Abstract

This report was written in 2001 and it is a translation of work that was originally published in Greek, in the author’s diploma thesis in July 1998. It may contain minor mistakes and should not be considered a complete study. It however touches upon several of the considerations that will be included in the complete paper. The work was done jointly with E. Gallopoulos and was presented at the FOCM99 conference, at the 5th IMACS conference on iterative methods in scientific computing, and at the 50th annual meeting of SIAM.

We present an iteration for the computation of simple eigenvalues using a pseudospectrum approach. The most appealing characteristic of the proposed iteration is that it reduces the computation of a single eigenvalue to a small number of eigenvalue computations on Hermitian matrices. We show that this number is directly associated with the matrix pseudospectrum. We present numerical results and we discuss advantages and drawbacks of the method. We also discuss its relationship with an iteration that was proposed independently in [Stewart, O’Leary, ETNA, Vol 8, 1998].

1 A pseudospectrum setting

We shortly describe some well known characteristics of matrix pseudospectrum. Denote with $\Lambda(A)$ the spectrum of a matrix $A$, with $\Lambda_\epsilon(A)$ the $\epsilon$-pseudospectrum of $A$, with $\sigma_{\text{min}} = \sigma_N \leq \sigma_{N-1} \leq \ldots \leq \sigma_1$ the singular values of $A$, and with $D(z, \rho)$ and $D^\circ(z, \rho)$ a closed disk and an open disk respectively, with center $z$ and radius $\rho$. Let $N$ denote a normal matrix.

Theorem 1

• $\Lambda(A) \subset \Lambda_\epsilon(A)$ for $\epsilon > 0$.
• $\epsilon < \epsilon_1 \iff \Lambda_\epsilon(A) \subset \Lambda_{\epsilon_1}(A)$.
• $\Lambda(N) = \Lambda(A) \Rightarrow \Lambda_\epsilon(N) \subseteq \Lambda_\epsilon(A)$.

These properties state that $\epsilon$-pseudospectrum forms closed curves around eigenvalues. The crucial property of subharmonicity of the norm of the resolvent $\| (zI - A)^{-1} \|$ (see [2]), assures that

$$\sigma_{\text{min}}(zI - A) = \text{local minimum} = 0 \iff z \in \Lambda(A) \tag{1}$$

This alternative characterization of an eigenvalue together with the properties of matrix pseudospectrum appeal for the corresponding optimization problem:

$$\min f(z) = \sigma_{\text{min}}(zI - A), \ z \in \mathbb{C}$$

Notice that in this formulation we are seeking for a minimizer over the complex plane. This is not usually the case in other methods for the computation of eigenvalues. The “heart” of any competent minimization algorithm can naturally be the following theorem by Sun [11].
Theorem 2 Denote with $\sigma_i$ the $i^{th}$ singular value and $u_i$, $v_i$ the corresponding left and right singular vectors. Let also $z = x + iy \in \mathbb{C} \setminus \Lambda(A)$. Then $g(x, y) = \sigma_i(zI - A)$ is real analytic in a neighborhood of $(x, y)$, if $\sigma_{\min}(zI - A)$ is a simple singular value. For the gradient of $g(x, y)$ we have

$$\nabla g(x, y) = (Re(v^*_i u_i), Im(v^*_i u_i))$$

What is interesting, is that $\nabla \sigma_{\min}(zI - A)$ can be computed almost as easy as $\sigma_{\min}$ itself. Given that $\sigma_{\min}$ can be computed by means of some of the well known methods for Hermitian matrices, we can readily setup the framework for a minimization algorithm. Using for example a steepest descent strategy we get the extremely compact Matlab routine shown below.

```matlab
function z=sdeig(A,starting_point)

z= starting_point; s_min= 1;
while (s_min > tol)
    [u_min, s_min, v_min] = svds(z*I-A);
    direction = v_min'*u_min / |v_min'*u_min|;
    step_size = ? ;
    z = z - step_size*direction;
end
```

The determination of the step size is obviously of critical importance for the effectiveness of the `sdeig`. In our experiments we used the general purpose minimization function `fminu` of Matlab Optimization Toolbox, supplemented with the gradient information. Alas, even for a moderate accuracy of the output approximate eigenvalue, the number of iterations (and $\sigma_{\min}$ evaluations) of `fminu`, usually exceeded the number of 100.

The main part of this paper aims to determine a strategy for selecting the step size. Using mainly results from our work for the efficient computation of the pseudospectrum [3], we give a simple and computationally efficient formula for the step size, which as we shall see, when incorporated in `sdeig` gives a powerful iteration.

2 Determining Step Size

In this section we will use theorems proven in [3]. Denote by $D^\epsilon(z, r)$ the open disk with center $z$ and radious $r$. We usually denote with $\sigma_{\min}(z)$ the minimum singular value of $zI - A$ and with $u_{\min}(z), v_{\min}(z)$ the corresponding left and right singular vectors.

Theorem 3 If $\sigma_{\min}(zI - A) = r > \epsilon$, then $D^\epsilon(z, r - \epsilon) \cap \Lambda_e(A) = \emptyset$. In the extreme case $\epsilon = 0$, we have $D^\epsilon(z, r) \cap \Lambda(A) = \emptyset$.

Is $\sigma_{\min}(zI - A)$ a good candidate for step size? The answer is affirmative in the case of normal matrices, as the following corollary shows:

Corollary 1 If $N \in \mathbb{C}^{n \times n}$ is normal, $z_i, i = 1, \ldots, n$ are its eigenvalues, and $\sigma_{\min}(zI - N) = r > \epsilon$ then the perimeter $\partial D(z, r - \epsilon)$ contains at least one point of $\Lambda_e(N)$. In the extreme case $\epsilon = 0$, the disk $D(z, r)$ “touches” at least one eigenvalue of $N$.

Corollary 1 along with the observation that pseudospectra of normal matrices are concentric circles around eigenvalues, guarantee that `sdeig` always finds in one step the eigenvalue closest to the starting point. However, in non-normal matrices the pseudospectra expansion can be very fast. In other words, the value of $\sigma_{\min}(z)$ can be very small comparing to the distance of $z$ from $\Lambda(A)$, so that the convergence of `sdeig` is very slow. Our basic effort will be to measure and cancel this fast pseudospectra expansion. To this aim we define the pseudospectrum sensitivity at a point $z$ to be
Definition 1

\[ pss(z) = |\mu_{\text{min}}^H(z) \cdot u_{\text{min}}(z)|^{-1} \]  

(2)

Using the above definition the effectiveness of Theorem 3 can be extended as follows.

Theorem 4 Let \( z = x + iy \in \mathbb{C} \setminus \Lambda(A) \) and \( L \) the line segment between \( z \) and the closest eigenvalue. If \( pss(z') \leq pss(z) \) for every point \( z' \in L \), then \( D^0(z, \sigma_{\text{min}}(z) \cdot pss(z)) \cap \Lambda_e(A) = \emptyset \).

Proof Let \( g(x, y) = \sigma_{\text{min}}((x + iy)I - A) \). By definition \( g(x, y) - g(x_0, y_0) = \oint_{(x_0, y_0)} \nabla g(x, y) \cdot \hat{n}_L \, dL \), where \( \hat{n}_L \) is a normalized vector parallel to \( L \). Then using Theorem 2 we have

\[ |g(x_0, y_0) - g(x_1, y_1)| = |\oint_{(x_0, y_0)} \nabla g(x, y) \cdot \hat{n}_L \, dL| \leq \oint_{(x_0, y_0)} |\nabla g(x, y) \cdot \hat{n}_L| \, dL \]

\[ = \oint_{(x_0, y_0)} pss(z)^{-1} \, dL \leq pss(z_0)^{-1} \oint_{(x_0, y_0)} \, dL = pss(z_0)^{-1} \cdot |z_0 - z_1|. \]

Of course, the key question concerning 4 is its applicability, given that its assumption does not hold in general. Notice first that even in cases where the assumption does not hold, the statement of the theorem can be true, since \( pss(z) \) is not in general constant in \( L \). In [3] we showed that the above statement is in general true, with the exception of some areas between eigenvalues. We could briefly explain this phenomenon by means of some basic theorems and observations.

Theorem 5 Let \( z_0 \) be a simple eigenvalue of \( A \) with \( y, x \) the corresponding left and right eigenvectors. If we define the eigenvalue condition as \( \kappa(z_0) = \frac{||y^H|| \cdot ||x||}{||y^Hx||} \), then

\[ \lim_{z \to z_0} pss_A(z) = \kappa(z_0)^{-1} \]

Observe now that in the limit \( |z| \to +\infty \), we have \( v_n^H u_n \to 1 \). This fact along with Theorem 5 and continuity of \( pss(z) \) is an indication of the \( pss(z) \) behavior with \( \text{dist}(z, \Lambda(A)) \) increasing. Of course, our claim gives no guarantee for the \( pss(z) \) behavior close to \( \Lambda(A) \). The following theorem taken from [10] gives a local description around simple eigenvalues.

Theorem 6 Let \( z_e \) be a simple eigenvalue of \( A \) with \( y, x \) the corresponding left and right eigenvectors and \( \tilde{A} = A + E \) be a perturbation of \( A \). Then there is a unique eigenvalue \( \tilde{z}_e \) of \( \tilde{A} \) such that

\[ |\tilde{z}_e - z_e| \leq \frac{||y^H|| \cdot ||x|| \cdot ||E||}{||y^Hx||} + O(||E^2||) \]

(3)

Second order terms in Theorem 6 translate directly in a decrease of \( pss(z) \) locally around simple eigenvalues. Concerning areas between eigenvalues where the statement of Theorem 4 fails, we can use a basic result from [8].

\[ v_{\text{min}}^H(z) \cdot u_{\text{min}}(z) = 0 \iff \exists E \text{ such that } z \text{ is a double eigenvalue of } A + E. \]

(4)

In that case \( \sigma_n = \sigma_{n-1} \) is a necessary condition. Since \( pss(z) \) is continuous there are areas around \( z \) where \( pss(z) \) is very small and thus gives very large incorrect exclusions. We will defer further discussion on the behavior of pseudospectrum sensitivity behavior until section 7. The final argument of this section is given in Figure 1 which essentially shows that the assumption of Theorem 4 is very weak.

We have set grounds which justify our selection for the step size:

\[ \text{step size} = \sigma_{\text{min}}(z) \cdot pss(z) \]

(5)
3 Numerical Results

In this section we present numerical results that in principal show the effectiveness of sdeig. Starting points have been selected using the enclose algorithm of [3]. We use the complete svd decomposition, but essentially the same results are obtained with Arnoldi methods, for example with the function svds of Matlab. In the following, with \( \lambda \) we denote an eigenvalue computed by Eig, with "eig_sens" we denote the sensitivity of the corresponding eigenvalue computed by eigsens. All test matrices and function eigsens are from the Testmatrix Toolbox for Matlab.

The steepest descent is stopped when the first increase of the numerical values of \( \sigma_{\text{min}} \) occurs. In that sense, the implementation of a stopping criterion is straightforward. However as we can see in Table 1 convergence may have been obtained earlier. Hence, a better implementation of a stopping criterion could stop avoid some of the last iterations. An example of the steepest descent process and a zoom in the area of the eigenvalue is given in Figure 2.

In Table 2, we see that the number of iterations can be decreased with the choice of a "good" starting point (15/8), and of an appropriate stopping criterion tol (17/12).

In the examples of Table 3, we use a slightly different matrix changing a single parameter in function pentoep. The spectrum of the new matrix is of similar form with that discussed on Table 2, but eigenvalue sensitivities are clearly reduced. We use the starting points of Table 2. The effects are clear in the size of \( |\lambda - \hat{\lambda}| \) and more importantly in the number of iterations.
| Starting Point | Iterations | $\lambda$ | $|\lambda - \lambda|_*$ | $s_{\text{min}}$ | $\text{eig.sens}$ |
|----------------|------------|----------------|----------------|----------------|----------------|
| 0.6+0.5i       | 15         | 6.96686e-01   | 3.84137e-014  | 4.933e-018     | 9.45e+003     |
| 0.6+0.5i       | 14         |               | 9.23759e-014  | 1.383e-017     |               |
| 0.6+0.5i       | 12         |               | 1.29933e-006  | 1.374e-010     |               |

Table 1: Matrix pentoep(32,0,0.5,0,0,1)

| Starting Point | Iterations | $\lambda$ | $|\lambda - \lambda|_*$ | $s_{\text{min}}$ | $\text{eig.sens}$ |
|----------------|------------|----------------|----------------|----------------|----------------|
| 1.0+0.1i       | 8          | 1.02409e+00   | 1.90412e-014  | 8.191e-019     | 2.75e+004     |
| 1.0+0.5i       | 15         | 9.32779e-01   | 1.85407e-014  | 2.091e-019     | 2.32e+004     |
| 1.3+0.0i       | 17         | 1.17998e+00   | 5.10702e-015  | 6.897e-019     | 5.21e+003     |
| 1.3+0.0i       | 12         |               | 1.35447e-014  | 1.770e-018     |               |
| -0.4+0.5i      | 9          | -(3.48-6.03i)e-01 | 3.57989e-014 | 2.018e-018 | 9.45e+003     |

Table 2: Matrix pentoep(32,0,0.5,0,0,1)

| Starting Point | Iterations | $\lambda$ | $|\lambda - \lambda|_*$ | $s_{\text{min}}$ | $\text{eig.sens}$ |
|----------------|------------|----------------|----------------|----------------|----------------|
| 1.0+0.2i       | 10         | 9.32039e-01   | 4.04639e-022  | 1.586e-018     | 2.82e+002     |
| 0.8+0.2i       | 13         | 7.03348e-01   | 2.22044e-016  | 4.832e-019     |               |
| 0.6+0.2i       | 15         | 4.94699e-01   | 3.51803e-016  | 3.08e-018      | 1.86e+002     |
| 0.4+0.2i       | 17         | 3.47946e-01   |               |               |               |
| 0.2+0.2i       | 18         | 1.72127e-01   |               |               |               |

Table 3: Matrix pentoep(32,0,0.7,0,0,1)

| Starting Point | Iterations | $\lambda$ | $|\lambda - \lambda|_*$ | $s_{\text{min}}$ | $\text{eig.sens}$ |
|----------------|------------|----------------|----------------|----------------|----------------|
| 1.0+0.2i       | 10         | 9.32039e-01   | 8.88178e-015  | 2.727e-017     | 9.09e+001     |
| 0.8+0.2i       | 13         | 7.03348e-01   | 1.14330e-012  | 3.041e-017     | 3.98e+003     |
| 0.6+0.2i       | 15         | 4.94699e-01   | 8.37324e-012  | 2.023e-017     | 7.38e+004     |
| 0.4+0.2i       | 17         | 3.47946e-01   | 3.01335e-011  | 1.727e-017     | 1.08e+006     |
| 0.2+0.2i       | 18         | 1.72127e-01   | 1.71558e-011  | 1.634e-019     | 3.26e+007     |

Table 4: Matrix kahan(32)
In the examples of Table 4 we use a nice property of matrix kahan(32). Its eigenvalues lie on the real axis in the range [0, 1.11, 1], and their sensitivities satisfy \( e_i < e_j \iff \text{sens}(e_i) > \text{sens}(e_j) \). We observe that the increase of eigenvalue (and pseudospectrum) sensitivity reflects in a monotone way in the number of iterations and in the size of \( |\lambda - \lambda'| \). However, an O(10^6) increase of the eigenvalue sensitivity does not even double the number of iterations. We also observe that independently from eigenvalue sensitivity, \( \sigma_{\min}(z - A) < 10^{-16} \). For a variety of similar results refer to [?].

4 The role of clustering

In the previous section we observed a connection between the number of iterations and eigenvalue sensitivity (or closeness of the original matrix to defective matrices – see an argument in [10]). But, how clusters of eigenvalues on the complex plane can affect the number of iterations? We settle the question by means of a numerical example, and an extreme case theorem.

In Figure 3 we plot spectra of \texttt{rand(32)} and \texttt{rand(100)}. It is obvious that eigenvalues of \texttt{rand(100)} exhibit a more intense geometric clustering. However, sensitivity of eigenvalues is less than 100 in both cases. In particular \( \text{mean(eigsens(rand(32)))=4.59} \) and \( \text{mean(eigsens(rand(100)))=6.25} \). For a small number of starting points inside the cluster, we obtained \( \text{mean(iterations(rand(32)))=6.8} \) and \( \text{mean(iterations(rand(100)))=6.9} \). We now give an extreme case theorem.

**Theorem 7** Let \( N \) be a normal matrix with eigenvalues \( \lambda_1, \ldots, \lambda_n \), with \( |\lambda_1| > \ldots > |\lambda_n| \), and singular values \( \sigma_1 > \ldots > \sigma_n \). The following hold:

1. \( |\lambda_i| = \sigma_i \).

2. For every \( z \in \mathbb{C} \), if \( zI - N = U\Sigma V^H \), there is a permutation \( \pi \), such that \( \lambda_{\pi(i)} = z - S(i, \cdot) * V(:, i)' * U(:, i) \), \( i = 1, \ldots, n \).

**Proof** For claim 1, see [5]. In the case of normal matrices we have \( u_i^H v_i \) for every singular value \( \sigma_i \). Let \( z_i \) be the eigenvalue for which \( |z_i - z| = \sigma_i(z) \). Let \( L \) be the line between \( z \) and \( z_i \). For each point \( z' \) of \( L \), there is some \( j < i \) such that \( |z' - z_i| = \sigma_j(z'I - A) \). We now split \( L \) in segments where the index \( j \) is constant and we consider the integral, as we did in proof of Theorem 4 for the corresponding \( \sigma_j \) along each segment. Observe that since \( N \) is normal, we have \( u_i(z')^H v_i(z') = 1 \), for every \( i, z' \), and the inequalities of the proof become strict equalities. Hence, the gradient of \( \sigma_j \) must be parallel to \( L \) at every point of it. \( \square \)
In Table 4 we give the eigenvalues of a normal $5 \times 5$ matrix with no trivial eigenvectors, computed using the algorithm of Theorem 7, for the point $z = 1.5$. We also compare with values computed by \texttt{eig}.

A well known result (see [4]), is that \texttt{svd} requires (by a factor) less flops than \texttt{eig}. In our 5x5 example, $\text{flops(eig)} = 4695, \text{flops(svd)} = 2293$. Theorem 7 directly suggests a way for exploiting normality in the computation of eigenvalues of normal matrices with direct or indirect methods.

This section established also, that the size of the matrix does not affect the number of iterations.

5 Using Exclusions

In the previous sections we established \texttt{sdeig}, a steepest descent algorithm for the computation of a simple eigenvalue. The central observation of this section is that the steepest descent procedure can give additional useful information. We repeat the key claim of Section 2.

Claim 1 $D^\sigma(z, \sigma_{\min}(zI - A) \cdot \text{pss}(z))$ and $\Lambda(A)$ have under weak conditions no common points.

This claim implies that we can use all the $\sigma_{\min}(z)$ computations of \texttt{sdeig} to obtain regions of the complex plan which do not contain eigenvalues. Figure 4 shows the area excluded after two runs of \texttt{eig}. The use of "localization information" could be an additional feature of an eigenvalue algorithm which will use our ideas. Of course, exclusions will be most informative in the case of hermitian and in general, normal matrices.

In Figure 4 also observe that exclusion disks intersect. A more sophisticated algorithm could choose a slightly bigger step size (at least in areas away from eigenvalues) in order to diminish the number of iterations. A natural
way to try such an improvement would be to use second order information for $\sigma_{\min}$. These are open issues for future research.

6 The Oleary-Stewart Result

The iteration of $sdeig$ is given in [9] slightly disguised. It is interesting that the iteration is derived from a very different perspective. The starting point is the following variant of the Rayleigh quotient method. Let $\lambda$ be a simple eigenvalue of $A$ with right and left eigenvectors $x$ and $y_H$. Let $\hat{v}$ and $\hat{w}^H$ be approximations to $x$ and $y^H$, and let $\tau$ be an approximation to $\lambda$. The new approximations $\hat{v}$, $\hat{w}^H$ and $\hat{\tau}$ are generated as follows:

1. $\hat{v} = (A - \tau I)^{-1}\hat{u}$
2. $\hat{w}^H = \hat{w}^H(A - \tau I)^{-1}$
3. $\hat{\tau} = \hat{w}^H A\hat{v}/\hat{w}^H \hat{v}$

The procedure is then iterated. The basic observation of [9] is that if $\tau$ is close to an eigenvalue the singular vectors should approximate the eigenvectors. Using only this observation the Rayleigh quotient iteration is transformed to the iteration of $sdeig$. Finally, it is given a proof that the iteration achieves local quadratic convergence.

Theorem 8 if $\epsilon = |\lambda - \tau|$ is sufficiently small, there is a constant $\mu$ such that:

$$\hat{\epsilon} \equiv |\lambda - \hat{\tau}| \leq C((\epsilon/\mu) + (\epsilon/\mu)(||\delta_u|| + ||\delta_w||)) + ||\delta_v|| ||\delta_w||, \quad (6)$$

where

$$C = \frac{2k^2||A||}{\sqrt{1 - (\epsilon/\mu)^2 - \kappa(2\epsilon/\mu + ||\delta_v|| + ||\delta_w||)}} \quad (7)$$

The constant $\mu$ is the lower bound of $\sigma_{n-1}(z)$ in a neighborhood of $\lambda$ and $\delta_u, \delta_w$ denote inaccuracies in the computation of the singular vectors $u, w$.

Unfortunately, the result of [9] holds only for (unbounded) small neighborhoods around simple eigenvalues, and fails to explain the general convergence exhibited by $sdeig$. It is however useful in proving rigorously the ultimate convergence of $sdeig$, and establishing a better stopping criterion.

7 Pseudospectrum Sensitivity Behavior

Figure 1 shows that pseudospectrum exhibits a behavior more structured than that implied from theorems and observations in Section 2. In this section we will attempt to give a more accurate picture of that structure. We first give a general theorem taken from [1] (see also [6]).

Theorem 9 Let $X$ be a Banach space and $\Omega$ an open subset of $C$. Consider a function $f : \hat{\Omega} \to X$ holomorphic in $\Omega$ and continuous in $\hat{\Omega}$. Then $||f||$ is subharmonic in $\hat{\Omega}$.

We will need one more basic result contained in [2] (see page 84).

Theorem 10 If $A(z) \in \mathbb{C}^{n \times n}$ is an holomorphic function of $z \in \mathbb{C}$, and $\lambda(z)$ is a simple eigenvalue of $A(z)$ in some domain $\Omega \subset \mathbb{C}$ then $\lambda(z)$ is holomorphic in $\Omega$. Moreover, the corresponding left and right eigenvectors $y^H(z), x$ are holomorphic in $\Omega$.

We are now ready to give the main theorem.

Theorem 11 If $A \in \mathbb{C}^{n \times n}$, $pss(z)$ is subharmonic in every domain $\Omega \in \mathbb{C}$, where $\sigma_{\min}(z)$ is simple.
The curves are slightly more steep for bigger sensitivities of eigenvalues. \( \alpha \) shows up, in the sense that despite the initial explosion, the expansion of pseudospectra stabilizes quickly. Corollary 2 naturally captures details about these expansion phenomena as the \( \alpha \) gives a very good tool for further theoretical investigation. In Figure 5 we plot the determinant of the Hessian of \( \Phi = \sum_A \sigma^2 \). Hence \( u_1^H(z) \cdot v_1(z) \) is holomorphic. Subharmonicity follows from Theorem 10 and the definition of \( pss(z) \).

The Maximum Principle is an elementary property of subharmonic functions. Specifically, the following theorem holds.

**Theorem 12** Let \( \Omega \) be a bounded domain in \( \mathbb{C} \) and \( \partial \Omega \) be its boundary. Suppose \( f \) is subharmonic in \( \Omega \). Then

\[
\sup_{z \in \Omega} f(z) = \max_{\zeta \in \partial \Omega} f(z) \tag{8}
\]

The Maximum Principle can be directly applied to \( pss(z) \). Notice also, that since \( pss(z) = 0 \) \( \Rightarrow \) \( \sigma_n = \sigma_n-1 \), the function \( pss(z)^{-1} \) is subharmonic in the same domain. Hence, the Maximum Principle can also be applied to \( pss(z)^{-1} \). These observations are summarized in the following corollary.

**Corollary 2** Let \( \Omega = \mathbb{C} \setminus \{ z : \sigma_n(z) \neq \sigma_n-1(z) \} \). Then

\[
\sup_{z \in \Omega} pss(z) = \max_{\zeta \in \partial \Omega} pss(z) \tag{9}
\]

\[
\inf_{z \in \Omega} pss(z) = \min_{\zeta \in \partial \Omega} pss(z)
\]

We can strengthen the result by taking into consideration the behavior of \( pss(z) \) close to points where \( \sigma_n(z) = \sigma_n-1(z) \). These are exactly the points where disjoint curves of \( \Lambda_n(A) \) collide.

Corollary 2 together with some of the observations of Section 2 plausibly explains why \( pss(z) \) decreases in a monotonic way as \( dist(z, \Lambda(A)) \) increases. However, the similarity of \( pss(z) \) contours with \( \Lambda_n \) contours is striking and obviously more structured. We will need the extension of Sun’s Theorem.

**Theorem 13** Let \( U(x, y) \Sigma V^H(x, y) = A - (x + iy)I \), where \( \sigma = \sigma_n(x, y_0) \) is simple and non-zero. Let \( \tilde{U} = (u_1 u_2 \ldots u_n-1), \tilde{V} = (v_1 v_2 \ldots v_n-1) \) and \( \tilde{\Sigma} = \text{diag}(\sigma_1, \ldots, \sigma_n) \). We then have

\[
\frac{\partial^2 \sigma}{\partial x^2}(x_0, y_0) = Re\{r^H \Phi r + l^H \Phi l + 2l^H \Psi r \} + Im\{u_n^H v_n\}^2 / \sigma_n,
\]

\[
\frac{\partial^2 \sigma}{\partial x \partial y}(x_0, y_0) = -Im\{2l^H \Psi r \} + Im\{u_n^H v_n\} Re\{u_n^H v_n\} / \sigma_n,
\]

\[
\frac{\partial^2 \sigma}{\partial y^2}(x_0, y_0) = Re\{r^H \Phi r + l^H \Phi l - 2l^H \Psi r \} + Re\{u_n^H v_n\}^2 / \sigma_n,
\]

where \( \Phi = \sigma_n(\sigma_n^2 I - \tilde{\Sigma}^2)^{-1}, \Psi = \tilde{\Sigma}(\sigma_n^2 I - \tilde{\Sigma}^2)^{-1}, r = \tilde{U}^H v_n \) and \( l = \tilde{V}^H u_n \).

Unlike the first order case, computation of second order derivatives is prohibitive for practical purposes. However, it gives a very good tool for further theoretical investigation. In Figure 5 we plot the determinant of the Hessian of \( \sigma_{\min}(z) \).

Obviously, the pattern is similar with that of \( \Lambda_n \) and \( pss(z) \), but clearly, we cannot use a subharmonicity argument. However, we can observe that expansion is slower than that of \( pss(z) \). Intuitively, we could expect that the sensitivity of analogous constructions for derivatives of order \( k \) asymptotically approaches 1 when \( k \to \infty \). A quantity that can naturally capture details about these expansion phenomena is the **pseudospectrum area**, defined in the obvious way.

In Figure 5 we measure the area (as the number of grid points) of \( \Lambda_n \) as a function of \( \epsilon \), of matrix \( \text{pen}(32, 0, \alpha, 0, 0, 1) \), for three different values of parameter \( \alpha \). This family of matrices has the nice property that the spectra are almost identical for different values of \( \alpha \), but the sensitivities of eigenvalues change significantly. Thus, the \( \Lambda_n \) area depends mainly on \( pss(z) \). We also measure the area of \( \Lambda_n \) for the matrix \( \text{gcar}(32) \). It is clear that a general "inverse exponential law" shows up, in the sense that despite the initial explosion, the expansion of pseudospectra stabilizes quickly. The curves are slightly more steep for bigger sensitivities of eigenvalues.

We now give some theorems which give a way for reasoning about the pseudospectra expansion and its relation to \( pss(z) \). First, a general theorem of Konrod.

Proof Let \( zI - A = U(z)^H \Sigma(z)V(z) \). It is well known that the hermitian matrix \((zI - A)^H(zI - A)\) has eigenvalues \( \sigma_1(z) \geq \ldots \geq \sigma_n(z) \), and corresponding left and right eigenvectors \( u_1(z), \ldots, u_n(z) \) and \( v_1(z), \ldots, v_n(z) \). Clearly \( \sigma_n(z) = \sigma_{\min}(z) \) is simple if \( \sigma_{n-1}(z) \neq \sigma_n(z) \). In that case, from Theorem 10 \( \sigma_n \) and \( u_i(z)^H v_i(z) \) are holomorphic in \( z \). Hence \( u_i^H(z) \cdot v_i(z) \) is holomorphic. Subharmonicity follows from Theorem 9.
Theorem 14  Let $G \subset \mathbb{R}^n$ be a domain and $f : G \rightarrow \mathbb{R}$ a smooth function, $E_t = \{ x \in G | f(x) = t \}$ the level set of the function $f$ and $ds$ the $(n-1)$-dimensional surface element on $E_t$. Then

$$\text{meas}(G) = \int_{\min f}^{\max f} \left( \int_{E_t} |\nabla f| \right) dt$$

Theorem 14 directly applies to our case giving the following corollary.

Corollary 3  Let $\partial \Lambda_t$ be the boundary of $\Lambda_t$ and $dz$ be the 1-dimensional surface element on $\partial \Lambda_t$. Then

$$\text{area}(\Lambda_t(A)) = \int_0^t \left( \int_{\partial \Lambda_t} (pss(z))dz \right) dt$$
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