The localization of Arnoldi Ritz values for real normal matrices

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Approximations to (a few of) the eigenvalues (and eigenvectors) of large sparse non-symmetric matrices are often computed with (variants of) the Arnoldi process

One of the most popular software is ARPACK. It is used, for instance, in Matlab

It uses the Implicitly Restarted Arnoldi algorithm

In this talk we consider the standard Arnoldi process

The Arnoldi process

This method builds an orthogonal basis of the Krylov space

$$\mathcal{K}_n(A, v) = span\{v, \quad Av, \quad \cdots, \quad A^{n-1}v\}$$

Given A of order n and starting from a vector v of unit norm (with $Ve_1 = v$), it computes an upper Hessenberg matrix H and an orthogonal (or unitary) matrix V such that

$$AV = VH$$

The approximations of the eigenvalues of A (the Ritz values) at iteration k are the eigenvalues $\theta_i^{(k)}$ of H_k, the principal submatrix of order k of H

The recurrence to compute the basis vectors v_j and the columns of H is

$$AV_{n,k} = V_{n,k}H_k + h_{k+1,k}v_{k+1}e_k^T$$

$V_{n,k}$: k first columns of V

The matrices V and H are constructed column by column

We assume that the process does not stop before iteration n

Let K be the Krylov matrix $K = \begin{pmatrix} v & Av & \cdots & A^{n-1}v \end{pmatrix}$. Then

$$K = VU$$

where U is upper triangular with a positive real diagonal and $U_{1,1} = 1$ (because $\|v\| = 1$). Moreover

$$U = \begin{pmatrix} e_1 & He_1 & \cdots & H^{n-1}e_1 \end{pmatrix}$$

As a consequence of $AK = KC$ we have

$$H = UCU^{-1}$$

where C is the companion matrix corresponding to the eigenvalues λ_i of A

$$C = \begin{pmatrix} 0 & \cdots & 0 & -\alpha_0 \\ & & & -\alpha_1 \\ & I_{n-1} & & \vdots \\ & & & -\alpha_{n-1} \end{pmatrix}$$

The symmetric case

When A is symmetric (or Hermitian), the matrix H is tridiagonal (Arnoldi $\Rightarrow$ Lanczos - which was introduced before the Arnoldi process)
Then we have the Cauchy interlacing theorem

$$\theta_1^{(k+1)} < \theta_1^{(k)} < \theta_2^{(k+1)} < \theta_2^{(k)} < \cdots < \theta_k^{(k)} < \theta_{k+1}^{(k+1)}$$

and

$$\lambda_j < \theta_j^{(k)}, \quad \theta_{k+1-j}^{(k)} < \lambda_{n+1-j}, \ 1 \leq j \leq k$$

The convergence is well understood

The situation is not the same in the non-symmetric case

A negative result

Theorem (Duintjer Tebbens and GM (2012))

Assume we are given a set of tuples of complex numbers

$$\begin{aligned}\mathcal{R} = \{ \quad & \theta_1^{(1)}, \\ & (\theta_1^{(2)}, \theta_2^{(2)}), \\ & \vdots \\ & (\theta_1^{(n-1)}, \dots, \theta_{n-1}^{(n-1)}), \\ & (\lambda_1, \dots\dots\dots, \lambda_n)\},\end{aligned}$$

and $n-1$ *positive real numbers* $\sigma_1, \dots, \sigma_{n-1}$
Then there exist a matrix A *and a starting vector* v *such that: the Hessenberg matrix* H *generated by the* *Arnoldi* *process applied to* A *and initial vector* v *has eigenvalues* $\lambda_1, \dots, \lambda_n$*, subdiagonal entries* $\sigma_1, \dots, \sigma_{n-1}$ *and* $\theta_1^{(k)}, \dots, \theta_k^{(k)}$ *are the eigenvalues of its* k*th leading principal submatrix for all* $k = 1, \dots, n-1$

Moreover the previous theorem is constructive

It means that we can construct examples for which the Ritz values *do not* converge to the eigenvalues (before the last step)

However, the theorem does not tell what are the properties of the matrix A

In most practical cases, we *do* observe convergence of the Ritz values

In order to better understand convergence, it is interesting to study the locations of the Ritz values in the complex plane for a *given* matrix A
This problem has recently received some attention

- Z. Bujanovic, On the permissible arrangements of Ritz values for normal matrices in the complex plane, LAA v 438 (2013), pp. 4606–4624
- R. Carden and D.J. Hansen, Ritz values of normal matrices and Ceva's theorem, LAA v 438 (2013), pp. 4114–4129
- R. Carden and M. Embree, Ritz value localization for non-Hermitian matrices, SIMAX v 33 (2012), pp. 1320–1338
- J. Duintjer Tebbens and GM, Any Ritz value behavior is possible for Arnoldi and for GMRES, SIMAX v 33 (2012), pp. 958–978

The matrices H_k

Since $H = UCU^{-1}$ one can prove that

$$H_k = U_k \left[E_k + \begin{pmatrix} 0 & U_k^{-1} U_{[1:k],k+1} \end{pmatrix} \right] U_k^{-1}$$

with U_k the principal submatrix of U of order k and

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

Then

$$U_k \begin{pmatrix} \beta_0^{(k)} \\ \vdots \\ \beta_{k-1}^{(k)} \end{pmatrix} = -U_{[1:k],k+1}$$

and the Ritz values are the roots of the polynomial
$q_k(\lambda) = \lambda^k + \sum_{j=0}^{k-1} \beta_j^{(k)} \lambda^j = \prod_{i=1}^{k} (\lambda - \theta_i^{(k)})$

Multiplying by U_k^* we obtain

$$M_k \begin{pmatrix} \beta_0^{(k)} \\ \vdots \\ \beta_{k-1}^{(k)} \end{pmatrix} = -M_{[1:k],k+1}$$

with $M = K^*K = U^*U$, $M_k = U_k^*U_k$

This characterizes the coefficients of the characteristic polynomial of H_k

The interest is that (in some cases) we know the entries of M in terms of the eigenvalues and eigenvectors of A

The matrix $M = K^*K$

Assume that A is diagonalizable $A = X\Lambda X^{-1}$. Then if $c = X^{-1}v$

$$K = \begin{pmatrix} v & Av & \cdots & A^{n-1}v \end{pmatrix} = X \begin{pmatrix} c & \Lambda c & \cdots & \Lambda^{n-1}c \end{pmatrix}$$

and

$$M_{\ell,m} = \sum_{i=1}^{n}\sum_{j=1}^{n}(X^*X)_{i,j}\, \bar{c}_i c_j\, \bar{\lambda}_i^{\ell-1}\lambda_j^{m-1}$$

If A is normal, we have $X^*X = I$, $c = X^*v$ and

$$M_{\ell,m} = \sum_{i=1}^{n} |c_i|^2\, \bar{\lambda}_i^{\ell-1}\lambda_i^{m-1}$$

The inverse problem

Given a matrix A and complex values $\theta_1, \cdots, \theta_k$, the inverse problem is to know if there is a starting vector v such that $\theta_1, \cdots, \theta_k$ are the Arnoldi Ritz values at iteration k

The unknowns will be the components of $c = X^{-1}v$

We will first restrict ourselves to normal matrices and then to real normal matrices. We will mainly consider the simplest case $k = 2$

The Ritz values are contained in the field of values which is for normal matrices the convex hull of the eigenvalues

A normal, $k = 2$

Let θ_1, θ_2 given and $p = \theta_1\theta_2$, $s = \theta_1 + \theta_2$, $\beta_0^{(2)} = p$, $\beta_1^{(2)} = -s$
We have to consider M_2

$$\sum_{i=1}^{n} |c_i|^2 = 1, \quad p - s\sum_{i=1}^{n} |c_i|^2 \lambda_i = -\sum_{i=1}^{n} |c_i|^2 \lambda_i^2$$

$$s\sum_{i=1}^{n} |c_i|^2 |\lambda_i|^2 = \sum_{i=1}^{n} |c_i|^2 |\lambda_i|^2 \lambda_i + p\sum_{i=1}^{n} |c_i|^2 \bar{\lambda}_i$$

The unknowns are $|c_i|^2$, $i = 1, \ldots, n$

The first equation corresponds to $\|v\| = 1$

We have a $3 \times n$ linear system

There exists a vector v such that θ_1, θ_2 are Ritz values if and only if this linear system has a solution with positive real components
This result can be extended to $k > 2$

A normal real, $n = 3$, $k = 2$

Let A be real

Assume that we have two complex conjugate eigenvalues λ_1, $\bar{\lambda}_1$ and a real eigenvalue λ_3

The matrix is 3×2 and we have an overdetermined system for $\omega_1 = \omega_2 = |c_1|^2$, $\omega_3 = |c_3|^2$

$$\begin{pmatrix} 2 & 1 \\ 2s\mathrm{Re}(\lambda_1) - 2\mathrm{Re}(\lambda_1^2) & s\lambda_3 - \lambda_3^2 \\ 2s|\lambda_1|^2 - 2|\lambda_1|^2\mathrm{Re}(\lambda_1) - 2p\mathrm{Re}(\lambda_1) & s\lambda_3^2 - \lambda_3^3 - p\lambda_3 \end{pmatrix} \begin{pmatrix} \omega_1 \\ \omega_3 \end{pmatrix} = \begin{pmatrix} 1 \\ p \\ 0 \end{pmatrix}$$

with $s = \theta_1 + \theta_2$ and $p = \theta_1\theta_2$

Since everything is real, we must have $\theta_2 = \bar{\theta}_1$ and the question is: what are the possible locations of θ_1 (those which yield a positive solution)?

Let us consider θ_1 complex, $\theta_1 = a + ib$. We eliminate ω_1 and ω_3 from the equations and we obtain

$$2(\mathrm{Re}(\lambda_1) - \lambda_3)b^4 - (\beta + 2\alpha(\mathrm{Re}(\lambda_1) - \lambda_3) + \delta\lambda_3)b^2 + \alpha\beta - \gamma\delta = 0$$

with

$$\alpha = \lambda_3(2a - \lambda_3) - a^2$$

$$\beta = 4a(|\lambda_1|^2 - \lambda_3^2) - 2|\lambda_1|^2\,\mathrm{Re}(\lambda_1) + 2\lambda_3^3 - 2a^2(\mathrm{Re}(\lambda_1) - \lambda_3)$$

$$\gamma = -2a\lambda_3^2 + a^2\lambda_3 + \lambda_3^3$$

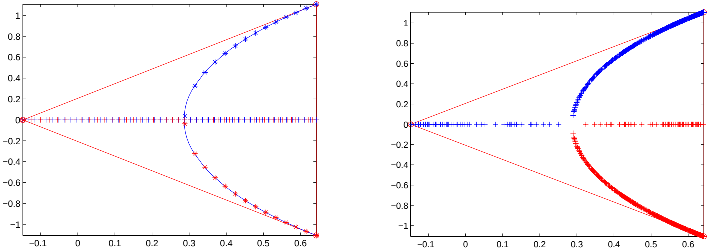
$$\delta = -4a(\mathrm{Re}(\lambda_1) - \lambda_3) + 2\mathrm{Re}(\lambda_1^2) - 2\lambda_3^2$$

It implicitly defines a curve $b(a)$ in the complex plane

We can compute points on the curve by solving the quadratic equation for b for a given a

Example, $n = 3, k = 2$

The field of values is a triangle



left: locations of θ_1, right: random starting vectors

A normal real, $n = 4$, $k = 2$

Let us consider the case with one pair of complex conjugate eigenvalues $(\lambda_1, \bar{\lambda}_1)$ and two real eigenvalues λ_3 and λ_4
The matrix is 3×3 and we have a square system for
$\omega_1 = \omega_2 = |c_1|^2$, $\omega_3 = |c_3|^2$, $\omega_4 = |c_4|^2$

$$\begin{pmatrix} 2 & 1 & 1 \\ 2s\mathrm{Re}(\lambda_1) - 2\mathrm{Re}(\lambda_1^2) & s\lambda_3 - \lambda_3^2 & s\lambda_4 - \lambda_4^2 \\ 2s|\lambda_1|^2 - 2|\lambda_1|^2\mathrm{Re}(\lambda_1) - 2p\mathrm{Re}(\lambda_1) & s\lambda_3^2 - \lambda_3^3 - p\lambda_3 & s\lambda_4^2 - \lambda_4^3 - p\lambda_4 \end{pmatrix} \begin{pmatrix} \omega_1 \\ \omega_3 \\ \omega_4 \end{pmatrix} = \begin{pmatrix} 1 \\ p \\ 0 \end{pmatrix}$$

with $s = \theta_1 + \theta_2 = 2\mathrm{Re}(\theta_1)$ and $p = \theta_1\theta_2 = |\theta_1|^2$

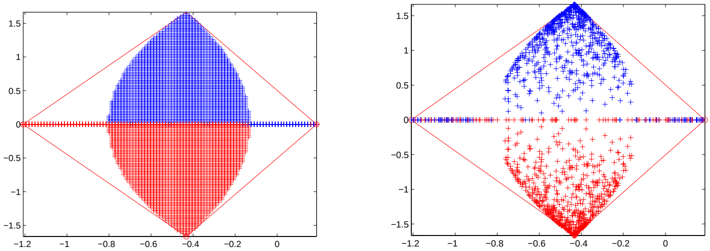
We cannot proceed as before

What we can do is, given a value of θ_1, solve the square linear system and check if the components of the solution are positive. If this is the case, then θ_1 is a feasible Ritz value. By discretizing the field of values, this yields the possible locations of the Ritz values

Example, $n = 4$, $k = 2$

Random normal real matrix

The left figure is obtained by discretization of the field of values



left: locations of θ_1, right: random starting vectors

Can we compute the boundary of the feasible region? Let the matrix be symbolically

$$\begin{pmatrix} 2 & 1 & 1 \\ a & c & e \\ b & d & f \end{pmatrix}$$

The inverse is given by

$$\frac{1}{D}\begin{pmatrix} cf - ed & d - f & e - c \\ eb - af & 2f - b & a - 2e \\ ad - cb & b - 2d & 2c - a \end{pmatrix}, \quad D = a(d-f)+c(2f-b)+e(b-2d)$$

and

$$\omega = \frac{1}{D}\begin{pmatrix} cf - ed + (d - f)p \\ eb - af + (2f - b)p \\ ad - cb + (b - 2d)p \end{pmatrix}$$

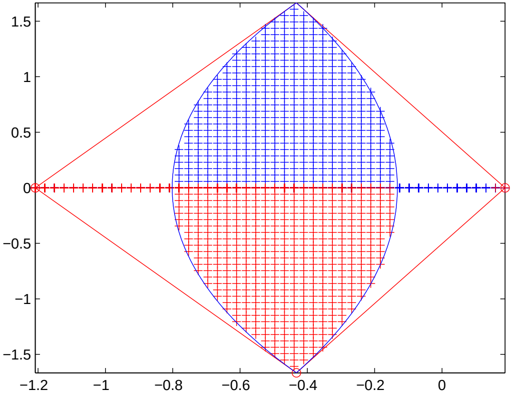
The boundary must be given by the components being zero

$$\begin{aligned} cf - ed + (d - f)p &= 0 \\ eb - af + (2f - b)p &= 0 \\ ad - cb + (b - 2d)p &= 0 \end{aligned}$$

The coefficients a, b, c, d, e, f are functions of unknowns quantities $s = 2x = 2\mathrm{Re}(\theta_1)$ and $p = x^2 + y^2 = |\theta_1|^2$

It yields 3 curves in the (x, y) complex plane

Example, $n = 4$, $k = 2$



Boundary of the feasible region

Here we use a coarser grid. The third curve is outside of the window

The situation is more or less the same for $n = 5$ with two pairs of complex conjugate eigenvalues and a real eigenvalue (the matrix is still 3×3)

For $n \geq 6$ we generally have an underdetermined linear system for the ω_j's

For a given θ_1 the feasibility can be checked with the SVD of the rectangular matrix

Pieces of the boundary correspond to some of the ω_j's being 0

Therefore we can put all the components to zero except for 3 of them. Then we can do the same as before for all the 3×3 matrices obtained by choosing 3 columns and solving the 3×3 linear systems

Of course we could obtain some curves which are not relevant for the boundary

It corresponds to what is done to handle the constraints in linear programming (LP) whose solution components must be positive

Let us assume that we have linear equality constraints $Cx = b$ defined by a real $m \times n$ matrix C of full rank with $m < n$ we can write $C = [B\ E]$ with B square nonsingular of order m

$$x = \begin{pmatrix} B^{-1}b \\ 0 \end{pmatrix}$$

is called a basic solution

This is just taking m independent columns, putting the other components of the solution to zero and solving

A basic feasible solution (BFS) is a basic solution that satisfies the constraints of the LP

The feasible region is a polyhedron and the BFS are the vertices of the polyhedron

We have a polyhedron defined by the rectangular matrix and considering all the 3×3 matrices (provided they are nonsingular) is computing symbolically the basic solutions

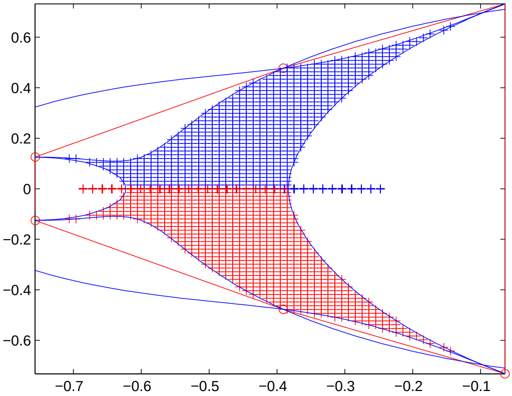
The feasible ones (with $\omega_j \geq 0$) correspond to vertices of the polyhedron

The curves we obtain are where components of ω change signs as a function of $x = \mathrm{Re}(\theta_1)$ and $y = \mathrm{Im}(\theta_1)$

They also give a parametric description of the vertices of the polyhedron

Example, $n = 6, k = 2$

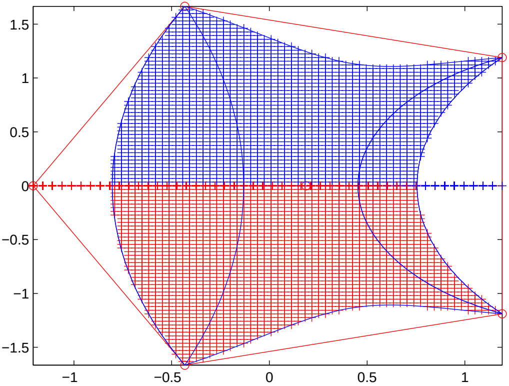
3 pairs of complex conjugate eigenvalues (square matrix), only 3 curves



Boundary of the feasible region

Example, $n = 6, k = 2$

2 pairs of complex conjugate eigenvalues, 2 real eigenvalues (3×4 matrix)



Boundary of the feasible region

We have some "spurious" curves

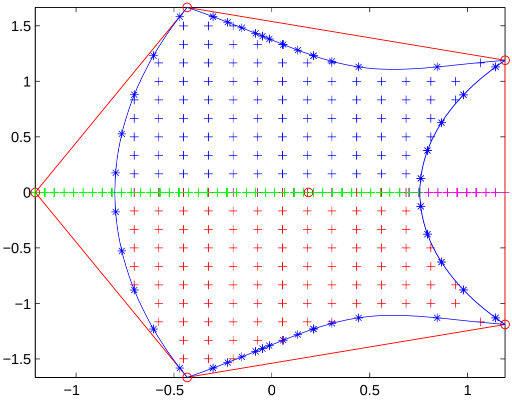
We can get rid of the “spurious” curves by computing some points on the boundary, considering some points around and seeing if those are inside or outside the feasible region (using the signs of the solution components)

This can be difficult close to the eigenvalues and some misclassifications may occur

However, we will see that the “spurious” curves may have some interest

Example, $n = 6$, $k = 2$

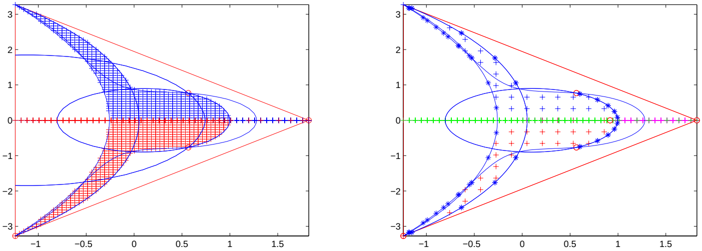
2 pairs of complex conjugate eigenvalues, 2 real eigenvalues (3×4 matrix)



Boundary of the feasible region

Example, $n = 6$, $k = 2$

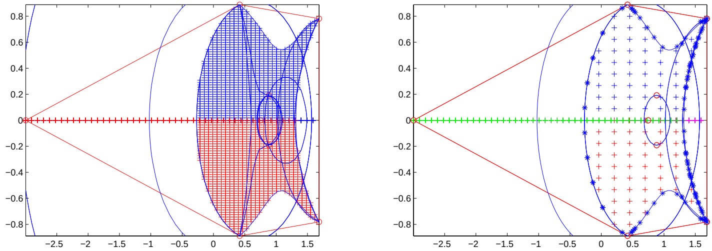
2 pairs of complex conjugate eigenvalues (one pair inside the convex hull), 2 real eigenvalues (3×4 matrix)



Boundary of the feasible region

Example, $n = 8$, $k = 2$

3 pairs of complex conjugate eigenvalues (one pair inside the convex hull), 2 real eigenvalues (3×5 matrix)



Boundary of the feasible region

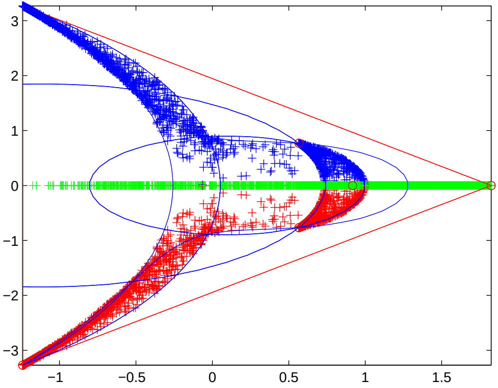
Open problems

What can we do for $k > 2$?

One can fix the location of all the Ritz values except for $\theta_1, \bar{\theta}_1$ and check for their possible locations (if any); see Bujanovic

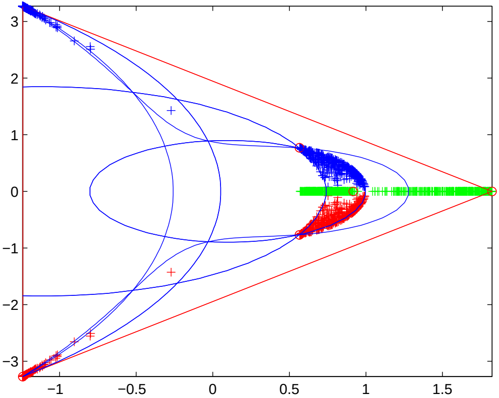
Let us do some experiments with random starting vectors

Example, $n = 6$



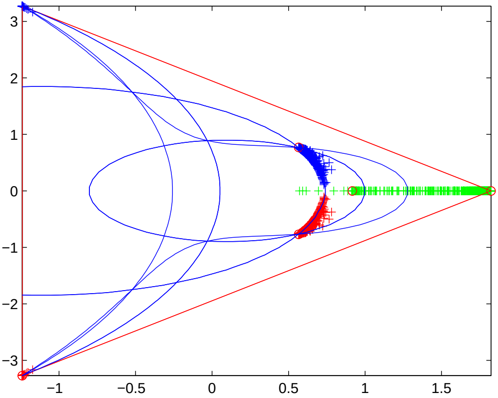
all $k = 2:5$, A normal real, location of the Ritz values, random starting vectors

Example, $n = 6$



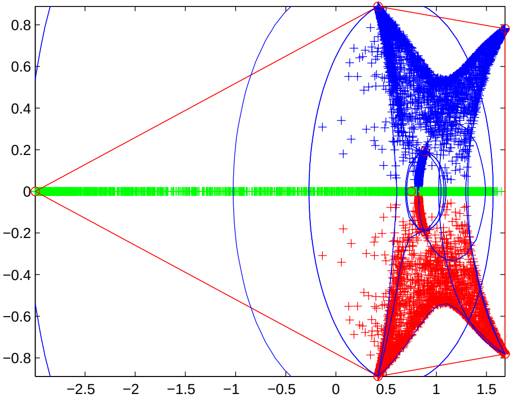
$k = 4$, A normal real, location of the Ritz values, random starting vectors

Example, $n = 6$



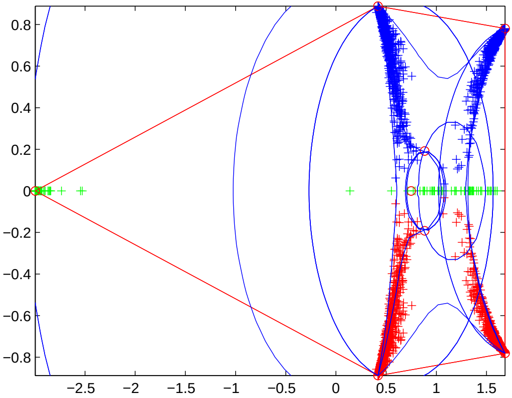
$k = 5$, A normal real, location of the Ritz values, random starting vectors

Example, $n = 8$



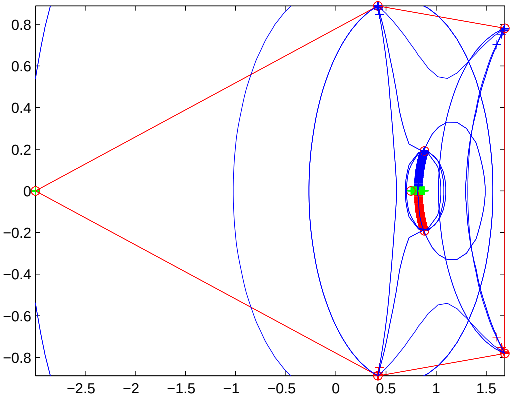
all $k = 2 : 7$, A normal real, location of the Ritz values, random starting vectors

Example, $n = 8$



$k = 5$, A normal real, location of the Ritz values, random starting vectors

Example, $n = 8$



$k = 7$, A normal real, location of the Ritz values, random starting vectors

An interesting open question is:

Why are some Ritz values for $k > 2$ preferably located near some of the “spurious” curves obtained for $k = 2$?

Conclusion

We have a necessary and sufficient condition for a set of complex values to be the Arnoldi Ritz values at some iteration

For normal matrices this condition involves finding a real positive solution of a (rectangular) linear system

For real normal matrices we were able to compute the boundary of the feasible region for $k = 2$

Even in simple cases, there are still many remaining open questions about the location of the Ritz values for $k > 2$