Ritz values, Sorensen showed that the implicitly restarted Arnoldi method with exact shifts would converge. As symmetric matrices are encountered in numerous applications, Sorensen's proof validated the utility of the implicitly restarted Arnoldi method for determining eigenvalues of symmetric matrices.

1.7 Convergence of Restarted Arnoldi for Nonsymmetric Matrices

Nonsymmetric eigenvalue problems arise frequently, and the use of the implicitly restarted Arnoldi method with exact shifts to solve them is common practice. Though the behavior of Ritz values for nonsymmetric problems is poorly understood, exact shifts perform well in practice. This thesis will identify and characterize the Ritz values of particular nonsymmetric matrices for which the Arnoldi method will converge. This is a difficult problem because, for one, there are matrices and starting vectors for which the method will fail to converge in exact arithmetic; the restart polynomial annihilates the components of the starting vector in the direction of desired eigenspaces [6]. Matrices that allow for this type of failure are characterized by having wanted eigenvalues that lie in the numerical range of the portion of the matrix associated with the unwanted eigenvalues. Understanding Ritz value behavior alone is not sufficient to establish convergence, as the starting vector must be properly oriented to guarantee convergence. Even for the case of normal nonsymmetric matrices with perfectly conditioned eigenvalues, little is known about what is necessary for convergence.

Various lines of research have developed for understanding convergence of the restarted Arnoldi method. The most direct attacks on the problem focus on bounding convergence of the method using optimal shifts [2, 3]. The convergence of the restarted Arnoldi method is best measured by calculating the containment gap, which is associated with the sine of the largest canonical angle between the current subspace and the desired subspace,

$$\delta(\mathcal{W}, \mathcal{V}) = \max_{w \in \mathcal{W}} \min_{v \in \mathcal{V}} \frac{\|v - w\|}{\|w\|},$$

where typically \mathcal{W} will be an invariant subspace and \mathcal{V} some approximating subspace (possibly of unequal dimensions). These approaches involve seeking polynomials that are small not only on the spectrum but also on larger sets that contain the spectrum, such as the pseudospectrum. The main result [3] of the convergence analysis for restarted Arnoldi gives the following bound for the containment gap between a desired invariant subspace \mathcal{U}_g and the restarted Krylov subspace as

$$\delta(\mathcal{U}_g, K_k(A, \Psi(A)v)) \leq C_1(A, v)C_2(A, \Omega_b) \max_{z \in \Omega_b} |1 - \Psi(z)\alpha_g(z)|.$$

The first term accounts for the starting vector v . The second term accounts for the nonnormality of A associated with the unwanted eigenvalues contained in the complex set Ω_b . The last term, where Ψ is product of all the restart polynomials and α_g is a polynomial with roots at the wanted eigenvalues, captures the convergence behavior associated with constructing restart polynomials that are small on a set containing the unwanted portion of the spectrum and yet large on the wanted portion of the spectrum. The disadvantage of this approach is that, though it does bound the rate of convergence and essentially identifies what would be ideal behavior for exact shifts, it does not provide insight into what is necessary for such ideal behavior to occur. By localizing Ritz values, this thesis will provide insights into why exact shifts should exhibit ideal behavior.

1.8 Ritz Values and Restarted Arnoldi Convergence

This thesis will identify criteria that give rise to localization of Ritz values, particularly Arnoldi Ritz values, for nonsymmetric matrices. In the symmetric case, the classical interlacing result of Cauchy [16, §10.1] restricts the location of Ritz values with respect to the spectrum. The optimality of Arnoldi Ritz values gives rise to the

separation of Ritz values by eigenvalues. These properties restrict the set of possible Arnoldi factorizations. To recover similar properties in the nonsymmetric case, this thesis will characterize the set of possible Arnoldi factorizations for particular nonsymmetric matrices. I will show both numerically and analytically that even for the most nonnormal matrix, a Jordan block, the Ritz values can be localized in the sense that repeated Ritz values cannot occur throughout the entire numerical range.

The results of this thesis will allow for further analysis of methods that rely upon Ritz values for eigenvalue approximation. A better understanding of the behavior of Ritz values for nonsymmetric matrices can potentially aid in the analysis of deflated and augmented Krylov techniques, such as Morgan's GMRES-DR algorithm [5, 15]. These methods use information about eigenspaces derived from Ritz pairs to improve the rate of convergence. In the standard restarted GMRES algorithm, at each restart information associated with certain eigenvalues (such as those closest to the origin) must be rediscovered before the algorithm can continue to make progress [20]. By supplementing the method with Ritz value information from previous steps, the time spent rediscovering the troublesome eigenvalues can be minimized. The question is, How well can one expect the Ritz values to localize these eigenvalues?

This thesis will also establish criteria that are sufficient for convergence of the restarted Arnoldi method for certain scenarios in which the wanted eigenvalues are not in the numerical range of the portion of the matrix associated with the unwanted eigenvalues. For this class of matrices, the type of failure demonstrated by Embree cannot occur [6]. Without loss of generality, the possible Ritz values will be characterized using the Schur decomposition, an invaluable tool in understanding many different eigenvalue problems. In 2001 Stewart generalized the notion of an Arnoldi decomposition, introducing what he called *Krylov decompositions* [24]. With this

generalization and the Schur decomposition, he introduced a Krylov–Schur algorithm for determining eigenvalues. The algorithm is equivalent to the Arnoldi method but the resulting factorization is upper triangular rather than upper Hessenberg and allows for a simpler application of the exact-shift restart polynomial. This thesis will characterize Ritz value behavior partly by determining the possible Krylov–Schur factorizations.

To the set of possible Krylov–Schur factorizations for a particular matrix there corresponds the set of equivalent matrices that can generate the same factorizations. This thesis will use equivalent matrices, matrices that can generate the same Arnoldi factorization, for characterizing Ritz values and Arnoldi convergence of block diagonal matrices with shifted skew-symmetric blocks. This result can possibly provide insight into how to show convergence of the restarted Arnoldi method for sectorial matrices, matrices whose eigenvalues or numerical range lie in a cone in the complex plane.

Chapter 2

Ritz Value Localization for Jordan Blocks

The interlacing theorem ensures that Ritz values of a Hermitian matrix cannot cluster near the rightmost eigenvalue. The absence of this property for non-Hermitian matrices is a significant obstacle preventing the development of a convergence theory for the restarted Arnoldi algorithm. Indeed, the presence of multiple Ritz values beyond the rightmost eigenvalue is essential to examples of extreme eigenvalue failure [6]. In this chapter, I evaluate the potential for clustered Ritz values by analyzing a Jordan block, the most extreme deviation from a Hermitian matrix. Even for this highly nonnormal matrix, a defective matrix having only one eigenvector, the Ritz values can be localized, i.e., the Ritz values cannot cluster throughout the entire numerical range.

I will determine regions in the complex plane in which particular Ritz values may occur. The following questions will be addressed: when determining $n - 1$ Ritz values of a $n \times n$ Jordan block, where in the complex plane can the second rightmost Ritz value occur, and where in the complex plane can Ritz values with multiplicity $n - 1$ occur? To help answer these questions I study numerical ranges. As the Ritz values of a matrix are the eigenvalues of a smaller matrix determined via projection, I will need to know how the numerical range of the full matrix relates to the numerical range of the projected matrix. Real projections will provide a surprising amount of insight into how the Ritz values may be distributed. For the smallest interesting case, which involves determining two Ritz values of a 3×3 Jordan block, I determine the

region in which the leftmost Ritz value must lie and the region in which repeated Ritz values may occur. Results for the $n = 3$ case will provide weak bounds for similar regions for localizing $n - 1$ Ritz values of a $n \times n$ Jordan block. To derive sharper bounds, the numerical range of the adjugate of $\lambda I - J_n$ will be used [11, 13].

2.1 Numerical Range of a Jordan Block

A Jordan block, J_n , is a square matrix with ones along the first superdiagonal and zeros elsewhere. For insight into the numerical range of J_n , consider matrices of the form

$$B_n = \begin{pmatrix} 0 & 1 & & & \\ & 1 & 0 & 1 & \\ & & \ddots & \ddots & \ddots \\ & & & 1 & 0 & 1 \\ & & & & 1 & 0 \end{pmatrix}.$$

Note that this is simply a translation of the matrix used to form finite difference approximations of the second derivative. The largest eigenvalue of such a matrix is $\rho(B_n) = 2 \cos(\pi/(n + 1))$. How do matrices of this form relate to matrix A ? The Hermitian part of J_n is given by

$$\mathrm{H}(J_n) \equiv \frac{J_n + J_n^*}{2} = \frac{1}{2}B_n.$$

A technique used for determining the boundary of the numerical range of a matrix requires determining the extreme eigenvalues of $\mathrm{H}(Ae^{i\theta})$ for values of θ ranging from 0 to π [10]. The extreme eigenvalues of $\mathrm{H}(Ae^{i\theta})$ determine the interval

$$\{\mathrm{Re}(ze^{i\theta} : z \in W(A)\} \subseteq \mathbb{R}$$

and thus bounds the numerical range of A .

For J_n , $W(H(J_n e^{i\theta})) = W(D^{-1}H(J_n)D) = \frac{1}{2}W(B_n)$, where D is a diagonal matrix with diagonal entries $[D]_{jj} = e^{ij\theta}$. The first equality follows because the numerical range is invariant under unitary similarity transformations. The second equality shows that the extreme eigenvalues of $H(e^{i\theta} J_n)$ do not vary with θ and are equal to the extreme eigenvalues of B_n . Hence the numerical range of J_n is the disk centered about the origin of radius $\cos(\pi/(n+1))$ [8, §1.3].

2.2 The Case $n = 3$

In this case I wish to characterize the Ritz values of J_3 generated from orthogonal projections of J_3 onto a two dimensional subspace. This is equivalent to analyzing the eigenvalues of $H = P^* J_3 P$ for all $P \in \mathbb{C}^{3 \times 2}$ such that $P^* P = I_2$. Since H is a 2×2 matrix, it will have two eigenvalues, λ_1 and λ_2 , which I will refer to as left and right eigenvalues, in the sense that $\text{Re}(\lambda_1) \leq \text{Re}(\lambda_2)$. The main concerns are, Where in \mathbb{C} may λ_1 lie? and, Where in \mathbb{C} may $\lambda_1 = \lambda_2$?

To build some intuition, one can generate matrices P using random complex vectors. After sampling thousands of such randomly generated matrices, one finds that the region in which λ_1 may lie, Ω , has a kidney bean shape, as seen in Figure 2.1.

Using a trace argument one can determine a bound for Ω ,

Lemma 2.1 *The region Ω in the numerical range of J_3 must be bounded by*

$$\{z \in \mathbb{C} : |z| \leq \sqrt{2}/2, \text{Re}(z) \leq \sqrt{2}/4\}.$$

Proof. Consider any unitary matrix $\hat{P} \in \mathbb{C}^{3 \times 3}$. Then $H = [\hat{P}^* J_3 \hat{P}]_3$ where $[\cdot]_3$ denotes the principal submatrix formed from removing column 3 and row 3. As all Ritz values are in the numerical range, the left boundary of Ω should coincide with a semicircle of radius $\sqrt{2}/2$, which is the left boundary of $W(J_3)$. The extent of the

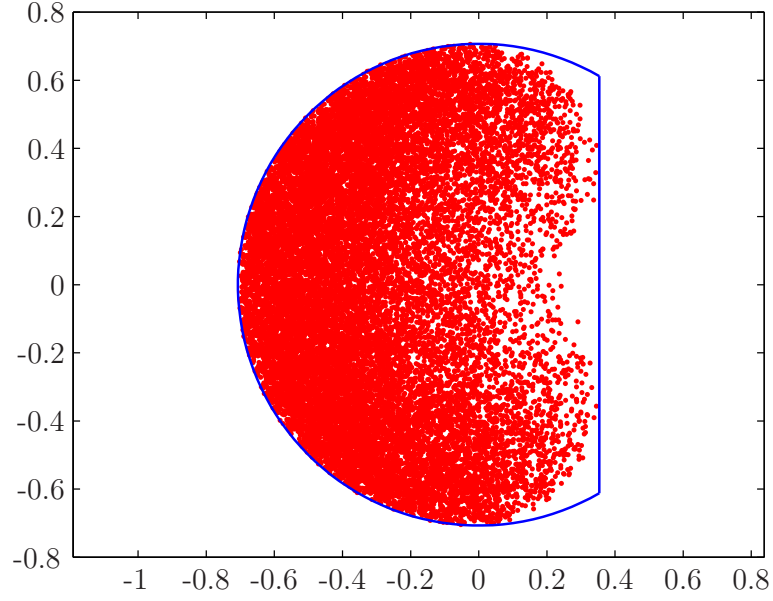


Figure 2.1 : Points in Ω , the region where left Ritz values of J_3 may lie. The blue line indicates the bound based on the trace argument.

right boundary is constrained by the trace of H . As the trace of a matrix is invariant under similarity transformations,

$$\text{tr}(\hat{P}^* J_3 \hat{P}) = \text{tr}(J_3).$$

Since the trace of a matrix is equal to the sum of the diagonal entries, and the diagonal entries of J_3 are all zero,

$$\text{tr}(\hat{P}^* J_3 \hat{P}) = 0.$$

From the properties of the trace,

$$\text{tr}(H) + [\hat{P}^* J_3 \hat{P}]_{33} = 0,$$

where $[\hat{P}^* J_3 \hat{P}]_{33}$ denotes entry $(3, 3)$ of the matrix $\hat{P}^* J_3 \hat{P}$. Taking the absolute value and noting that $[\hat{P}^* J_3 \hat{P}]_{33}$ is simply a point in the numerical range and thus must

have a magnitude no greater than $\sqrt{2}/2$, so

$$|\mathrm{tr}(H)| = |[\hat{P}^* J_3 \hat{P}]_{33}| \leq \frac{\sqrt{2}}{2}$$

Hence the magnitude of the trace of H can be no greater than $\sqrt{2}/2$.

As Ω consists of the points where left Ritz values may occur, if the left Ritz value has a real part of $\sqrt{2}/4$, then the real part of the right Ritz value must be greater than or equal to $\sqrt{2}/4$ by definition, and less than or equal to $\sqrt{2}/4$ to satisfy the constraint on the trace of H . ■

This result is sufficient to rigorously illustrate that the leftmost Ritz value cannot fall just anywhere in the numerical range: see Figure 2.1. I will now use a combination of numerics and analysis to estimate the finer structure of Ω . The result agrees with what is observed using random complex orthogonal projections. Indeed, there is more structure to the right half of Ω than can be gleaned solely from invariance of the trace of J_3 .

A better understanding of the boundary of Ω requires a parametrized, rather than random, means of selecting the matrices P with orthonormal columns. Selecting a matrix $P \in \mathbb{C}^{3 \times 2}$ corresponds to selecting a vector $p \in \mathbb{C}^3$ to which the columns of P are orthogonal. With p chosen and the fact that eigenvalues are invariant under unitary similarity transformations, I can then choose the columns of P to have a structure that will facilitate analysis. The natural parametrization involves a complex variant of spherical coordinates. The additional structure imposed upon P by unitary similarity is that its second column has a zero in its first entry. The reasoning above

yields

$$P = \begin{bmatrix} \cos(\theta_1) & 0 \\ -\sin(\theta_1) \cos(\theta_2) e^{i\theta_3} & \sin(\theta_2) e^{i\theta_3} \\ -\sin(\theta_1) \sin(\theta_2) e^{i\theta_4} & -\cos(\theta_2) e^{i\theta_4} \end{bmatrix}, \quad p = \begin{bmatrix} \sin(\theta_1) \\ \cos(\theta_1) \cos(\theta_2) e^{i\theta_3} \\ \cos(\theta_1) \sin(\theta_2) e^{i\theta_4} \end{bmatrix}, \quad (2.1)$$

where I have also required that the first entry of each column be real. Based on this parametrization of P , expressions for the trace of H and the determinant of H in terms of $\theta_1, \theta_2, \theta_3$ and θ_4 are as follows:

$$\text{tr}(H) = -\sin(\theta_1) \cos(\theta_1) \cos(\theta_2) e^{i\theta_3} - \cos^2(\theta_1) \cos(\theta_2) \sin(\theta_2) e^{i(\theta_4 - \theta_3)} \quad (2.2)$$

$$\det(H) = \cos(\theta_1) \sin(\theta_1) \sin(\theta_2) e^{i\theta_4}. \quad (2.3)$$

Expressing the eigenvalues of H as $\lambda_1 = r_1 e^{i\phi_1}$ and $\lambda_2 = r_2 e^{i\phi_2}$, I determine expressions that can be used to determine the right portion of the boundary of Ω . Results from the random projections indicate that along the right portion of the boundary of Ω the eigenvalues have equal real components, $r_1 \cos \phi_1 = r_2 \cos \phi_2$. As I will show, this assumption leads to convincing numerical results. With this assumption and the fact that the above equations may be complex valued and thus make up altogether four equations, one can derive an expression relating r_1, ϕ_1, ϕ_2 and θ_1 :

$$\begin{aligned} r_1^{12} k_5^6 - r_1^8 (k_5^4 \cos^2 \theta_1 \sin^2 \theta_1 + 2k_5^4 \sin^4 \theta_1) + r_1^6 k_3^2 k_5^2 \sin^4 \theta_1 \\ + r_1^4 (2k_4^2 k_5 \sin^6 \theta_1 + k_5^2 \sin^8 \theta_1 + 2k_5^2 \cos^2 \theta_1 \sin^6 \theta_1) \\ + r_1^2 k_3^2 \sin^8 \theta_1 - \cos^2 \theta_1 \sin^{10} \theta_1 = 0, \end{aligned} \quad (2.4)$$

with

$$\begin{aligned}
k_1^2 &= (1 - k_5)^2 & k_2^2 &= (1 + k_5)^2 \\
k_3^2 &= k_1^2 \sin^2 \left(\frac{\phi_1 - \phi_2}{2} \right) + k_2^2 \cos^2 \left(\frac{\phi_1 + \phi_2}{2} \right) \\
k_4^2 &= k_1^2 \sin^2 \left(\frac{\phi_1 - \phi_2}{2} \right) - k_2^2 \cos^2 \left(\frac{\phi_1 + \phi_2}{2} \right) \\
k_5 &= \frac{\cos \phi_1}{\cos \phi_2}.
\end{aligned}$$

Using the relationship (2.4), I numerically estimate the maximum r_1 for each ϕ_1 , which determines the right boundary of Ω : see Figure 2.2.

As expressions often simplify when dealing with only real arithmetic, I considered the boundary for solely real projections ($\theta_3 = \theta_4 = 0$), as it would include all Ritz values produced by the Arnoldi method applied to J_3 with a real starting vector. I found the right portion of the boundary for real projections almost coincides with the right portion of the boundary of Ω . In this case the above equation reduces to

$$\begin{aligned}
&r_1^8 + r_1^6 \sin^2 \theta_1 + r_1^4 (\sin^4 \theta_1 - \sin^2 \theta_1 \cos^2 \theta_1) \\
&\quad + r_1^2 \sin^4 \theta_1 (4 \cos^2 \phi_1 - 2 \cos^2 \theta_1) - \sin^6 \theta_1 \cos^2 \theta_1 = 0. \quad (2.5)
\end{aligned}$$

Using numerical methods to determine the largest r_1 for a given ϕ_1 , in the real case I determined that all the complex conjugate eigenvalues fall in a region bounded by circles $\{x + iy\}$ in the complex plane represented by the equations,

$$\begin{aligned}
x^2 + \left(y - \frac{\sqrt{2}}{4} \right)^2 &= \frac{1}{8} \\
x^2 + \left(y + \frac{\sqrt{2}}{4} \right)^2 &= \frac{1}{8} \\
(x - 1)^2 + y^2 &= \frac{1}{2} \\
(x + 1)^2 + y^2 &= \frac{1}{2},
\end{aligned}$$

as illustrated in Figure 2.2.

The difference between the boundary for the complex case and the real case can be seen in Figure 2.3. The deviation occurs in the region where the third equation above holds for the real case. In spite of being able to determine smooth approximations to the boundary, I have not yet found an equation that can describe the middle portion of the right boundary of Ω .

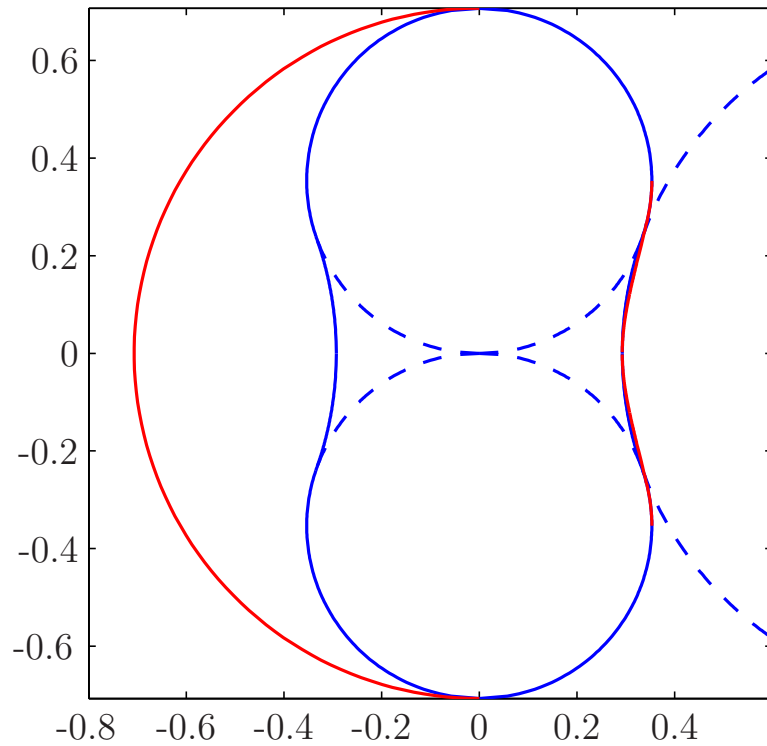


Figure 2.2 : Boundary for Ω . Boundary for real projections in blue, complex in red. Dashed blue lines indicate arcs of the circles that make up the boundary of real projections.

For the question of equal Ritz values, in rotating Ω about the origin in the complex plane, the region where equal Ritz values can occur must be the interior of the circle of radius $1 - \sqrt{2}/2$. The expressions above for the determinant and the trace of H

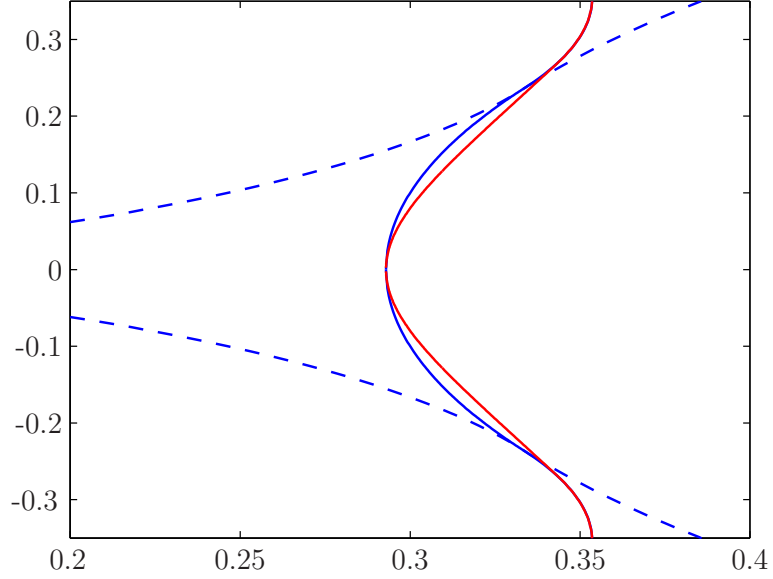


Figure 2.3 : Close up of Figure 2.2.

do indeed allow us to rotate Ω . By inspection, one can see that for a given pair of Ritz values corresponding to some H , one can rotate the Ritz values by ϕ simply by increasing θ_3 and θ_4 by ϕ and 2ϕ , respectively. In other words, a rotation by ϕ requires the angle of the trace of H to increase by ϕ while the angle of the determinant must increase by 2ϕ . Since the point $1 - \sqrt{2}/2$ on the boundary of Ω can be attributed to real projections, all that remains is to eliminate the possibility of a complex projection giving equal Ritz values of larger magnitude.

Since the Ritz values can always be rotated such that the determinant is real, for determining properties of the Ritz Values of J_3 only the case where $\theta_4 = 0$ need be considered. If H has equal eigenvalues and a determinant that is real, then the trace must be either purely real or purely imaginary. If the Ritz values lie on anything other than the positive half of the real axis, then a rotation can make them real and positive. This leads to the question, For $\theta_4 = 0$, is there any $\theta_3 \neq 0$ such that $\text{tr}(H)$

is real and positive? Based on (2.2) the following must hold in order for the trace of H to be real:

$$\text{Im}(\sin(\theta_1) \cos(\theta_1) \cos(\theta_2) e^{i\theta_3} + \cos^2(\theta_1) \cos(\theta_2) \sin(\theta_2) e^{-i\theta_3}) = 0$$

$$\sin(\theta_1) = \cos(\theta_1) \sin(\theta_2)$$

$$\tan(\theta_1) = \sin(\theta_2).$$

If this holds, then the implications for the trace and determinant are

$$\begin{aligned} \text{tr}(H) &= \cos(\theta_3) \cos(\theta_1) \sqrt{1 - \tan^2(\theta_1)} (-\sin(\theta_1) - \cos(\theta_1) \tan(\theta_1)), \\ &= -2 \sin(\theta_1) \cos(\theta_3) \sqrt{\cos^2(\theta_1) - \sin^2(\theta_1)}; \\ \det(H) &= \cos(\theta_1) \sin(\theta_1) \tan(\theta_1) \\ &= \sin^2(\theta_1). \end{aligned}$$

Since I am concerned with equal eigenvalues, then $\text{tr}(H) = 2\sqrt{\det(H)}$. Using the expressions above leads to:

$$\begin{aligned} 2 \sin(\theta_1) &= -2 \sin(\theta_1) \cos(\theta_3) \sqrt{\cos^2(\theta_1) - \sin^2(\theta_1)} \\ 1 &= -\cos(\theta_3) \sqrt{\cos^2(\theta_1) - \sin^2(\theta_1)} \\ \frac{-1}{\sqrt{\cos(2\theta_1)}} &= \cos(\theta_3). \end{aligned}$$

The above equation only holds where θ_1 and θ_3 involve integer multiples of π , in which case the determinant must be zero. Thus complex projections do not allow for equal Ritz values of magnitude greater than $1 - \sqrt{2}/2$.

If I can indeed generate some H that has equal eigenvalues, what can be said of the normality of such matrices? Further analysis shows that if H is normal then H has Ritz values such that $\lambda_1 = -\lambda_2$. This result shows that the set known as the $k = 2$ numerical range of J_n is empty [13].

2.3 Observations for $n > 3$

For $n > 3$, deriving equations that characterize the regions I wish to bound becomes difficult. However, I can determine bounds for these regions.

To identify where in the numerical range one can have Ritz values of multiplicity $n - 1$, one may again use a trace argument. Since all the Ritz values are equal, the radius of the desired region is bounded by the radius of the numerical range of J_n divided by $n - 1$.

$$|z| \leq \frac{\cos(\frac{\pi}{n+1})}{n-1}.$$

Thus as n becomes large, the region within the numerical range of J_n corresponding to equal ritz values shrinks to zero. Based on the results for $n = 3$, this may be a weak bound.

2.3.1 Interlacing Polynomials

To determine the region where the left Ritz values, $\theta_1, \dots, \theta_{n-2}$, must lie, I cannot use a trace argument to develop a useful bound. A trace approach would discard information regarding how the Ritz values must distribute themselves about the numerical range. With the tools utilized thus far, the possibility of developing any sort of bound is rather bleak. Thus some new tools must be found. A glimmer of hope was found in applying results of Johnson on interlacing polynomials of Hermitian matrices [11].

Johnson made the observation that for a Hermitian matrix A the set of polynomials in λ whose roots interlace the eigenvalues of A is equal to the numerical range of the adjugate of $\lambda I - A$. Recall that the adjugate of a matrix is equal to its inverse multiplied by its determinant, $\text{adj}(A) = \det(A)A^{-1}$. Also, each (i, j) entry in the adjugate of a matrix is proportional to the determinant of the matrix with rows j and column i deleted. The interlacing polynomials for a Hermitian matrix form a

convex set. For a general matrix, the interlacing property is lost, and the meaning of the polynomials derived from the numerical range of $\text{adj}(\lambda I - A)$ is not clear, nor is this set of polynomials convex for general matrices [13]. However, for a Jordan block $\text{adj}(\lambda I - A)$ can be easily computed.

For $n = 3$ the following holds,

$$\text{adj}(\lambda I - J_3) = \begin{pmatrix} \lambda^2 & \lambda & 1 \\ 0 & \lambda^2 & \lambda \\ 0 & 0 & \lambda^2 \end{pmatrix}.$$

From this matrix and the properties of powers of J_3 , one can form the equivalent expression

$$\text{adj}(\lambda I - J_3) = \lambda^2 I + \lambda J_3 + J_3^2.$$

Glancing back at equations (2.3) and (2.2) for the determinant and the trace, one can see that the characteristic polynomial of a projection of J_3 can be determined by the vector p in (2.1) that is in the null space of the projection:

$$p_H(\lambda) = p^* \text{adj}(\lambda I - J_3) p.$$

Thus for $n = 3$, this formula determines all possible characteristic polynomials of our projected matrices. This same technique can be used for $n > 3$. For any given $n - 1$ dimensional projection, I can construct a unitary matrix U such that the (n, n) entry of the adjugate of $U^*(\lambda I - A)U$ is the characteristic polynomial of the corresponding H , and the appropriate p would be the unit vector spanning the null space of the projection. With this new perspective I can construct a bound for how far to the right the second rightmost Ritz value can be. For the $n = 3$ case, the boundary includes a point on the positive real axis where the rightmost real Ritz value of multiplicity two occurs, $1 - \sqrt{2}/2$. For this point there is a corresponding p^0 that determines the

projection and characteristic polynomial. In the general case the coefficients of the characteristic polynomial will have the form

$$c_k = \sum_{i=1}^{k+1} p_i p_{i+n-1-k} = p^* J_n^{n-1-k} p, \quad \text{for } k = 0, \dots, n-1,$$

where c_k is the coefficient of the λ^k term. From the $n = 3$ case, I have a p^0 that determines a polynomial with a real repeated root. I can use the entries in this p^0 to construct vectors for $n > 3$ that also have real repeated roots. The entries will be as follows: $p_1 = p_1^0$, $p_{\lceil n/2 \rceil} = p_2^0$ and $p_{n+\text{mod}(n+1,2)} = p_3^0$ with the rest of the entries in p equal to zero. This particular p will give a double root of $(1 - \sqrt{2}/2)^{2/(n-1)}$ for n even and at $(1 - \sqrt{2}/2)^{2/n}$ for n odd. Thus I have a lower bound for how far to the right the second rightmost Ritz value can occur.

With some effort, the above bound can be checked numerically. Table 2.3.1 and Figure 2.4 show the results for $n \leq 20$. As n becomes large the bound is not sharp: some second rightmost Ritz values fall to the right of the lower bound. This is shown in Figure 2.4 by the blue dots, which represent the numerical results, being above the green crosses, the bound.

2.4 Discussion

My goal in this chapter was to show that the Ritz values of a Jordan block could be localized. I determined regions in the numerical range of a Jordan block where Ritz values of high multiplicity can occur. I also determined how far to the right the second rightmost Ritz value of a $n-1$ restriction of a n th order Jordan block can be. For the $n = 3$ case I determined these regions precisely. For $n > 3$, I provided bounds for these regions, which are not necessarily sharp. Nonetheless I have shown that the Ritz values of a Jordan block can be localized. A Jordan block is a highly specialized,

Table 2.1 : Numerical estimates and bounds for how far to the right the second rightmost Ritz value from an $n - 1$ dimensional subspace can be for $n = 3, \dots, 20$

n	numerical	bound
3	0.29289322	0.29289322
4	0.46821319	0.44103482
5	0.58278965	0.54119610
6	0.66214216	0.61190461
7	0.71960811	0.66410452
8	0.76268337	0.70409496
9	0.79591334	0.73566032
10	0.82214652	0.76118629
11	0.84328207	0.78224332
12	0.86057854	0.79990435
13	0.87495276	0.81492609
14	0.88702230	0.82785691
15	0.89638493	0.83910366
16	0.90568113	0.84897436
17	0.91350451	0.85770643
18	0.92020649	0.86548575
19	0.92606332	0.87245991
20	0.93575519	0.87874757

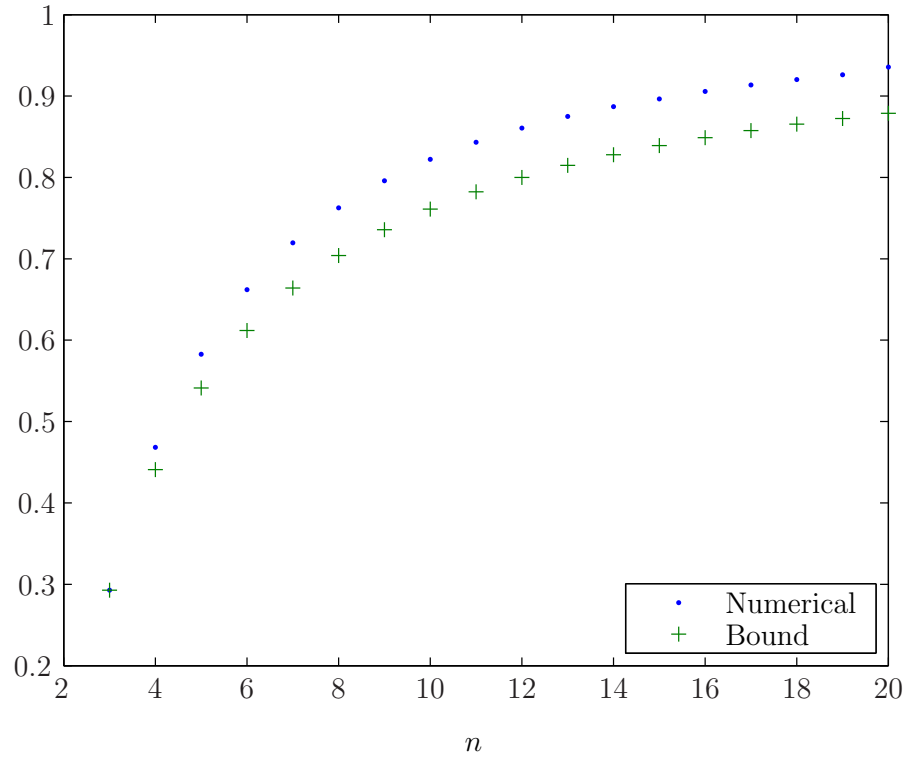


Figure 2.4 : Plot of numerical estimate and bound on how far to the right the second rightmost Ritz value from $n - 1$ dimensional subspace can be for $n = 3, \dots, 20$.

particularly nasty, nonnormal matrix having just one eigenvalue and one eigenvector. Jordan blocks are defective matrices that are difficult for many numerical methods to handle in practice. If Ritz values for such a nasty matrix can be localized, then there is good hope that Ritz values may also be localized for more general nonsymmetric matrices. I address this issue in the next chapter.

Chapter 3

Block Diagonal with a Normal Eigenvalue

Having observed in the last chapter that Ritz values can obey some localization behavior even for nonsymmetric matrices, I exploit this general idea to develop some sufficient conditions for the convergence of the restarted Arnoldi method with exact shifts. In this chapter I consider a class of block diagonal matrices that address some of the issues that arise in the convergence of restarted Arnoldi iterations.

The problem of determining a few eigenvalues of a matrix using an iterative method such as restarted Arnoldi is complicated by the nonnormality of the eigenvalues both desired, which restarted Arnoldi seeks to compute, and undesired, which restarted Arnoldi suppresses via the restart polynomial, and also by the possibility of failure or stagnation. The nonnormality of eigenvalues reflects how sensitive the eigenvalues are to perturbations in the matrix. The possibility of failure is dependent upon whether there are starting vectors that could lead to either a “lucky breakdown,” in which case an eigenspace has been found, or misconvergence to undesired eigenvalues. In applications, additional issues arise due to the finite precision of floating point arithmetic and the cost of performing real versus complex arithmetic. Such concerns necessitate modifications to the algorithm, such as reorthogonalization to counteract the loss of orthogonality due to finite precision and double shifts to avoid complex arithmetic.

Addressing all the factors above would be a rather daunting task; in this chapter I address some of these issues. First I present examples demonstrating two different

types of failure. The first example demonstrates the possibility of stagnation: the Ritz values converge but not to eigenvalues. This type of failure is dependent on the starting vector. The second example comes from Embree [6] and involves extreme breakdown: the restart polynomial annihilates the desired eigenvector from the starting vector, thereby precluding the possibility of convergence to the desired eigenvalue. This type of failure is due to the wanted eigenvalue being in the numerical range associated with the unwanted eigenvalues. Towards avoiding extreme breakdown, I make restrictions on the numerical range associated with the unwanted eigenvalues. To address the possibility of stagnation, I establish criteria for the starting vector. Throughout I assume exact arithmetic, in which case the implicitly restarted Arnoldi, restarted Arnoldi and restarted Krylov–Schur methods are all mathematically equivalent.

Since in practical applications the desired eigenvalues tend to be relatively normal, I consider matrices that have a simple normal eigenvalue, an eigenvalue with an algebraic multiplicity of one whose eigenvector is orthogonal to the complement of its invariant subspace. Hence, the class of matrices I consider are all unitarily similar to a block diagonal matrix with diagonal entries λ and D ,

$$A = \begin{pmatrix} \lambda & 0 \\ 0 & D \end{pmatrix}, \quad (3.1)$$

where λ is real and nonnegative and D contains all the unwanted eigenvalues. Future work would allow for more wanted eigenvalues and also for nonnormal coupling between the wanted eigenvalue and the block associated with the unwanted eigenvalues.

The development of a convergence theory for the matrices I consider will proceed in the following manner. I will establish that there is a Ritz value near the wanted eigenvalue. Then I will show that the other Ritz values cannot be arbitrarily close

to the wanted eigenvalue. Using these results I will determine conditions on the spectrum and the starting vector that will together ensure convergence. To test my results I will consider the case where D is skew symmetric, $D^* = -D$.

3.1 Examples

In this section, two examples will be considered. One demonstrates extreme breakdown and the other demonstrates stagnation. All these involve computing the eigenvalue with largest real part. In each example the wanted eigenvalue is simple and normal and thus the matrices in question could each be presented in the block diagonal form (3.1).

3.1.1 Stagnation

In this section I will present a matrix and starting vector for which the restarted Arnoldi method stagnates.

Consider the matrix

$$A = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix},$$

a circulant matrix whose largest real eigenvalue $\lambda = 1$ has an eigenvector with equal components in each entry. Using the restarted Arnoldi method with one exact shift to compute the largest eigenvalue with the starting vector

$$v_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

gives $K_2(A, v_1) = \text{span}\{v_1, Av_1\} = \text{span}\{v_1, v_2\}$, where

$$v_2 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

Forming the the upper Hessenberg matrix H_2 , the restriction of A onto $K_2(A, v_1)$ using $V_2 = [v_1 \ v_2]$, gives

$$H_2 = V_2^* A V_2 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

Clearly H_2 has but one eigenvalue, thus $\theta_1 = \theta_2 = 0$. Using an exact shift of zero to generate the new starting vector,

$$v_1^{(2)} = v^+ = Av_1 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix},$$

where the superscript denotes that $v_1^{(2)}$ is the starting vector for the second iteration of the restarted Arnoldi method.

For the second iteration, the Arnoldi basis vectors are

$$v_1^{(2)} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad v_2^{(2)} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}.$$

As in the previous iteration, the restriction of A to the current Krylov subspace is

$$H_2^{(2)} = (V_2^{(2)})^* A V_2^{(2)} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

As before, both Ritz values are zero. Proceeding with further restarted Arnoldi cycles produces the successive starting vectors

$$v_1^{(3)} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad v_1^{(4)} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}.$$

Thus at the fourth cycle of restarted Arnoldi, the starting vector $v_1^{(4)} = v_1^{(1)}$, the new starting vector is equal to the first starting vector. Hence, for this example the restarted Arnoldi method stagnates, and the Ritz value never converges to an eigenvalue, wanted or unwanted.

This example is particularly striking because A is a normal matrix with a unique rightmost eigenvalue $\lambda = 1$. If put into the form (3.1), then $\lambda \notin W(D)$. The starting vector v_1 has a significant component in the desired eigenvector direction; in fact, the problem arises because v_1 is equally weighted in each of the eigenvectors. Moreover, this example readily generalizes to n -dimensional circulant shift matrices with Krylov subspaces of dimension k for $2 \leq k < n$. This matrix is also a well known example of stagnation for GMRES; see [4].

If one were to alter the starting vector slightly, making it closer to the desired eigenvector, then restarted Arnoldi would converge. This example suggests that for some matrices there exist criteria for local convergence. In other words, if the starting vector is sufficiently rich, as in the desired eigenvector, then the restarted Arnoldi method will converge. Later in this chapter, I will consider a class of matrices for which local convergence as well as stagnation can occur.

3.1.2 Extreme Breakdown

This example is taken from Embree [6] and demonstrates extreme breakdown.

Consider the matrix

$$A = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 6 & -2 \\ 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

of the form (3.1) with largest eigenvalue $\lambda = 1$ and corresponding eigenvector e_1 . Using the restarted Arnoldi algorithm with one exact shift to compute the largest eigenvalue with a starting vector that has equal components in each entry leads to the following Arnoldi basis for $K_2(A, v_1)$:

$$v_1 = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \quad v_2 = \frac{1}{2\sqrt{35}} \begin{pmatrix} -3 \\ 9 \\ 1 \\ -7 \end{pmatrix}.$$

Restricting the matrix A to $K_2(A, v_1)$ gives

$$H_2 = V_2^* A V_2 = \begin{pmatrix} 7/4 & 3/(4\sqrt{35}) \\ \sqrt{35}/4 & 5/4 \end{pmatrix}.$$

The characteristic polynomial of H_2 is

$$p_H(\lambda) = \det(\lambda I - H_2) = \lambda^2 - 3\lambda + 2 = (\lambda - 1)(\lambda - 2).$$

Thus the eigenvalues of H_2 are $\theta_1 = 1$, $\theta_2 = 2$. The strategy for computing the rightmost eigenvalue would use θ_1 as the exact shift. Since $\theta_1 = \lambda$, this particular

shift results in the new starting vector

$$v^+ = (A - \theta_1 I)v_1 = \begin{pmatrix} 0 \\ 3 \\ 1 \\ -1 \end{pmatrix},$$

which does not have a component in e_1 , the eigenvector associated with the rightmost eigenvalue. Due to the structure of A , all further starting vectors of the restarted Arnoldi method will be orthogonal to e_1 . Hence convergence to e_1 for this particular starting vector, v_1 , is impossible. This failure is not unique to just this particular starting vector. Failure can also occur for any vector of the form

$$v_1 = \frac{1}{\sqrt{\alpha^2 + 3}} \begin{pmatrix} \alpha \\ 1 \\ 1 \\ 1 \end{pmatrix},$$

where α is any scalar. This form shows that the starting vector can be arbitrarily rich in the desired eigenvector and yet restarted Arnoldi can still fail to converge to the desired eigenvalue. Such examples are troubling for convergence theory of the restarted Arnoldi for general matrices. Unlike the previous example involving stagnation, local convergence is not possible for this matrix.

Embree went on to generalize this example allowing for more desired eigenvalues and more shifts. In all his examples, this type of failure occurs where the wanted eigenvalues are in the numerical range of the portion of the matrix associated with the unwanted eigenvalues. Note that in the notation of (3.1), $\lambda \in W(D)$. It is not known if $\lambda \notin W(D)$ is sufficient to prevent extreme Arnoldi failure (i.e. where v_1 is arbitrary close to e_1).

3.2 The General Case

Having shown two types of failure for the restarted Arnoldi method, in this section I develop a convergence theory for a class of matrices that addresses the more serious type of failure. Throughout this section assume that λ is not in the numerical range of D , and that $\|D\| < \lambda$. For simplicity, I always assume we are computing a single rightmost eigenvalue and hence will use all but one Ritz value as exact shifts.

The development of the convergence theory rests upon the localization of the Ritz values. I show there must be a Ritz value within a certain distance of the wanted eigenvalue, and that the rest of the Ritz values are bounded away from the desired Ritz value. Sufficient criteria for convergence are then based upon these localization results. Throughout this section I assume A has the form (3.1) and the starting vector v is represented as

$$v = \begin{pmatrix} c \\ r \end{pmatrix},$$

where $c \in \mathbb{C}$ is a nonzero scalar and represents the component of the starting vector in the direction of desired eigenvector, e_1 , and $r \in \mathbb{C}^{n-1}$ is the rest of the starting vector.

3.2.1 Ritz Value Localization

In this subsection I prove three lemmas that localize the Ritz values. The first lemma shows that not all the Ritz values can be arbitrarily far away from the desired eigenvalue.

Lemma 3.1 For a Krylov subspace $K_k(A, v)$, there must exist at least one Ritz value,

θ_1 , that is within η of the desired eigenvalue, $|\theta_1 - \lambda| \leq \eta$, where

$$\eta = (\|D\| + \lambda) \left(\frac{\|r\|}{|c|} \right)^{\frac{1}{k}}.$$

Proof. Ritz values from a Krylov subspace are optimal in the sense that they are the roots of the monic polynomial that minimizes

$$\left\| \prod_{i=1}^k (A - \theta_i I) v \right\| = \min_{p \in P_k} \|p(A)v\|,$$

where P_k is the set of all monic polynomials of degree k ; [18]. Suppose that all the Ritz values, θ_i , are such that $|\lambda - \theta_i| \geq \epsilon$. Due to the block diagonal structure of A ,

$$\begin{aligned} \left| \prod_{i=1}^k (\lambda - \theta_i) c \right|^2 &\leq \left| \prod_{i=1}^k (\lambda - \theta_i) c \right|^2 + \left\| \prod_{i=1}^k (D - \theta_i I) r \right\|^2 \\ &= \min_{p \in P_k} \|p(A)v\|^2. \end{aligned}$$

Then due to the nature of ϵ ,

$$\epsilon^k |c| \leq \min_{p \in P_k} \|p(A)v\|.$$

Since the Ritz values are optimal, no other polynomial $\hat{p}(z)$ with different roots can produce a smaller norm, so taking $\hat{p}(z) = (z - \lambda)^k$, one obtains

$$\min_{p \in P_k} \|p(A)v\| \leq \|(D - \lambda)^k r\|;$$

this comes from the fact that this particular $\hat{p}(z)$ annihilates the first component of the starting vector. Applying the definition of the operator norm and the triangle inequality, the term on the right gives

$$\min_{p \in P_k} \|p(A)v\| \leq (\|D\| + \lambda)^k \|r\|.$$

Combining the bounds from above and below for $\min_{p \in P_k} \|p(A)v\|$ yields

$$\epsilon^k |c| \leq (\|D\| + \lambda)^k \|r\|.$$

This implies that $\epsilon \leq (\|D\| + \lambda) \left(\frac{\|r\|}{|c|} \right)^{\frac{1}{k}}$, indicating that not all of the Ritz values can be greater than $\eta = (\|D\| + \lambda) \left(\frac{\|r\|}{|c|} \right)^{\frac{1}{k}}$ from λ . Denoting the closest Ritz value to λ as θ_1 , we see $|\lambda - \theta_1| \leq \eta$. ■

The next two lemmas localize the exact shifts, i.e., the Ritz values θ_j , $j = 2, \dots, k$. The first utilizes a trace argument, whereas the second makes use of a Schur decomposition.

Lemma 3.2 If $\operatorname{Re} W(D) \subset [-\alpha, \beta]$, then for each θ_j , $j = 2, \dots, k$,

$$\operatorname{Re} \theta_j \leq f(\alpha, \eta) := \eta + \operatorname{Re}(\operatorname{tr}(D)) + (n - 2)\alpha.$$

Furthermore

$$|\theta_j| \leq \rho := \sqrt{f(\alpha, \eta)^2 + \mu(D)^2}, \quad (3.2)$$

where $\mu(D) := \max_{z \in W(D)} |z|$ is the numerical radius of D .

Proof. From the matrix of k Arnoldi basis vectors V_k , form a unitary matrix such that $V = [V_k \ V_k^\perp] \in \mathbb{C}^{n \times n}$, where the range of V_k^\perp spans the space orthogonal to the range of V_k . Then V^*AV is a matrix that is similar to A and has for its k th principal submatrix H_k . Use θ_i for $i = k + 1, \dots, n$ to denote the Ritz values of the $(n - k) \times (n - k)$ submatrix of $\hat{H}_k = (V_k^\perp)^*AV_k^\perp$. Since the trace of a matrix is invariant under similarity transformation,

$$\begin{aligned} \lambda + \operatorname{tr}(D) &= \operatorname{tr}(H_k) + \operatorname{tr}(\hat{H}_k) \\ &= \sum_{i=1}^k \theta_i + \sum_{i=k+1}^n \theta_i \end{aligned}$$

Rearranging to form an equation for θ_j for $j = 2, \dots, n$ and regrouping the terms in the summation,

$$(\lambda - \theta_1) + \operatorname{tr}(D) - \sum_{\substack{i=2 \\ i \neq j}}^n \theta_i = \theta_j,$$

Taking the real part of this equation and then using the bound for the first quantity from Lemma 3.1,

$$\begin{aligned} \operatorname{Re} \theta_j &= \operatorname{Re}(\lambda - \theta_1) + \operatorname{Re}(\operatorname{tr}(D)) - \sum_{\substack{i=2 \\ i \neq j}}^n \operatorname{Re} \theta_i \\ &\leq \eta + \operatorname{Re}(\operatorname{tr}(D)) + (n-2)\alpha, \end{aligned}$$

where I have used $\operatorname{Re} \theta_i \in \operatorname{Re} W(D) \subseteq [-\alpha, \beta]$. ■

The following lemma gives a bound for how close the shifts, θ_j for $j = 2, \dots, k$, can be to the desired eigenvalue λ . The proof uses a Schur decomposition of H .

Lemma 3.3 The Ritz values θ_j for $j = 2, \dots, k$, all satisfy

$$\operatorname{Re} \theta_j \leq \frac{\lambda + \mu(D)}{2}.$$

Proof. Recall that Ritz values are simply the eigenvalues of $H_k = V_k^* A V_k$, where the columns of $V_k \in \mathbb{C}^{n \times k}$, the Arnoldi basis vectors for the k th Krylov subspace, are orthonormal.

The Schur decomposition implies there exists a unitary $U \in \mathbb{C}^{k \times k}$ such that

$$U^* V_k^* A V_k U = U^* H_k U = T,$$

where $T \in \mathbb{C}^{k \times k}$ is an upper triangular matrix and the diagonal entries of T are the Ritz values. As U is unitary, $Z = V_k U \in \mathbb{C}^{n \times k}$ has orthonormal columns. The columns of U are Schur vectors for H_k and denote the j th column of Z by z_j , which I call a *Krylov-Schur vector*. The matrix T is not unique; the Ritz values can appear in any order along the diagonal of T . Assume they are ordered such that

$$\operatorname{diag}(T) = (\theta_1, \theta_2, \theta_3, \dots, \theta_k),$$

where $\operatorname{diag}(T)$ denotes the diagonal entries of T [24].

Expressing the Krylov–Schur vectors as

$$z_j = \begin{pmatrix} \hat{z}_j \\ r_j \end{pmatrix},$$

where $\hat{z}_j \in \mathbb{C}$, $r_j \in \mathbb{C}^{n-1}$, then each Ritz value satisfies

$$\theta_j = z_j^* A z_j = |\hat{z}_j|^2 \lambda + r_j^* D r_j.$$

This expression yields a bound for the magnitude of each Ritz value,

$$\operatorname{Re} \theta_j \leq \lambda |\hat{z}_j|^2 + \mu(D) \|r_j\|^2.$$

Since the columns of Z are orthonormal,

$$|\hat{z}_j|^2 + \|r_j\|^2 = 1, \quad \sum_{j=1}^k |\hat{z}_j|^2 \leq 1. \quad (3.3)$$

If the last inequality were attained then that would imply that the wanted eigenvector is in the Krylov subspace.

Using equations (3.3) in the inequality for $|\theta_j|$, observe that

$$\begin{aligned} \operatorname{Re} \theta_j &\leq (\lambda - \mu(D)) |\hat{z}_j|^2 + \mu(D) \\ &\leq (\lambda - \mu(D))(1 - |\hat{z}_1|^2) + \mu(D). \end{aligned}$$

However, θ_j must also satisfy $\operatorname{Re} \theta_j < \operatorname{Re} \theta_1$, hence the bound for $|\theta_j|$ solves

$$\max_{\hat{z}_1} \min \left\{ \lambda |\hat{z}_1|^2 + \mu(D)(1 - |\hat{z}_1|^2), (\lambda - \mu(D))(1 - |\hat{z}_1|^2) + \mu(D) \right\}.$$

This bound for $|\theta_j|$ is largest when $|\hat{z}_j|^2 = 1/2$. Thus

$$\operatorname{Re} \theta_j \leq \hat{\theta} := \frac{\lambda + \mu(D)}{2}. \quad \blacksquare$$

Implications for Arnoldi Convergence

Building upon the lemmas above, in this section I demonstrate two separate conditions sufficient for convergence of the restarted Arnoldi method with exact shifts. The first result holds only in the case that the starting vector is sufficiently rich in the desired eigenvector. In other words, I will first show criteria that are sufficient for local convergence in the sense that the Ritz vector is sufficiently close to the desired eigenvector.

To ensure convergence of the restarted Arnoldi method, I seek conditions where the containment gap, the angle between the desired eigenspace and the Krylov subspace, will decrease at each restart. For the model problem (3.1), the desired eigenspace is spanned by the first canonical vector e_1 . Write the starting vector, v , as in the previous section, as

$$v = \begin{pmatrix} c \\ r \end{pmatrix},$$

where $c \in \mathbb{C}$ and $r \in \mathbb{C}^{n-1}$ are such that $\|v\| = 1$, so that for convergence the norm of r must be driven to zero by successive restarts. The relationship between the starting vector from one cycle to the next involves the restart polynomial, $\psi(x)$, so that

$$v^+ = \frac{\psi(A)v}{\|\psi(A)v\|}.$$

Note that due to the structure of A ,

$$\psi(A)v = \begin{pmatrix} c\psi(\lambda) \\ \psi(D)r \end{pmatrix}.$$

Using $p = k - 1$ exact shifts, the result from the previous section indicates that the p shifts will all have a magnitude less or equal to both $\hat{\theta} = (\lambda + \mu(D))/2$ and $\rho = \sqrt{f(\alpha, \eta)^2 + \mu(D)^2}$. The first quantity, $\hat{\theta}$, is independent of the starting vector,

whereas the second, ρ , incorporates information from the starting vector via η . Having the containment gap decrease at each step is equivalent to having

$$\frac{\|(I - e_1 e_1^*)v^+\|}{|e_1^* v^+|} = \frac{\|\psi(D)r\|}{|c\psi(\lambda)|} \leq \gamma < \frac{\|r\|}{|c|}.$$

for some fixed $\gamma \in [0, 1]$ at each iteration. Thus for convergence,

$$\frac{\|\psi(D)r\|}{\|r\||\psi(\lambda)|} < 1. \quad (3.4)$$

With this notation in place, the following two theorems employ the different bounds for the shifts θ_j for $j = 2, \dots, k$ to determine sufficient conditions to ensure convergence of restarted Arnoldi.

Theorem 3.1 *If $\|D\| + 2\mu(D) < \lambda$ and the starting vector is sufficiently close to the desired eigenvector then, the containment gap will decrease at each step.*

Proof. The bound (3.4) implies the more stringent convergence criterion

$$\frac{\|\psi(D)r\|}{\|r\||\psi(\lambda)|} \leq \frac{\|\psi(D)\|}{|\psi(\lambda)|} < 1.$$

To generate an even stronger criterion, recall that $\psi(z) = \prod_{i=2}^k (z - \theta_i)$, where the θ_i are the exact shifts, the unwanted Ritz values. Then the worst possible scenario would be that all the shifts occur at $\hat{\theta} := (|\lambda| + \mu(D))/2$, for this would minimize the denominator. A bound for the numerator term involves $\|D - \hat{\theta}\| < \|D\| + \hat{\theta}$. By requiring

$$\frac{\|\psi(D)\|}{|\psi(\lambda)|} \leq \frac{(\|D\| + \hat{\theta})^p}{(\lambda - \hat{\theta})^p} < 1,$$

or equivalently

$$\frac{\|D\| + \hat{\theta}}{\lambda - \hat{\theta}} < 1, \quad (3.5)$$

the containment gap will decrease and v^+ will better approximate the desired eigenvector e_1 . Rearranging equation (3.5) leads to a criterion for $\hat{\theta}$:

$$\hat{\theta} < \frac{\lambda - \|D\|}{2}.$$

Using the inequality from the previous section as a bound for the magnitude of all the unwanted Ritz values, one finds

$$|\hat{\theta}| < (\lambda - \mu(D))(1 - |z_{i1}|^2) + \mu(D) < \frac{\lambda - \|D\|}{2}.$$

The criterion above implies that if λ is greater than $\|D\| + 2\mu(D)$ then if the original starting vector is sufficiently rich in the desired eigenvector, then the new starting vector will better approximate the desired eigenvector. This criterion is sufficient for local convergence of the restarted Arnoldi method using p shifts. ■

The next theorem uses the bound involving ρ from equation (3.2) to generate a sufficient condition for convergence.

Theorem 3.2 *If A and v are such that $\|D\| < \lambda - 2\rho$, then the component of the starting vector in the desired eigenvector will increase with each iteration and thus the restarted Arnoldi method will converge.*

Proof. By requiring

$$\frac{\|\psi(D)\|}{|\psi(\lambda)|} \leq \frac{(\|D\| + \rho)^p}{\lambda - \rho} < 1,$$

the result follows. ■

The criteria in both these theorems are not particularly sharp, that is, there are most certainly matrices that do not satisfy these criteria and yet restarted Arnoldi converges. The above theorems involve bounding $\|\psi(D)r\|/\|r\|$ with $\|\psi(D)\|$. Requiring $\|\psi(D)r\|/\|r\|$ to be small, depending on r , may necessitate only that $\psi(z)$ be

small on some of the eigenvalues of D , whereas requiring $\|\psi(D)\|$ means $\psi(z)$ must be small on all the unwanted eigenvalues. In bounding $\|\psi(D)\|/|\psi(\lambda)|$, each of the shifts was treated independently, and they were allowed to cluster as close as possible to λ . Such clustering is unlikely to occur in practice. A sharper bound would require treating the shifts as an ensemble rather than independently. The quantity ρ is an extremely weak bound; for one, it does not reduce to $\mu(D)$ in the case of v^+ being extremely rich in the desired eigenvector, due to the use of the trace argument, but at least it does incorporate the starting vector. The quantity $\hat{\theta}$ is overly pessimistic, for its derivation involved the assumption that $\hat{z}_1 = \hat{z}_j = 1/2$, which would imply that the desired eigenvector is in the current Krylov subspace. Nonetheless the theorems above do indeed give criteria that ensure convergence of the restarted Arnoldi algorithm with exact shifts, the first such results of which I am aware.

3.3 Skew Symmetric D

Here I demonstrate some of the notions developed in the previous section for a small normal matrix for which everything can be determined.

Given a real matrix with $D = -D^*$ of the form (3.1),

$$A = \begin{pmatrix} \lambda & 0 \\ 0 & D \end{pmatrix} = \begin{pmatrix} \lambda & 0 & 0 \\ 0 & 0 & \alpha \\ 0 & -\alpha & 0 \end{pmatrix},$$

which has eigenvalues λ , αi and $-\alpha i$, I answer the following questions concerning Ritz values of 2×2 real restrictions of A .

- Where in the field of values of A can complex conjugate Ritz values occur?
- How rich must the starting vector, v , be in e_1 in order to guarantee convergence

to λ for restarted Arnoldi with exact shifts (RA)?

- Are there any restrictions that must be placed on the magnitude of α to ensure it is possible for RA to converge to λ ?

First I determine where complex conjugate Ritz values may lie, and then I show how Ritz values for a general restriction of A can be related to the Ritz values from a Krylov subspace. These results lead to conditions on the angle between the starting vector and the desired eigenspace, the containment gap, that ensure a desirable shift for RA. I will refer to the cosine of the angle Θ between e_1 and v as the richness in e_1 ,

$$\cos(\Theta) = \frac{|e_1^* v|}{\|v\|}.$$

To consider the Ritz values of all possible real projections of A , it suffices to parametrize a matrix $P \in \mathbb{R}^{3 \times 2}$ with two orthonormal columns as

$$P = \begin{pmatrix} \cos \theta & 0 \\ \sin \theta \cos \phi & \sin \phi \\ \sin \theta \sin \phi & -\cos \phi \end{pmatrix}.$$

The sufficiency of this form follows from the invariance of eigenvalues under unitary similarity transformations.

From this special P the restriction of A , $P^T A P$, takes the form

$$P^T A P = \begin{pmatrix} \lambda \cos^2 \theta & -\alpha \sin \theta \\ \alpha \sin \theta & 0 \end{pmatrix}.$$

Immediately one can see that

$$\begin{aligned} \text{tr}(P^T A P) &= \lambda \cos^2 \theta \\ \det(P^T A P) &= \alpha^2 \sin^2 \theta. \end{aligned}$$

Thus the roots of the characteristic polynomial for $P^T A P$ are given by

$$\frac{\lambda \cos^2 \theta \pm \sqrt{\lambda^2 \cos^4 \theta - 4\alpha^2 \sin^2 \theta}}{2}. \quad (3.6)$$

The Ritz values will be a complex conjugate pair if and only if

$$\lambda^2 \cos^4 \theta - 4\alpha^2 \sin^2 \theta < 0.$$

To determine where complex conjugate pairs may lie, consider

$$\begin{aligned} x &= \frac{\lambda \cos^2 \theta}{2} \\ y &= \frac{\sqrt{4\alpha^2 \sin^2 \theta - \lambda^2 \cos^4 \theta}}{2}. \end{aligned}$$

Combining these equations, the relationship between x and y is

$$y^2 + \left(x + \frac{\alpha^2}{\lambda}\right)^2 = \alpha^2 \left(1 + \frac{\alpha^2}{\lambda^2}\right).$$

Hence the possible complex conjugate Ritz values all lie on a circle centered at $(x, y) = (-\alpha^2/\lambda, 0)$ with radius $\alpha\sqrt{1 + \alpha^2/\lambda^2}$; see Figure 3.1. Note that this circle is tangent to the boundary of the numerical range of A at $\pm\alpha i$.

At this point one might be tempted to parametrize the starting vector for RA in a manner similar to that of P . However, due to the size of the problem, one can do much better. To determine a Krylov subspace that spans the range of P , let p_1 and p_2 denote the columns of P and p_3 the vector orthogonal to the range of P . Then a starting vector v for which $K_2(A, v) = \text{Ran}(P)$ must satisfy the equations

$$\begin{aligned} p_3^T v &= 0 \\ p_3^T A v &= 0. \end{aligned}$$

The first equation indicates that v should be a linear combination of p_1 and p_2 , $v = c_1 p_1 + c_2 p_2$. The second equation then gives

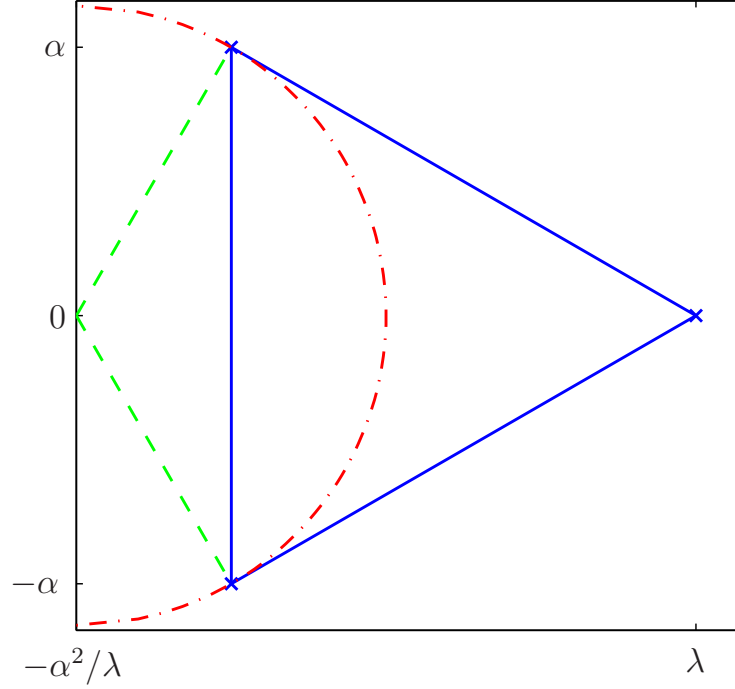


Figure 3.1 : Blue solid lines outline $W(A)$; the dot-dash line indicates the arc of a circle in $W(A)$, along which complex conjugate Ritz values may occur; the dashed green line indicates the center of this circle.

$$\begin{pmatrix} p_3^T A p_1 & p_3^T A p_2 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = 0.$$

Thus $(c_1, c_2)^T$ must lie in the null space of $(p_3^T A p_1, p_3^T A p_2)$. With the exception of $\theta = \pi/2$, which corresponds to P being completely deficient in e_1 , the null space has a dimension of 1 and is spanned by the vector $(p_3^T A p_2, -p_3^T A p_1)^T$. For our chosen basis $p_3 = (\sin \theta, -\cos \theta \cos \phi, -\cos \theta \sin \phi)^T$. Thus one can conclude that

$$c = \begin{pmatrix} -\alpha \cos \theta \\ \lambda \cos \theta \sin \theta \end{pmatrix}.$$

Hence the angle, Θ , between e_1 and the starting vector $v = Pc$ is given by

$$\cos^2(\Theta) = \frac{\alpha^2 \cos^2 \theta}{\lambda^2 \sin^2 \theta + \alpha^2}. \quad (3.7)$$

Using this formula for the bias of v requires knowing where the left Ritz value must lie for the restarted starting vector v^+ to be richer than v in the eigenvector e_1 .

Representing v as in previous sections, $v = (c, r)^T$, where c is a scalar and $r \in \mathbb{C}^2$, consider a real shift $\tilde{\theta}$,

$$v^+ = (A - \tilde{\theta})v = \begin{pmatrix} (\lambda - \tilde{\theta})c \\ (D - \tilde{\theta})r \end{pmatrix}.$$

For progress, the richness of v^+ must be greater than the richness of v . As in the previous section this amounts to

$$\frac{\|\psi(D)r\|}{\|r\|\|\psi(\lambda)\|} < 1. \quad (3.8)$$

For the single exact shift $\tilde{\theta}$ and the skew-symmetric D , $\|\psi(D)r\| = \sqrt{\tilde{\theta}^2 + \alpha^2}\|r\|$.

Hence the inequality above is equivalent to

$$\frac{\tilde{\theta}^2 + \alpha^2}{|\lambda - \tilde{\theta}|^2} < 1. \quad (3.9)$$

Manipulating the inequality to determine a criterion for the shift gives

$$\tilde{\theta} < \frac{\lambda^2 - \alpha^2}{2\lambda} = \left(\frac{\lambda + \alpha}{\lambda}\right) \left(\frac{\lambda - \alpha}{2}\right), \quad (3.10)$$

where the last expression should be contrasted with the result of Theorem 3.2,

$$\rho < \frac{\lambda - \|D\|}{2},$$

in this case $\|D\| = \alpha$. Hence for this example the shift can actually be larger than prescribed by Theorem 3.2 and still lead to convergence.

If the leftmost Ritz value satisfies inequality (3.10), then the new starting vector will be richer in e_1 and the containment gap will decrease. Note that this inequality is useful only if $\alpha < \lambda$.

Using our formula for the Ritz values, equation (3.6) with inequality (3.10) yields an inequality for $\cos^2(\theta)$:

$$\cos^2 \theta > \frac{\lambda^2 + \alpha^2}{2\lambda^2}. \quad (3.11)$$

Recalling equation (3.7) for the richness of the starting vector in terms of θ , the inequality in equation (3.11) can be manipulated to determine a criterion for the richness of v in e_1 such that the new starting vector, v^+ , will be richer in e_1 :

$$|e_1^* v|^2 = \frac{\alpha^2 \cos^2 \theta}{\lambda^2 \sin^2 \theta + \alpha^2} > \frac{\alpha^2}{\lambda^2} \quad (3.12)$$

If the richness of the starting vector is greater than α/λ , then restarted Arnoldi will make progress at this step.

Suppose the richness of the starting vector satisfies this criterion, and denote Θ_i as the angle between the starting vector at the i th step and the desired eigenvector. Then for progress, equation (3.8) is equivalent to requiring that

$$\tan(\Theta_{i+1}) < \tan(\Theta_i).$$

If the criterion for the shift is met, then in terms of $\tan(\Theta_i)$, the following must hold:

$$1 > \frac{\tan(\Theta_{i+1})}{\tan(\Theta_i)} = \sqrt{\frac{\tilde{\theta}^2 + \alpha^2}{|\lambda - \tilde{\theta}|^2}}.$$

The quantity on the right is the rate at which progress is made at this step. The question is then, If the criterion for the shifts is met at one step, will it also be met for all subsequent steps?

To show that all subsequent steps will also satisfy the criterion, note that the formula for the rate of progress, which depends on $\hat{\theta}$, and the formula for the shift,

which is dependent upon $\cos(\theta)$, are given by

$$\sqrt{\frac{\tilde{\theta}^2 + \alpha^2}{|\lambda - \tilde{\theta}|^2}}, \quad \frac{\lambda \cos^2 \theta - \sqrt{\lambda^2 \cos^4 \theta - 4\alpha^2 \sin^2 \theta}}{2}.$$

The formula for the shift is a monotonically decreasing function of $\cos(\theta)$. If the shift meets the convergence criteria, then equation (3.12) indicates that $\cos(\theta)$ will increase at this step and thus the shift will decrease (move to the left). The rate of progress is a monotonically increasing function of θ , which means that method will make more progress at the next step. The asymptotic rate of progress is α/λ . Hence if the starting vector is sufficiently biased in the desired eigenvector and $\lambda > \alpha$, then restarted Arnoldi will converge and yield the desired eigenvector.

Figure 3.2 presents an example of the Ritz values at each step of RA for $\alpha = \sqrt{3}/3$, $\lambda = 1$ and $|e_1^* v| = \alpha/\lambda + .001$. For this example the numerical range of A is an equilateral triangle and the starting vector is just barely rich enough to meet the criterion. Figure 3.3 for the same example shows the convergence of $\tan(\Theta_i)$. Note that the matrix for this example is just a shifted and scaled version of the matrix given to demonstrate stagnation in Section 3.1.1.

Having developed a criterion for RA convergence for this test problem, one must ask, Is the criterion sharp? The sharpness of the bound as well as the possibility of stagnation are addressed by the following lemma.

Lemma 3.4 If $\alpha > \frac{\sqrt{3}}{3}\lambda$, then there exists starting vectors such that restarted Arnoldi method can stagnate. If $\alpha < \frac{\sqrt{3}}{3}\lambda$, then there exist starting vectors which do not satisfy (3.12) such restarted Arnoldi will converge.

Proof. Note that from equation (3.9) the condition of having

$$\frac{\tilde{\theta}^2 + \alpha^2}{|\lambda - \tilde{\theta}|^2} = 1$$

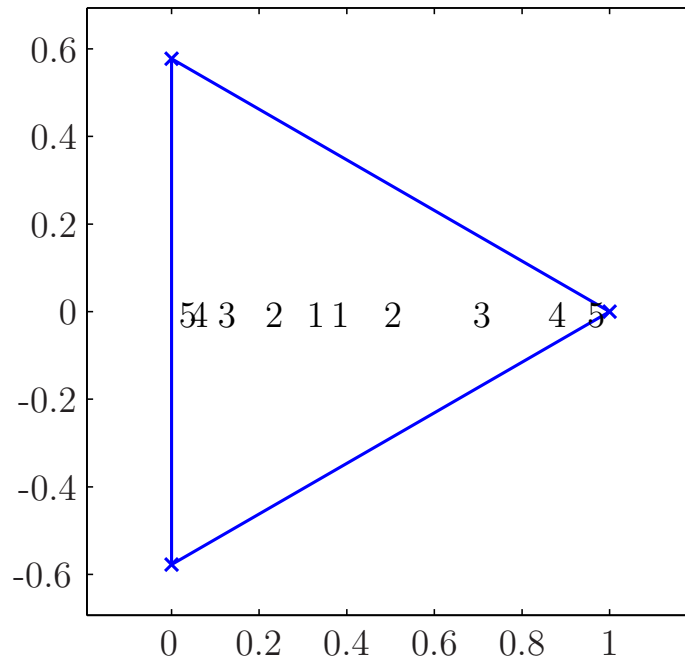


Figure 3.2 : Ritz values for five cycles of RA for $\lambda = 1$ and $\alpha = \sqrt{3}/3$. The two Ritz values at each cycle are denoted in the plot by the value of k .

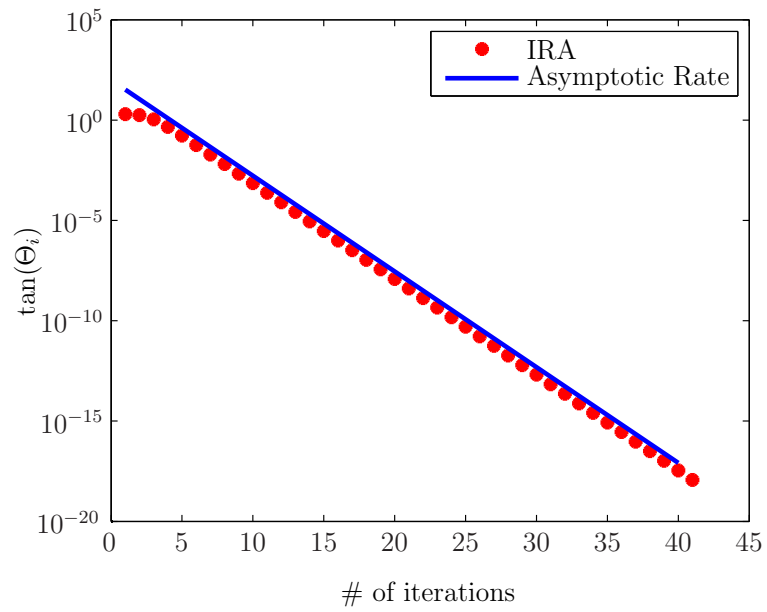


Figure 3.3 : Dots indicate $\tan(\Theta_i)$ in RA for $\lambda = 1$ and $\alpha = \sqrt{3}/3$. The blue line shows the asymptotic rate of convergence.

is equivalent to having $\tilde{\theta}$ be equidistant from all the eigenvalues. The point on the real axis that is equidistant to all the eigenvalues is

$$\ell := \frac{\lambda^2 - \alpha^2}{2\lambda}.$$

The question then becomes, Is there a real orthogonal projection for A such that the leftmost Ritz value is equidistant from all the eigenvalues? Using the expression for the circle on which the conjugate Ritz values must lie, equation (3.7) gives

$$\hat{x} := \alpha \sqrt{1 + \frac{\alpha^2}{\lambda^2}} - \frac{\alpha^2}{\lambda},$$

where $(\hat{x}, 0)$ is the point on the real axis where a double Ritz value can occur. So if $\ell > \hat{x}$, then there are no real projections such that RA can stagnate. For a given λ , manipulating the expressions for ℓ and \hat{x} gives an inequality for α such that stagnation cannot occur:

$$\alpha \sqrt{1 + \frac{\alpha^2}{\lambda^2}} - \frac{\alpha^2}{\lambda} < \frac{\lambda^2 - \alpha^2}{2\lambda},$$

which, after some algebra, reduces to

$$\lambda > \sqrt{3}\alpha,$$

the desired result. Note that if $\lambda = \sqrt{3}\alpha$, then the numerical range of A is an equilateral triangle. If the numerical range is narrow, so that $\lambda > \sqrt{3}\alpha$, then any starting vector such that the resulting Ritz values are real will lead to convergence. In this case a sharper convergence criterion is determined from (3.7):

$$4\alpha^2 \sin^2 \theta - \lambda^2 \cos^4 \theta > 0. \quad \blacksquare$$

Higher Dimensions

In this section I extend the results for D of dimension 2 to larger matrices. In this case $D \in \mathbb{C}^{n \times n}$ with spectrum such that $\sigma(D^2) \subset [-\alpha_{\max}^2, -\alpha_{\min}^2]$ with $\pm\alpha_{\max}i, \pm\alpha_{\min}i$ being eigenvalues of D . First I determine where all the Ritz values may lie, then show sufficient criteria for convergence.

To determine where the Ritz values may lie, I will construct a matrix of dimension 3 that generates the same Hessenberg matrix as A for a particular starting vector. The matrix will be of the same form as the matrix analyzed in the previous section. This matrix will be constructed by projecting A onto a subspace that contains the current Krylov subspace. Consider the subspace

$$K_2(A, v) + e_1,$$

which is equivalent to

$$\left\{ \begin{pmatrix} c \\ r \end{pmatrix} : c \in \mathbb{C}, r \in K_2(D, r) \right\},$$

where r is such that $v = [c; r]$. Construct an orthogonal matrix whose columns span this subspace:

$$Q = \begin{bmatrix} 1 & 0 \\ 0 & \tilde{Q} \end{bmatrix},$$

where the columns of \tilde{Q} form an orthonormal basis for $K_2(D, q)$. If V_2 and H_2 are respectively the Arnoldi basis and resulting usual upper Hessenberg matrix from $K_2(A, v)$. Then because the columns of V_2 are in the span of the columns of Q , $QQ^*V_2 = V_2$. Define $\hat{A} = Q^*AQ$ and $\hat{V} = Q^*V_2$. Then we have

$$\hat{V}^*\hat{A}\hat{V} = V_2^*QQ^*AQQ^*V_2 = H_2.$$

Note that \hat{V} and H_2 together with the vector orthogonal to the range of \hat{V} form an Arnoldi decomposition, starting from the Arnoldi decomposition associated with $K_2(A, v)$:

$$\begin{aligned} AV &= VH + fe_2^T \\ Q^*AQQ^*V &= Q^*VH + Q^*fe_2^T \\ \hat{A}\hat{V} &= \hat{V}H + \hat{f}e_2^T. \end{aligned}$$

Due to the structure of Q , \hat{A} will have the form

$$\hat{A} = Q^*AQ = \begin{bmatrix} \lambda & 0 \\ 0 & \tilde{Q}^*D\tilde{Q} \end{bmatrix}.$$

Since D is skew-symmetric

$$\hat{A} = Q^*AQ = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & 0 & \alpha \\ 0 & -\alpha & 0 \end{bmatrix},$$

where $\alpha = q_1^*Dq_2$.

So $\hat{A} := Q^T A Q$ is a 3×3 matrix that would generate the same H_2 for the appropriate starting vector, Q^*v . This matrix indicates where all possible Ritz values of RA using one exact shift can lie. Proceeding as in the previous section, where in $W(A)$ can complex conjugate Ritz values occur? From the properties of Krylov subspaces for skew-symmetric matrices, $-\alpha^2 \in W(D^2)$. Using knowledge from the dimension-2 case, all the complex Ritz values must lie between the arcs of two circles determined by the largest and smallest eigenvalues of D^2 .

The rest of this section will develop criteria for convergence for general skew-symmetric D . As in the 2-dimensional case, a criterion for convergence is that

$$\frac{\|\psi(D)\|}{|\psi(\lambda)|} < 1.$$

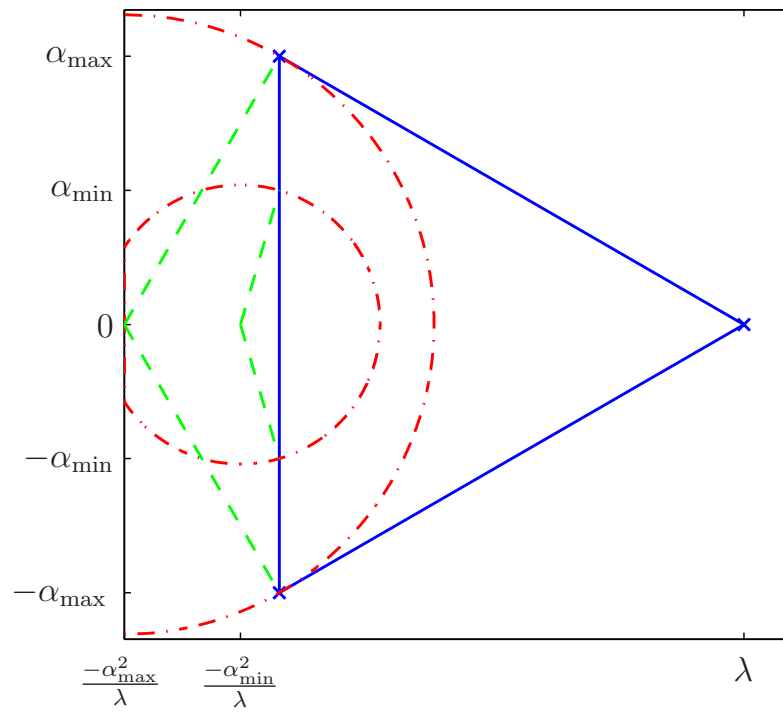


Figure 3.4 : Blue solid lines outline $W(A)$; the red dot-dash line indicates the arcs of circles that bound the region in $W(A)$, in which complex conjugate Ritz values may occur; the dashed green line indicates the centers of this circles.

In this case, $\|\psi(D)\| = \sqrt{\theta^2 + \alpha_{\max}^2}$. Hence the shift criterion is dependent only upon the largest magnitude eigenvalue of D . Recall the corresponding richness criterion from the 2-dimensional case:

$$|e_1^* v|^2 = \frac{\alpha^2 \cos^2 \theta}{\lambda^2 \sin^2 \theta + \alpha^2} > \frac{\alpha^2}{\lambda^2}.$$

In the worst case, $\alpha = \alpha_{\max}$. Then, by the arguments used for the dimension-2 case, if the richness of the starting vector is greater than α_{\max}/λ then RA will converge regardless of what the component of the starting vector is in the other eigenvectors. In practice, the component of the starting vector in the unwanted eigenvectors may lead to rapid initial convergence; however, the asymptotic rate will be determined by the extreme eigenvalues of D .

3.4 Discussion

In this chapter I developed sufficient conditions for the convergence of the restarted Arnoldi algorithm for a matrix with one simple normal eigenvalue for which the wanted eigenvalue is not in the numerical range associated with the desired eigenvalues. The requirements on the numerical range of the matrix are essential for eliminating the possibility of extreme breakdown. Some of the criteria are rather weak in that they ask that the wanted eigenvalue be well separated from the unwanted eigenvalues. The localization of the Ritz values involved in the conditions relied upon the inability of Ritz values to cluster arbitrarily close to the desired eigenvalue. Developing less stringent criteria will require accounting for not just how the Ritz values may cluster about the wanted eigenvalue, but also how the Ritz values must distribute themselves throughout the rest of the numerical range.

I developed sharp convergence criteria for matrices in which the unwanted eigen-

values come from a skew-symmetric block. In this case, the criteria ultimately address the issue of local convergence; if the starting vector has a large enough component in the desired eigenvector, then restarted Arnoldi will converge. Also, only one shift was considered for the skew-symmetric case, Future work could involve handling more shifts as well as complex conjugate shifts. The skew-symmetric results may prove useful for showing convergence for matrices whose spectrum is sectorial, i.e. ,the numerical range lie in a cone in a sector of the complex plane.

Chapter 4

Conclusion

This thesis has shown that under certain conditions the Ritz values of nonsymmetric matrices can be localized and that the localization of the Ritz values can be used to determine sufficient conditions for convergence of the restarted Arnoldi method.

The results of Chapter 2 concerning the Ritz values of a Jordan block raised questions about possible generalizations of the numerical range that would be useful for characterizing matrices for which Arnoldi will converge. From the example of extreme failure we know that if the numerical range associated with the unwanted eigenvalues can contain the desired eigenvalue, then there may well exist a vector for which restarted Arnoldi will fail. Perhaps the requirement on the numerical range may be relaxed or sharpened by requiring that the desired eigenvalues must not fall in the $k = 2$ numerical range, $W^k(A)$, where the $\lambda \in W^k(A)$ means that λ is a Ritz value of A of multiplicity k for some k dimensional subspace. Note this is not how the $k = 2$ numerical range is defined in the literature; in the literature the algebraic and geometric multiplicity of the Ritz values in $W^k(A)$ must be equal. As Arnoldi factorizations allow for only defective Ritz values, a more useful generalization of the numerical range for analyzing the Arnoldi method would allow for defective Ritz values.

The use of the numerical range of the adjugate of $\lambda I - A$ to determine the characteristic polynomial of a restriction of A is a polynomial numerical range approach to characterizing Ritz values. Generalizations to polynomial numerical ranges for

$k < n - 1$ dimensional subspaces do exist [13]. The polynomials in such sets would certainly provide insight into Ritz value behavior. However, they may be too difficult to compute to be of practical use. Any connection between the polynomial numerical range and the polynomial numerical hull would be interesting [7].

The Arnoldi convergence criteria for matrices with one simple normal eigenvalue developed in Chapter 3 are but a first step toward the development of a sharper convergence theory for the restarted Arnoldi method with exact shifts. The criteria do address the important issues such as the distribution of the spectrum relative to the desired eigenvalues and the richness of the starting vector. Sharper criteria must be more precise in the handling of the shifts. The criteria developed assumed the worst possible distribution for the shifts, but it seems likely that the shifts, when analyzed as an ensemble, will provide a convergence theory that is applicable to a wider range of matrices.

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