ON THE BOUNDARY OF THE PSEUDOSPECTRUM
AND ITS FAULT POINTS

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Abstract. The study of pseudospectra of linear transformations has become a significant part of numerical linear algebra and related areas. A large body of research activity has focused on how to compute these sets for a given spectral problem with, possibly, certain underlying structure. The theme of this paper was motivated by the question: How effective are path-following procedures for tracing the pseudospectral boundary? The present study of the mathematical properties of the boundary of the pseudospectrum is the result. Although this boundary is generally made up smooth curves, it is shown how the Schur triangular form of the matrix can be used to analyse the singular points of the boundary.

1. PRELIMINARIES

In this manuscript we discuss regularity properties of the boundary of the pseudospectrum of a matrix \( A \in \mathbb{C}^{n \times n} \). This boundary turns out to be a piecewise smooth curve. Our main concern is how the structure of the Schur triangular form of \( A \) determines the singular points on this curve.

Let us begin by adapting the results of [2] on general matrix polynomial to the particular case of the linear monic polynomial. Below, \( \text{Spec} A \) denotes the spectrum of \( A \) and \( \| \cdot \| \) denotes the (maximum) norm of \( A \) as a linear operator in the Euclidean space \( \mathbb{C}^n \). For a given \( \delta \geq 0 \), the pseudospectrum of \( A \) is the set

\[
\text{Spec}_\delta A := \bigcup_{\| E \| \leq \delta} \text{Spec} (A + E).
\]

By construction \( \text{Spec}_0 A = \text{Spec} A \). For \( \delta > 0 \) sufficiently small, \( \text{Spec}_\delta A \) consists of “small” connected components around \( \text{Spec} A \). As \( \delta \) increases, these components enlarge, collide and eventually intersect in various complicated ways and the boundary of \( \text{Spec}_\delta A \), \( \partial \text{Spec}_\delta A \), becomes more complex. Typically, corners will appear in \( \partial \text{Spec}_\delta A \) as a consequence of two or more of these components intersecting. As we shall see below, the least singular values of \( P(\lambda) = (\lambda - A) \) plays an important role in the dynamics of this process.

Let \( \lambda = x + iy \equiv (x, y) \) be in the complex plane (\( \equiv \mathbb{R}^2 \)). The singular values of \( P(\lambda) \) are the nonnegative square roots of the \( n \) eigenvalue...
functions of $P(\lambda)^*P(\lambda)$. They are denoted by
$$s_1(\lambda) \geq \ldots \geq s_n(\lambda) \geq 0.$$ Both the spectrum and the pseudospectra of $A$ are characterised by the
real-valued function $s_n : \mathbb{C} \rightarrow [0, \infty)$, given by the smallest singular
value. Indeed, it is well known [9] that for all $\delta \geq 0$,
\begin{equation}
\text{Spec}_\delta A = \{ \lambda \in \mathbb{C} : s_n(\lambda) \leq \delta \}.
\end{equation}
It will be seen that this characterisation is crucial for the study of
smoothness properties of the boundary, $\partial \text{Spec}_\delta A$. They are the subject
of the next section and the main conclusions are contained in Theorem 3. In particular, the notion of fault points (at which the least singular
value is multiple) is introduced and developed. In Section 3 the Schur
triangular form is studied and it is shown that, by defining a certain
equivalence relation on the eigenvalues of $A$, the general Schur triangle
can be reduced to a block diagonal form. It is natural to ask whether the
equivalence classes of eigenvalues generated in this way are independent
of the particular unitary transformation used. This is shown to be
the case when all eigenvalues of $A$ are distinct.

Section 4 includes a classification and study of singular points on
the boundary of a pseudospectrum and, finally, Section 5 is devoted to
a study of these singular points in the case of matrices with size not
exceeding $n = 3$.

2. Regularity properties of the pseudospectral boundary

Let us first consider regularity properties of $s_n(\lambda)$ as a function
defined on the complex plane. Let
$$\Sigma_j := \{(x, y, s_j^2(x, y)) \in \mathbb{R}^3 : (x, y) \in \mathbb{R}^2\}.$$ 

**Lemma 1.** $\bigcup_{j=1}^n \Sigma_j$ is a real algebraic variety.

**Proof.** Define the function
\begin{equation}
d(x, y, S) = \det [I S - P(x + iy)^*P(x + iy)], \hspace{1em} (x, y, S) \in \mathbb{R}^3.
\end{equation}
As the matrix $P(x+iy)^*P(x+iy)$ is hermitian, $d(x, y, S)$ is a polynomial
in $x, y, S$ with real coefficients, and since
$$\bigcup_{j=1}^n \Sigma_j = \{(x, y, S) \in \mathbb{R}^3 : d(x, y, S) = 0\},$$
the result follows. $\square$

Real algebraic surfaces usually have strong smoothness properties,
but self intersections and cusps of various types may also occur as the
following two examples demonstrate.
Example 1. If \( A = \text{diag}[1, e^{2i\pi/3}, e^{-2i\pi/3}] \), then
\[
\text{Spec}[P(\lambda)^*P(\lambda)] = \{|\lambda - 1|^2, |\lambda - e^{2i\pi/3}|^2, |\lambda - e^{-2i\pi/3}|^2\}.
\]
Thus \( \Sigma_1 \cup \Sigma_2 \cup \Sigma_3 \) is the union of three paraboloids of revolution with minima at \( 1, e^{2i\pi/3} \) and \( e^{-2i\pi/3} \) respectively. These paraboloids intersect each other in three different planes parallel to the vertical axis. The only point where the three surfaces intersect simultaneously is \((0, 0, 1)\).

Example 2. If
\[
A = \begin{pmatrix} 3/4 & 1 & 1 \\ 0 & 5/4 & 1 \\ 0 & 0 & -3/4 \end{pmatrix},
\]
\( \Sigma_1 \cup \Sigma_2 \cup \Sigma_3 \) has a conic double point at \((0, 0, 5/16)\). At this point \( s_3(0) = s_2(0) = \sqrt{5}/4 \).

It will be seen below that the occurrence of isolated singularities such as that of Example 2 is rare. In this example, the matrix \( A \) had to be carefully crafted to allow the conic double point around the origin. Any slight change in the coefficients of \( A \) would eliminate this degeneracy.

It is well known [4, Theorem S6.3] that, for each \( j \), \( s_j(\gamma(t))^2 \) is a real analytic function of \( t \in \mathbb{R} \) whenever \( \gamma : \mathbb{R} \rightarrow C \) is analytic. Thus, \( s_j(\lambda) = s_k(\lambda) \) for \( j \neq k \) on a non-empty open set \( \mathcal{O} \) only when \( \mathcal{O} = \mathbb{C} \). Therefore two different surfaces \( \Sigma_j \) can intersect only in a set of (topological) dimension at most one (see also [2]).

To describe these surfaces more precisely, let \( p_A \equiv p : \{1, \ldots, n\} \rightarrow \{1, \ldots, n\} \) (not always onto) satisfy the following properties:
(a) \( \Sigma_j = \Sigma_{p(j)} \).
(b) \( \bigcup_{j=1}^n \Sigma_j = \bigcup_{j=1}^n \Sigma_{p(j)} \) and
(c) \( \Sigma_{p(j)} = \Sigma_{p(k)} \iff p(j) = p(k) \).

The map \( p \) is a choice of the indexes of the different \( \Sigma_j \) and only these. We denote by \( m_A(j) \equiv m(j) = m(p(j)) \) the (constant) value of the algebraic multiplicity of \( s_j(\lambda) \) for almost all \( \lambda \in \mathbb{C} \).

We are now ready to identify the region of the plane where \( s_j(\lambda) \) is differentiable. Here and below \( \partial \) denotes partial differentiation with respect to \( S \). With the determinant function \( d \) as in [2], let
\[
\mathcal{G}_A^j := \{(x, y) \in \mathbb{R}^2 : \partial_S d^{1/m(j)}(x, y, s_j^2(x, y)) = 0\}.
\]

Lemma 2. Let \( \mathcal{O} \subseteq \mathbb{R}^2 \) be an open set such that \( \mathcal{O} \cap (\mathcal{G}_A^1 \cup \text{Spec } A) = \emptyset \). Then \( s_j^2(x, y) \) is differentiable in \( \mathcal{O} \).
Proof. This lemma is a consequence of the implicit function theorem applied to the function \(d(x, y, S)\). Clearly, the polynomial \(d(x, y, S)\) is continuously differentiable and, since \(\mathcal{O} \cap \text{Spec} \mathcal{A} = \emptyset\), \(d(x, y, s_2^j(x, y)) \neq 0\) for \((x, y) \in \mathcal{O}\). These two facts ensure that \(d^{1/m(j)}(x, y, S)\) is also continuously differentiable in a suitable \(\mathbb{R}^3\) neighbourhood of \(\Sigma_j \cap (\mathcal{O} \times \mathbb{R})\). Since \(\mathcal{O} \cap \mathcal{G}_A^j = \emptyset\), the hypotheses of the implicit function theorem applied to \(\Sigma_j\) are fulfilled. Since \(s_2^j(x, y)\) is the actual “implicit” function given locally (and hence globally) by this theorem, the result follows. \(\square\)

Note that we can compute \(\nabla s_2^j\) on \(\mathcal{O}\) by implicit differentiation.

The sets \(\mathcal{G}_A^j\) introduced above are closely related to the set of “fault points” introduced in [2]. For \(j = 1, \ldots, n\), let

\[
\mathcal{F}_A^j := \{ (x, y) : s_{p(j)}(x, y) = s_{p(k)}(x, y) \text{ for some } k \text{ s.t. } p(j) \neq p(k) \}.
\]

Here, we call \(\mathcal{F}_A := \mathcal{F}_A^n\) the set of fault points of \(A\). Typically \(\mathcal{F}_A\) is made up of fault lines or curves where \(\nabla s_n(\lambda)\) is undefined.

Let \(\{p_1, \ldots, p_l\} := p\{1, \ldots, n\}\). By construction, \(s_{p_i} \neq s_{p_k}\) almost everywhere and

\[
d(x, y, S) = (S - s_2^{p_1})^{m(p_1)} \cdots (S - s_2^{p_l})^{m(p_l)}.
\]

Also

\[
\partial_S d^{1/m(p_i)}(x, y, S) = \sum_{j=1}^{l} \frac{m(p_j)}{m(p_i)} (S - s_2^{p_j})^{-\frac{m(p_j)}{m(p_i)}} \prod_{k \neq j, 1 \leq k \leq n} (S - s_2^{p_k})^{-\frac{m(p_k)}{m(p_i)}}.
\]

So \((\tilde{x}, \tilde{y})\) satisfies \(s_{p_i}(\tilde{x}, \tilde{y}) \neq s_{p_j}(\tilde{x}, \tilde{y})\) for all \(i \neq j\) if and only if

\[
\partial_S d^{1/m(p_i)}(\tilde{x}, \tilde{y}, s_{p_i}(\tilde{x}, \tilde{y})) \neq 0.
\]

It follows from this observation that

\[
(3) \quad \mathcal{G}_A^j = \mathcal{F}_A^j, \quad j = 1, \ldots, n.
\]

In particular \(s_n(\lambda)\) will be differentiable outside \(\mathcal{F}_A\). This justifies the name chosen for the latter set.

Clearly [2],

\[
(4) \quad \partial \text{Spec}_\delta A \subseteq \{ z \in \mathbb{C} : s_n(\lambda) = \delta \}.
\]

Note that equality in (4) does not hold in general. In Example 1 above the origin is in the right hand set, but it is an interior point of \(\text{Spec}_1 A\).

**Theorem 3.** For any \(\delta > 0\) the boundary of \(\text{Spec}_\delta A\) is a piecewise smooth portion of an algebraic curve. In particular, it has a finite number of singularities. These singularities are either cusps or self-intersections. If \(\lambda_0 \in \partial \text{Spec}_\delta A\) is a cusp, then \(\lambda_0 \in \mathcal{F}_A\).
Proof. The first part of the theorem is Theorem 7 of [2]. For the latter part note that if a singularity occurs at $\lambda_0 \in \partial \text{Spec}_\delta A$, then either $\lambda_0 \in F_A$ or $\nabla s_n(\lambda_0) = 0$. If $\nabla s_n(\lambda_0) = 0$, then either $\lambda_0$ is a point of self-intersection or $\lambda_0 \in \text{Spec} A$. Since no eigenvalue of $A$ lies on the pseudospectral boundary, the result follows. □

Theorem 3 extends to matrix polynomials without much effort.

3. Refinement of the Schur triangular form

We denote a Schur factorisation of $A$ by $A = USU^*$, where

$$S = \begin{pmatrix}
\alpha_1 & t_{12} & \cdots & t_{1n} \\
0 & \alpha_2 & \ddots & \vdots \\
\vdots & \ddots & \ddots & t_{(n-1)n} \\
0 & \cdots & 0 & \alpha_n
\end{pmatrix}$$

and $U$ is a unitary matrix. Note that Spec $A$ consists of the distinct $\alpha_j$, and that $S$ and $U$ are not uniquely defined. The singular values of $P(\lambda)$ are invariant under unitary similarity transformation, so the Schur form is an invariant as far as spectrum, pseudospectrum and fault points are concerned.

The characterisation of all possible Schur triangular forms of a general matrix $A$ is certainly beyond the scope of this manuscript. However, Theorems 5 and 6 below suggest how this issue can be approached. Some preliminary considerations are required.

Definition 1. Let $A = U^*SU$ be a Schur factorisation of $A$ with $S$ as in (5):

(a) We write $\alpha_i \simeq \alpha_j$ and say that $\alpha_i$ is directly related to $\alpha_j$ if one of the following conditions holds:

(i) $i = j$, (ii) $i < j$ and $t_{ij} \neq 0$, (iii) $i > j$ and $t_{ji} \neq 0$.

(b) We write $\alpha_i \simeq \alpha_j$ and say that $\alpha_i$ is block equivalent to $\alpha_j$ if and only if there exists a subset $\{\sigma_1, \ldots, \sigma_m\}$ of $\{1, \ldots, n\}$ such that

$$\alpha_i \simeq \alpha_{\sigma_1} \simeq \cdots \simeq \alpha_{\sigma_m} \simeq \alpha_j.$$

In this definition we consider that any two eigenvalues on the diagonal of $S$ are “different” even in the presence of multiplicity. The symbol “$\simeq$” obviously defines an equivalence relation on the set $\{\alpha_i\}_{i=1}^n$.

Let $D$ be the binary matrix obtained from $S$ by preserving the zeros of the latter and replacing the non-zero entries by 1. Then $D$ is the adjacency matrix (see [3]) of a graph, $G$. Two diagonal entries of $S$ will be block equivalent, $\alpha_i \simeq \alpha_j$, if and only if the nodes $i$ and $j$ of $G$ are connected with a path.
Lemma 4. Let $\sigma$ be any permutation of $\{1, \ldots, n\}$ and $S$ be upper triangular, as in (5). Then there is a unitary matrix $V$ such that

$$V^*SV = \begin{pmatrix}
\alpha_{\sigma(1)} & r_{12} & \cdots & r_{1n} \\
0 & \alpha_{\sigma(2)} & \ddots & \vdots \\
\vdots & \ddots & \ddots & r_{(n-1)n} \\
0 & \cdots & 0 & \alpha_{\sigma(n)}
\end{pmatrix}$$

and $\alpha_i \asymp \alpha_j$ if and only if $\alpha_{\sigma(i)} \asymp \alpha_{\sigma(j)}$.

**Proof.** By writing the permutation $\sigma$ as a product of transpositions (cycles of length 2), we see that the case $n = 2$ can play an important role. In this case $S = \begin{pmatrix} \alpha_1 & t \\ 0 & \alpha_2 \end{pmatrix}$ with $t \neq 0$ (so that $\alpha_1 \asymp \alpha_2$) and there is just one permutation $\sigma$ of interest: $(1, 2) \rightarrow (2, 1)$.

Let $\alpha_2 - \alpha_1 = be^{i\theta}$ ($b \geq 0$), and $a = |t|$ and consider the real orthogonal matrix

$$W := \frac{1}{\sqrt{a^2 + b^2}} \begin{pmatrix} a & -b \\ b & a \end{pmatrix}.$$ 

A little calculation shows that

$$W^*SW = \begin{pmatrix} \alpha_2 & |t|e^{i\theta} \\ 0 & \alpha_1 \end{pmatrix}.$$ 

Since $t \neq 0$, $|t|e^{i\theta} \neq 0$, and $\alpha_2 \asymp \alpha_1$, as required.

For the case $n > 2$ let $a_k = |t_{k,k+1}|$, $\alpha_{k+1} - \alpha_k = b_ke^{i\theta_k}$, ($b_k \geq 0$), and let

$$W_k = \frac{1}{\sqrt{a_k^2 + b_k^2}} \begin{pmatrix} a_k & -b_k \\ b_k & a_k \end{pmatrix}.$$ 

Define

$$V_k = \text{diag} (I_{k-1}, W_k, I_{n-k-1}).$$

Using a conforming block structure for $S$,

$$V_k^*SV_k = \begin{pmatrix} S_{11} & S_{12}W_k & S_{13} \\
0 & W_k^*S_{22}W_k & W_k^*S_{23} \\
0 & \text{tr} \end{pmatrix} =: R$$

and

$$W_k^*S_{22}W_k = \begin{pmatrix} \alpha_{k+1} & t_{k+1,k}e^{i\theta_k} \\ 0 & \alpha_k \end{pmatrix}.$$ 

By construction, the upper-right entry of the latter matrix is zero if and only if $t_{k+1,k} = 0$. Thus $\alpha_k \asymp \alpha_{k+1}$ (using $S$) if and only if $\alpha_{k+1} \asymp \alpha_k$ (using $R$).

Since the general permutation $\sigma$ can be expressed as a product of “contiguous” cycles as used above, the required transforming matrix $V$
can be expressed as a product of the elementary unitary matrices $V_k$ introduced above.

We now show that a block diagonal factorisation for $A$ can be obtained from the relation "$\approx$".

**Theorem 5.** Given any upper triangular matrix $S \in \mathbb{C}^{n \times n}$ there exists a unitary matrix $U$ preserving "$\approx$" such that

$$U^*SU = \text{diag} [B_1, \ldots, B_k],$$

where, for $l = 1, \ldots, k$,

$$B_l = \begin{pmatrix}
\tilde{\alpha}_1(l) & r_{12}(l) & \cdots & r_{1m_l}(l) \\
0 & \tilde{\alpha}_2(l) & \ddots & \vdots \\
\vdots & \ddots & \ddots & r_{(m_l-1)m_l}(l) \\
0 & \cdots & 0 & \tilde{\alpha}_{m_l}(l)
\end{pmatrix},$$

and $\tilde{\alpha}_i(l) \approx \tilde{\alpha}_j(l)$ for all $i, j$ and $l$.

**Proof.** Since "$\approx$" is an equivalence relation, it partitions $\text{Spec} S$ into a family of equivalence classes. So there is a permutation

$$\sigma = \{\sigma(1), \ldots, \sigma(n)\}$$

and there are positive integers $l_1 < l_2 < \ldots < l_k < n$ such that

$$\{\alpha_{\sigma(1)}, \ldots, \alpha_{\sigma(l_1)}, \{\alpha_{\sigma(l_1+1)}, \ldots, \alpha_{\sigma(l_2)}\}, \ldots, \{\alpha_{\sigma(l_k+1)}, \ldots, \alpha_{\sigma(n)}\}\}$$

is the partition of $\text{Spec} S$ under "$\approx$". The $U$ found in Lemma [4] for this $\sigma$ provides the desired conclusion. □

In this theorem, $\tilde{\alpha}_i(l) \approx \tilde{\alpha}_j(l)$ if and only if $l = \tilde{l}$. The blocks $B_l$ are not necessarily unique in the representation $U^*SU = \text{diag} [B_1, \ldots, B_k]$. The diagonal blocks can be permuted, for example.

Note that the equivalence classes given by "$\approx$" on the set $\{\alpha_i\}_{i=1}^n$, correspond to the connected components of the graph $G$ introduced above. When $S$ is sparse, strategies for computing the block diagonalisation [6] may be based on this observation.

It is natural to ask whether Definition [1] is independent of $U$ and $S$ in the Schur decomposition for $A$. We obtain a positive answer if all eigenvalues of $A$ are simple.

**Theorem 6.** Suppose that $A$ has no multiple eigenvalues, i.e. $\alpha_i \neq \alpha_j$ for $i \neq j$. Then the equivalence classes determined by the equivalence relation "$\approx$" of Definition [7] are independent of the Schur factorisation chosen for $A$.
Proof. This result is a direct consequence of the following observation. If $S$ and $T$ are two triangular matrices with the same diagonal entries $s_{ii} = t_{ii} = \alpha_i$ and with $\alpha_i \neq \alpha_j$ for $i \neq j$, such that $U^*TU = S$ for a suitable unitary matrix $U$, then $U$ must be diagonal. See [8, Theorem 2.3] or [7]. □

The results reviewed at length in [8] suggest that extension of this theorem to admit multiple eigenvalues of $A$ would be difficult.

4. The singular points on the pseudospectral boundary

As we shall see next, the block diagonalisation found in Theorem 5 provides a natural classification of the singular points on the boundary of the pseudospectra of $A$.

Let $S$ be a Schur triangular form of $A$ and $B_l$ be the blocks corresponding to the diagonalisation of $S$ given in (7). It is clear from the definition that the singular values of $P(\lambda) = \lambda - A$ are those of $(\lambda - B_l)$ for $l = 1, \ldots, k$. Then it follows from (7) that

$$\text{Spec}_\delta A = \bigcup_{l=1}^k \text{Spec}_\delta B_l,$$

for all $\delta \geq 0$.

This decomposition motivates the following classification of singular points on the boundary of the pseudospectrum:

Definition 2. We say that $\lambda_0 \in \partial\text{Spec}_\delta A$ is a

- stationary point if $\lambda_0 \notin \mathcal{F}_A$ but $\nabla s_n(\lambda_0) = 0$,
- essential fault point if $\lambda_0 \in \mathcal{F}_{B_l}$ for some $l = 1, \ldots, k$,
- regular fault point if $\lambda_0 \in \mathcal{F}_A$ but it is not an essential fault points.

Clearly a stationary point of $A$ must also be a stationary point of $B_l$ for some (not necessary unique) $l = 1, \ldots, k$.

If $\lambda_0 \in \mathcal{F}_A$, then either $\lambda_0 \in \bigcup_{l=1}^k \mathcal{F}_{B_l}$ or

$$\lambda_0 \in (\partial\text{Spec}_\delta B_k \cap \partial\text{Spec}_\delta B_l) \setminus \bigcup_{l=1}^k \mathcal{F}_{B_l}$$

for some $k \neq l$. In the former case, $\lambda_0$ is an essential fault point and in the latter it is a regular fault point.

Since it is formed as a consequence of two pseudospectra of different blocks $B_l$ intersecting, whenever non-empty, the regular portion of $\mathcal{F}_A$ is expected to be of topological dimension 1. On the other hand, we shall argue in Section 5 that blocks of small size have only a limited number of essential fault points.
The role played by the classification just introduced in the dynamics of the pseudospectrum of $A$ can be better visualised by means of concrete examples. However, let us first establish two elementary consequences of (7).

**Corollary 7.** If $A$ is a normal matrix, then all singular points on $\partial \text{Spec}_\delta A$ are regular fault points. Furthermore, $\mathcal{F}_A$ is the Voronoi diagram associated to $\text{Spec} A$.

**Proof.** The proof is straightforward. See Example 1 for illustration. 

**Corollary 8.** Let $A$ be unitarily similar to a bi-diagonal matrix. Then $\mathcal{F}_A = \emptyset$ if and only if no entry in the off-diagonal of $A$ vanishes.

**Proof.** Use the fact that $(\lambda - B)^*(\lambda - B)$ is a tri-diagonal symmetric matrix. See [10, §5.36].

Corollary 8 implies that bi-diagonal matrices have no essential fault points.

**Example 3.** A detailed analysis is made of a problem with two diagonal blocks ($k = 2$); see also Figure 2. Let

$$A = \begin{pmatrix} 3 & 0 & 0 \\ 0 & -1 & 1 \\ 0 & 0 & 1 \end{pmatrix}.$$ 

Any pseudospectrum of $A$ is the union of those of the blocks

$$B_1 = 3 \quad \text{and} \quad B_2 = \begin{pmatrix} -1 & 1 \\ 0 & 1 \end{pmatrix}.$$ 

The (only) singular value of $(x + iy - B_1)$ is $\sqrt{(x - 3)^2 + y^2}$, so $\text{Spec}_\delta B_1$ is a disk centred at $(x, y) = (3, 0)$ of radius $\delta$. The singular values of $B_2$ are

$$s_{\pm}(x + iy) = \left(\frac{3}{2} + x^2 + y^2 \pm \sqrt{5 + 20x^2 + 4y^2}\right)^{1/2}.$$ 

It is straightforward to see that the least singular value $s_-(x + iy) = \delta$ if and only if

$$(x^2 + y^2)^2 - 2(1 + \delta^2)x^2 + 2(1 - \delta^2)y^2 + 1 - 3\delta^2 + \delta^4 = 0.$$ 

This shows that $\text{Spec}_\delta B_2$ is a spiric section for all $\delta > 0$. It is also straightforward to see that $\mathcal{F}_A$ is a portion of the hyperbola given explicitly by

$$\mathcal{F}_A = \{(x, y) : 31x^2 - y^2 - 90x + 55 = 0, x > 1\}.$$
Any singularity on $\partial \text{Spec}_\delta A$ which arises as a consequence of $\partial \text{Spec}_\delta B_1$ intersecting with $\partial \text{Spec}_\delta B_2$, will be a regular fault point. Also, the curve $\partial \text{Spec}_\delta B_2$ has a stationary point at the origin when $\delta = \sqrt{\frac{3-\sqrt{5}}{2}}$.

Note that a further self-intersection occurs on $\partial \text{Spec}_\delta A$ at $(x, y) = (\frac{45+8\sqrt{5}}{31}, 0)$ for $\delta = \frac{48-8\sqrt{5}}{31}$ since the boundaries of $\text{Spec}_\delta B_1$ and $\text{Spec}_\delta B_2$ touch at this point. The pseudospectrum of $A$ will consist of three connected components for $0 \leq \delta < \sqrt{\frac{3-\sqrt{5}}{2}}$, two components for $\sqrt{\frac{3-\sqrt{5}}{2}} \leq \delta < \frac{48-8\sqrt{5}}{31}$ and a single component for all $\delta \geq \frac{48-8\sqrt{5}}{31}$.

The next observation may be relevant in the effective design of a corrector step in path-following algorithms for tracking $\partial \text{Spec}_\delta A$. The second part asserts that the corners in $\partial \text{Spec}_\delta A$ at regular fault points will always be re-entrant.

**Lemma 9.** Let $\lambda_0$ be a regular fault point in $\partial \text{Spec}_\delta A$. Assume that the curve $\partial \text{Spec}_\delta A$ fails to have a tangent line at $\lambda_0$ and does not self-intersect at this point. Then we can always find an $\alpha > \pi$, depending only on $\lambda_0$, satisfying the following property: If $0 < \beta < \alpha$, there exists $r > 0$ and $0 \leq \gamma < 2\pi$ such that the sector

$$\{ \lambda = \lambda_0 + \rho e^{i(\theta + \gamma)} : 0 \leq \theta \leq \beta, 0 \leq \rho \leq r \} \subset \text{Spec}_\delta A.$$  

**Proof.** This is a consequence of the fact that a regular fault point of $\partial \text{Spec}_\delta A$ is formed by two different intersecting connected components. \qed

**Theorem 10.** If $\alpha_i, \alpha_j \in \text{Spec}_A$ are in the same connected component of $\mathbb{C} \setminus \mathcal{F}_A$, then $\alpha_i \simeq \alpha_j$.

**Proof.** It suffices to show that if $\alpha_i \neq \alpha_j$, then any continuous trajectory $\phi : [0, 1] \rightarrow \mathbb{C}$ such that $\phi(0) = \alpha_i$ and $\phi(1) = \alpha_j$, intersects $\mathcal{F}_S$ (see (1)). We achieve this by noticing that $\alpha_i \in \text{diag}[B_l]$ and $\alpha_j \in \text{diag}[B_m]$ for $l \neq m$, and applying the mean value theorem inductively to $\rho_i - \rho_j$, where

$$\rho_k(t) := \min.\text{sing.val}(\phi(t) - B_p), \quad \alpha_k \in \text{diag}[B_p].$$  

The converse of Theorem 10 does not hold in general. It is easy to construct examples where $\alpha_i \simeq \alpha_j$, but $\alpha_i, \alpha_j$ both belong to different components of $\mathbb{C} \setminus \mathcal{F}_A$. One such example is the following.
Example 4. If

\[
A = \begin{pmatrix}
-1 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & -i & 1 \\
0 & 0 & 0 & i
\end{pmatrix},
\]

\[\mathcal{F}_A = \{\lambda \in \mathbb{C} : \text{Re } \lambda = \pm \text{Im } \lambda\}.\]

5. Essential fault points and the Schur structure of small matrices

Determining the structure of \(\mathcal{F}_A\) for a given matrix \(A\), is typically involved. As we confirmed in the previous section, the set of fault points can be empty or consist of a single point, but it can also be a complicated set such as a Voronoi diagram. By virtue of (7), the set of regular fault points is completely characterised once the pseudospectra of each of the blocks in the diagonal factorisation (6) are known. In this section we show that, for sufficiently small matrices, the number of essential fault points is finite.

It is easy to characterise the set of fault points of a \(2 \times 2\) triangular matrix

\[
B = \begin{pmatrix}
\alpha & r \\
0 & \beta
\end{pmatrix}.
\]

If \(\alpha \cong \beta\), then \(\mathcal{F}_B = \emptyset\). If \(\alpha \neq \beta\), then

\[\mathcal{F}_B = \{\lambda \in \mathbb{C} : |\lambda - \alpha| = |\lambda - \beta|\}\]

for \(\alpha \neq \beta\) and \(\mathcal{F}_B = \emptyset\) for \(\alpha = \beta\). By virtue of Corollary 8, no fault point of a \(2 \times 2\) matrix can be essential.

The \(3 \times 3\) case is more involved. This is illustrated in the following example (which is a generalisation of Example 2).

Example 5. See Figure 3. Let

\[
A = \begin{pmatrix}
a & 1 & 1 \\
0 & 5/4 & 1 \\
0 & 0 & c
\end{pmatrix},
\]

where \(|a| = |c| = 3/4\). Then \(\mathcal{F}_A = \{0\}\) and \(a \cong 5/4 \cong c\). Whenever \(0 \in \partial \text{Spec}_\delta A\), it will be an essential fault point. This can only occur at \(\delta = s_3(0) = \sqrt{5}/4\).

The complicated dynamic of the pseudospectral boundary as we move the parameters \(a\) and \(c\) on the circle with radius \(3/4\), is illustrated in Figure 3. There we show the evolution of the essential singularity when \(a = 3e^{i\theta}/4\) for \(\theta = k\pi/4\), \(k = 0, 1, 2, 3, 4\). When
$k = 0$, $\text{Spec}_{\sqrt{5}/4}A$ is connected and there is clear indication of a re-entrant corner on the left side of the boundary. The re-entrant angle at this corner becomes more pronounced when $k = 1$. For $k = 2, 3$ the concavity prevails. However there exist critical $\theta_1 \in (\pi/4, \pi/2)$ and $\theta_2 \in (3\pi/4, \pi)$, such that $0 \not\in \partial\text{Spec}_{\sqrt{5}/4}A$ for $\theta \in (\theta_1, \theta_2)$, and hence there is no corner on $\partial\text{Spec}_{\sqrt{5}/4}A$. At the final stage $k = 4$, the pseudospectrum now consists of two connected components, the concavity on the left side has vanished, however a new re-entrant corner forms in a different part of the boundary.

More generally, let

$$B = \begin{pmatrix} \alpha_1 & r & s \\ 0 & \alpha_2 & t \\ 0 & 0 & \alpha_3 \end{pmatrix}. \tag{8}$$

When $\alpha_j \neq \alpha_k$ for some $j \neq k$, $B$ can be reduced to a block diagonal form of smaller size, so the set of fault points is characterised by using (7). If $\alpha_1 \simeq \alpha_2 \simeq \alpha_3$, every point in $\mathcal{F}_B$ is an essential fault point and we have the following result.

**Theorem 11.** Let $B$ be as in (8) and assume that no two of the upper triangular entries $r, s, t$ vanish simultaneously (i.e. $\alpha_1 \simeq \alpha_2 \simeq \alpha_3$). If $rst = 0$, then $\mathcal{F}_B = \emptyset$. If $rst \neq 0$, then $\mathcal{F}_B$ is either empty or consists of a single point. In the latter case,

$$\mathcal{F}_B \subset \{ \lambda \in \mathbb{C} : \arg(\alpha_2 - \lambda) = \arg(rst) \}. \tag{9}$$

**Proof.** If $rst = 0$, the claimed assertion is a consequence of Corollary 8 and a suitable permutation of the rows and columns of $B$.

Let $a = (\alpha_1 - \lambda)$, $b = (\alpha_2 - \lambda)$, $c = (\alpha_3 - \lambda)$, and assume that $rst \neq 0$. Let

$$B_1 = \begin{pmatrix} a & r \\ 0 & b \end{pmatrix} \quad \text{and} \quad u = \begin{pmatrix} s \\ t \end{pmatrix},$$

so that

$$B - \lambda = \begin{pmatrix} B_1 & u \\ 0 & c \end{pmatrix},$$

and

$$(B - \lambda)^*(B - \lambda) = \begin{pmatrix} B_1^*B_1 & v \\ v^* & \|u^*\|^2 + |c|^2 \end{pmatrix},$$

where $v = B_1^*u$. By the Cauchy interlacing theorem, if $B^*B$ has a double eigenvalue $\sigma = s_3^2 = s_2^2$, then $\sigma$ is also the minimal eigenvalue of $B_1^*B_1$.  \diamond
Since \( r \neq 0 \), \( B_1^* B_1 \) has only simple eigenvalues. Let \( 0 \neq e \in \mathbb{C}^2 \) be an eigenvector such that \( B_1^* B_1 e = \sigma e \). A straightforward argument shows that, if \( \sigma \) is a double eigenvalue of \( B^* B \), then \( v \perp e \).

Now, \( v = \begin{pmatrix} \overline{t} s \\ \tau s + \overline{b} t \end{pmatrix} \),

\[
2\sigma = |a|^2 + |b|^2 + |r|^2 - \sqrt{(|a|^2 + |b|^2 + |r|^2)^2 - 4|a|^2|b|^2} \quad \text{and} \quad e = \begin{pmatrix} |b|^2 - |a|^2 + |r|^2 - \sqrt{(|a|^2 + |b|^2 + |r|^2)^2 - 4|a|^2|b|^2} \\ -2a\tau \end{pmatrix}.
\]

Note that all these three quantities depend on \( \lambda \). If \( v^* e = 0 \), then \( q(\lambda) = \overline{\tau}(|b|^2 - |a|^2 - |r|^2 - \sqrt{(|a|^2 + |b|^2 + |r|^2)^2 - 4|a|^2|b|^2}) - 2\tau \overline{t} b = 0 \).

As the coefficient of \( \overline{\tau} \) in the above expression is real, (9) is guaranteed.

Let \( \gamma(t) = \alpha t + \overline{t} e^{i \arg(\tau \overline{t})} \), \( -\infty < t < \infty \), be a parameterisation of the line where \( \mathcal{F}_A \) lies. Then \( q(\gamma(t)) = q_1(t) - \sqrt{q_2(t)} \) where \( q_1 \) depends linearly in \( t \) and \( q_2 \) is a quadratic polynomial in \( t \). Moreover, \( (q_1(t))^2 \) and \( q_2(t) \) have the same coefficient of order 2 in \( t \). Thus \( q(\gamma(t)) \) can only vanish at no more than one \( t \)-value, \( t_1 \). Since \( \gamma(t_1) \) is the only possible essential fault point of \( B \), the proof is complete.

In Example 5 the line described by the right hand expression in (9) is the real axis and \( \mathcal{F}_A \) is the origin.

It is natural to expect that the argument presented in the proof of Theorem 11 can be extended inductively to blocks of larger size. We have not explored this possibility in much detail. However our observations lead us to conjecture that, perhaps, the number of essential fault points is always finite for matrices of any size. This issue certainly requires further investigation.

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Figure 1. Pseudospectra of a randomly generated diagonal matrix along with the Voronoi diagram associated to the spectrum.

Figure 2. Example \( \text{Example} \) The thick lines are \( \partial \text{Spec}_\delta A \) for \( \delta = 2/5, \sqrt[4]{31}/8, 8/5 \). The thin line is \( \mathcal{F}_A \).
Figure 3. Evolution of the essential singularity on the pseudospectral boundary for the family of matrices given in Example 5. Here $a = \bar{c} = 3e^{ik\pi/4}/4$ for $k = 0, 1, 2, 3, 4$ (top to bottom). On the left side we depict $\partial\text{Spec}_\delta A$ for $\delta = \frac{3}{4\sqrt{5}}$, $\frac{\sqrt{5}}{4}$, $\frac{41}{4\sqrt{5}}$. On the right side we show details of the pseudospectral boundaries near the origin for $\delta$ close to the critical value $\sqrt{5}/4$. 