Eigenvalues and Pseudo-eigenvalues of Toeplitz Matrices

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ABSTRACT

The eigenvalues of a nonhermitian Toeplitz matrix A are usually highly sensitive to perturbations, having condition numbers that increase exponentially with the dimension N. An equivalent statement is that the resolvent $(zI - A)^{-1}$ of a Toeplitz matrix may be much larger in norm than the eigenvalues alone would suggest—exponentially large as a function of N, even when z is far from the spectrum. Because of these facts, the meaningfulness of the eigenvalues of nonhermitian Toeplitz matrices for any but the most theoretical purposes should be considered suspect. In many applications it is more meaningful to investigate the *ε-pseudo-eigenvalues*: the complex numbers z with $\|(zI - A)^{-1}\| \geqslant \varepsilon^{-1}$. This paper analyzes the pseudospectra of Toeplitz matrices, and in particular relates them to the symbols of the matrices and thereby to the spectra of the associated Toeplitz and Laurent operators. Our results are reasonably complete in the triangular case, and preliminary in the cases of nontriangular Toeplitz matrices, block Toeplitz matrices, and Toeplitz-like matrices with smoothly varying coefficients. Computed examples of pseudospectra are presented throughout, and applications in numerical analysis are mentioned.

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1. INTRODUCTION

Many of the nonhermitian matrices that arise in applications have eigenvalues that are highly sensitive to perturbations. Indeed, for a family of matrices with variable dimension N, the sensitivity of the eigenvalues often increases exponentially as $N \to \infty$. In such circumstances eigenvalue analysis may lead to misleading conclusions, and the reasons lie deeper than the possibility of rounding errors on a computer. Highly sensitive eigenvalues are a reflection of the fact that the basis of eigenvectors is highly ill conditioned, and when this is the case, it is unlikely that there is good reason for working with that basis. Yet any statement about eigenvalues depends ultimately on the properties of the associated eigenvectors, whether or not they are mentioned explicitly.

We believe that in problems like this, a fruitful alternative is the analysis of *pseudo-eigenvalues*. In particular, the purpose of this paper is to investigate the pseudospectra of various kinds of Toeplitz matrices, a special family of matrices with broad applications to integral equations, finite-difference equations, matrix iterations, spline approximation, signal processing, and other problems. Let A be a real or complex square matrix of dimension N, and let $\|\cdot\|$ denote the 2-norm. The definition of pseudo-eigenvalues is as follows:

DEFINITION. Given $\varepsilon > 0$, the number $\lambda \in \mathbb{C}$ is an *ε-pseudo-eigenvalue* of A if any of the following equivalent conditions is satisfied:

(i) λ is an eigenvalue of $A + E$ for some $E \in \mathbb{C}^{N\times N}$ with $\|E\| \leqslant \varepsilon$;
(ii) $\exists u \in \mathbb{C}^n$, $\|u\| = 1$, such that $\|(A - \lambda I)u\| \leqslant \varepsilon$;
(iii) $\|(\lambda I - A)^{-1}\| \geqslant \varepsilon^{-1}$;
(iv) $\sigma_N(\lambda I - A) \leqslant \varepsilon$.

The set of all ε-pseudo-eigenvalues of A, the *ε-pseudospectrum*, is denoted by $\Lambda_\varepsilon(A)$ or simply Λ_ε.

A pseudo-eigenvalue, in other words, need not be near to any exact eigenvalue, but it is an exact eigenvalue of some nearby matrix. The vector u in (ii) is a (normalized) *ε-pseudo-eigenvector*. The matrix $(\lambda I - A)^{-1}$ in (iii) is the *resolvent* of A at the point λ, and indeed, any statement about pseudo-eigenvalues is equivalent to a statement about norms of the resolvent. In condition (iv), $\sigma_N(\lambda I - A)$ denotes the smallest singular value of $\lambda I - A$. The proof of equivalence of (i)–(iv) is an easy matter.

If A is an operator of infinite dimension instead of a matrix, we take condition (iii) to be the definition of $\Lambda_\varepsilon(A)$. Equivalents of the other definitions can be obtained with slight modifications to ensure that the sets are closed. Our definitions generalize readily from matrices to operators, and also to other norms, but we shall not pursue such generalizations here; see [26].

Throughout this paper we shall use the following notation: D is the open unit disk in the complex plane, S is the unit circle, and $\Delta = D \cup S$ is the closed unit disk. The corresponding disks and circles of arbitrary radius r are denoted by D_r, S_r, and Δ_r.

To begin with the simplest possible example, consider the Jordan block[1]

$$A = \begin{pmatrix} 0 & 5 & & & \\ & 0 & 5 & & \\ & & 0 & 5 & \\ & & & 0 & 5 \\ & & & & 0 \end{pmatrix} \qquad (N \times N). \tag{1.1}$$

The spectrum $\Lambda = \Lambda_0$ of A is just the point $\{0\}$, but when N is large and ε is small, its pseudospectrum Λ_ε is approximately the disk Δ_r with radius

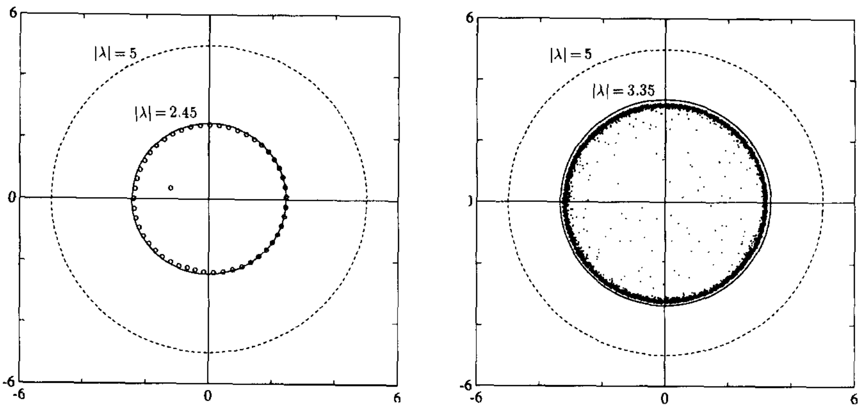
$$r = 5(\varepsilon/5)^{1/N} = 5 + O(N^{-1}) \tag{1.2}$$

(see Theorems 2.2 and 2.3). In many numerical experiments, Λ_ε represents a more meaningful spectrum for practical purposes than Λ. For an example of the relatively obvious kind involving rounding errors, suppose we take $N = 50$ and work with the numerically computed matrix $\tilde{A} := QAQ^T$, to ensure that rounding errors occur, where Q is a random unitary matrix. Figure 1(a) shows that most of the "exact" eigenvalues of $\tilde{A}$, computed numerically, lie near the circle S_r, where $r \approx 2.45$ is the value given by (1.2) with ε taken equal to $\sqrt{N}$ (to model accumulation of rounding errors) times machine epsilon.[2] This is consistent with the backward error analysis made famous by Wilkinson, which guarantees that a stable eigenvalue computation will yield the exact eigenvalues of a slightly perturbed matrix.

In Figure 1(b) we perturb A explicitly rather than relying on rounding errors. The figure shows a superposition of the eigenvalues of 100 matrices $A + E$, where each E contains independent normally distributed random

[1] Since this matrix is defective, any mathematician knows that analysis of eigenvalues alone is insufficient. However, our view is that whether or not a matrix happens to be exactly defective is of little practical importance (and indeed, is impossible to determine numerically). The behavior of this example would change negligibly if the diagonal elements were perturbed by sufficiently small quantities to make the matrix diagonalizable; the condition number of the basis of eigenvectors would become finite, but still arbitrarily close to ∞. The same comments apply to the triangular matrices of Section 2, all of which are defective. The matrices of Section 3 are in general nondefective, but their eigenvalues are still ill behaved.

[2] All calculations in this paper were carried out in Matlab on a Sun workstation with machine epsilon $2^{-52} \approx 2.2 \times 10^{-16}$. Except for Figures 1(a) and 2, all of our results would look the same in exact arithmetic.



(a) $\tilde{A} = QAQ^T$ (b) 100 matrices $A + E$, $\|E\| \approx \varepsilon = 10^{-8}$

FIG. 1. (a) Numerically computed eigenvalues of the 50×50 matrix $\tilde{A}$, numerically similar to the Jordan block A of (1.1). The exact eigenvalues of A are all 0. (b) Eigenvalues of 100 perturbed matrices $A + E$, where E is a random matrix with $\|E\| \approx \varepsilon = 10^{-8}$.

complete elements of standard deviation $10^{-8}/2\sqrt{N}$, hence with $\|E\| \approx 10^{-8}$ [8]. Much the same behavior is apparent as in Figure 1(a), except that r now takes the somewhat larger value ≈ 3.35 corresponding to (1.2) with $\varepsilon = 10^{-8}$.

It is not only explicit computation of eigenvalues that tends to detect the pseudospectra instead of the spectrum. For example, Figure 2 shows computed norms of powers $\|\tilde{A}^n\|$ as a function of n for the same 50×50 matrix $\tilde{A}$ as in Figure 1(a). Though nilpotent in theory, this matrix is evidently not even power-bounded in practice; the norms grow on average at a rate close to $r^n \approx (2.45)^n$.

In this paper we shall generalize this example to obtain a wide variety of pseudospectra of Toeplitz matrices. Our results are closely connected with the

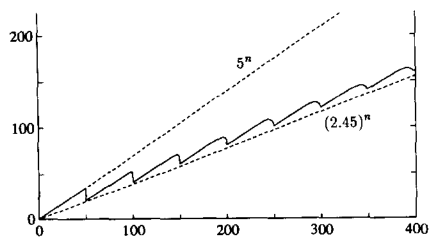


FIG. 2. Numerically computed norms of powers $\|\tilde{A}^n\|$ for the same matrix A as in Figure 1(a). In exact arithmetic $\|\tilde{A}^n\|$ would be zero for $n \geqslant 50$.

wealth of results that have arisen around Toeplitz matrices and operators since Otto Toeplitz first studied such problems at the beginning of this century. In particular, three sorts of operators and matrices have been of interest over the years:

(i) *Laurent operators* (doubly infinite matrices),
(ii) *Toeplitz operators* (infinite matrices),
(iii) *Toeplitz matrices* (finite matrices).

If the operator or matrix is hermitian, then the spectra are insensitive to perturbations and identical for Laurent and Toeplitz operators, and also for Toeplitz matrices in the limit $N \to \infty$. These problems have been studied by Szegö and others and are now very well understood [12, 15]. Our interest, however, is in the nonhermitian case (more precisely, nonnormal), where the spectra are highly sensitive to perturbations and very different for the three problems (i)–(iii). The pseudospectra, by contrast, are quite well behaved.

Our results, which are partly empirical, can be summarized as follows. For small ε and large N, the ε-pseudospectrum Λ_ε of a Toeplitz matrix is roughly the same as the spectrum of the associated Toeplitz operator, namely, a region in the complex plane bounded by the curve $f(S)$, where $f(z)$ is the *symbol* of the matrix. More precisely, Λ_ε is approximately a region bounded by $f(S_r)$ and $f(S_R)$, where $r < 1$ and $R > 1$ are parameters dependent on ε and N; the two families of curves reflect the existence of geometrically decaying $(r < 1)$ or increasing $(R > 1)$ pseudo-eigenvectors.

In our opinion these conclusions imply that the existing very different results on *exact* spectra of nonhermitian Toeplitz matrices, summarized after Theorem 3.1 below, are of dubious practical significance.

There are many further interesting problems involving spectra of perturbed matrices and operators that are not discussed here, such as eigenvalues of operators after infinitesimal perturbations (*approximate eigenvalues* as defined in [13]) or perturbations that are small in rank rather than in norm. In addition, there are other kinds of Toeplitz operators of interest besides (i)–(iii), particularly the family of *circulant matrices*, whose spectra behave much like those of Laurent operators but are also related to the spectra of Toeplitz matrices, a connection exploited elegantly by the preconditioned conjugate gradient iteration devised by Strang [5]. However, because circulant matrices are normal, their spectra are not very sensitive to perturbations, and these matrices will therefore not be discussed in this paper.

The idea of pseudo-eigenvalues seems to have been proposed first by Varah in 1979 [29]. Our own involvement began with [25], which discusses applications to matrix iterations. That paper was motivated by earlier work on the highly sensitive eigenvalue problems that arise in the numerical solution of partial differential equations by spectral methods, and an analysis of such problems from the point of view of pseudo-eigenvalues is given in [21]. A survey of the theory of pseudo-eigenvalues and their applications in numerical analysis is in preparation [26].

However, the roots of the idea of pseudo-eigenvalues in numerical analysis go deeper. In the Russian literature on numerical stability, especially, one finds various notions of the *spectrum of a family of matrices* $\{A_N\}$, which correspond to our ε-pseudospectra in a limit $\varepsilon \to 0$ [3, 9]. For example, the spirit of this paper is very much the same as in Section 6.5 of the book by Bakhvalov [3]. Our own formulation in terms of finite ε may seem cumbersome, but it is unavoidable if one wants to use spectral-type ideas to get sharp estimates of matrix behavior—for example, stability conditions for method-of-lines discretizations of partial differential equations that are necessary as well as sufficient [21]. See also [30], which contains some figures much like ours. Besides these theoretical advantages, we think that the finite-ε approach is a natural one for practical problems, since it enables one to make interesting statements about individual matrices.

2. TRIANGULAR TOEPLITZ MATRICES

Let A be an upper triangular Laurent operator, Toeplitz operator, or Toeplitz matrix defined by coefficients $a_k \in \mathbb{C}$, $0 \leqslant k \leqslant N-1 \leqslant \infty$,

$$A = \begin{pmatrix} a_0 & a_1 & a_2 & \cdots & a_{N-1} \\ & a_0 & a_1 & \ddots & \vdots \\ & & a_0 & \ddots & a_2 \\ & & & \ddots & a_1 \\ & & & & a_0 \end{pmatrix} \qquad (N \times N), \tag{2.1}$$

and let $f(z)$ be the *symbol* of this operator or matrix,

$$f(z) = \sum_{k=0}^{\infty} a_k z^k. \tag{2.2}$$

Since we are not concerned with sharp regularity conditions, we assume merely that $f(z)$ belongs to the *Wiener class* of functions with absolutely convergent Taylor coefficients,

$$\sum_{k=0}^{\infty} |a_k| < \infty, \tag{2.3}$$

so that in particular, $f(z)$ is analytic in D and continuous in Δ. In the case of a Toeplitz matrix this condition is vacuous, and we shall sometimes write the symbol as $f_N(z)$ to emphasize the finite dimensionality.

The spectrum $\Lambda(A)$ is well understood, and the results are summarized in the following theorem. For a highly readable presentation of the mathematics related to this theorem and to our analogous Theorem 3.1 for the nontriangular case, we recommend [31].

THEOREM 2.1. *Let A and f be as described above.*

(i) *If A is a Laurent operator*, $\Lambda(A) = f(S)$.
(ii) *If A is a Toeplitz operator*, $\Lambda(A) = f(\Delta)$.
(iii) *If A is a Toeplitz matrix*, $\Lambda(A) = f(\{0\}) = \{a_0\}$.

Proof. (i): The result for Laurent operators was first proved by Toeplitz in 1911 [23]. If A is a Laurent operator, then Au is a convolution a^*u, where a is the sequence of values $\{a_{-k}\}$. Since $u \in l^2$ and $a \in l^1 \subseteq l^2$ by assumption, the convolution is equivalent to an operation of pointwise multiplication in the Fourier domain $L^2[-\pi, \pi]$. To be precise, Au has semidiscrete Fourier transform $\mathrm{Au}(\theta) = \hat{a}(\theta)\hat{u}(\theta)$, and the vector $(\lambda I - A)^{-1}u$ has Fourier transform

$$\frac{\hat{u}(\theta)}{\lambda - \hat{a}(\theta)} = \frac{\hat{u}(\theta)}{\lambda - f(e^{i\theta})}.$$

Since $\hat{a}(\theta) = f(e^{i\theta})$ is a continuous function on a compact domain, the resolvent operator is evidently well defined and bounded in norm if and only if the denominator is never zero, i.e., $\lambda \notin f(S)$, as claimed.

(ii): The result for Toeplitz operators was first proved by Wintner in 1929 [34]. For any $z \in D$, the vector $(1, z, z^2, \ldots)^T$ belongs to l^2 and is obviously an eigenvector of A with eigenvalue $f(z)$. This proves that Λ includes $f(D)$, and since Λ must be compact, it includes $f(\Delta)$. Conversely, let $\lambda \in \mathbb{C} \setminus f(\Delta)$ be arbitrary. Then $[\lambda - f(z)]^{-1}$ is a bounded analytic function of the Wiener class in the unit disk, whose Taylor coefficients are easily seen to provide the matrix entries of an inverse (also Toeplitz) of the operator $\lambda I - A$. In other words, the resolvent $(\lambda I - A)^{-1}$ exists as a bounded operator, so λ is not in the spectrum.

(iii): Since A is triangular, the result for Toeplitz matrices is trivial. ■

Note that the fact that A is triangular was not used in the proof of (i) above, and thus the same statement carries over to nontriangular Toeplitz matrices and operators, as we shall discuss in the next section. An alternative proof of (ii) can be obtained as a corollary of Theorem 2.2 below.

So much for the standard results. Now, what about pseudospectra? A comparison of statements (ii) and (iii) of Theorem 2.1 shows that the limit $N \to \infty$ is a discontinuous one as far as exact spectra are concerned. The pseudospectra, however, behave continuously. The fundamental observation is that if ε is small and N is large, then Λ_ε looks not like $f(\{0\})$ but instead more like

$$\Lambda_\varepsilon \approx f(\Delta_r), \tag{2.4}$$

with

$$r = \left(\frac{\varepsilon}{c_N}\right)^{1/N} = 1 + O(N^{-1}), \qquad c_N = \sum_{k=1}^{N-1} |a_k|. \tag{2.5}$$

(The constant c_N is not exactly right, as we shall see below, but its precise value matters little because of the Nth root.) Thus as $N \to \infty$ we have $\Lambda_\varepsilon \approx f(\Delta)$, which is the same as the spectrum of the associated Toeplitz operator.

Before stating theorems to this effect, let us consider some examples. Figures 1 and 2 already dealt with the simplest nontrivial triangular Toeplitz matrix: a Jordan block. Here are three further matrices of interest:

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

$$B = \begin{pmatrix} 1 & \frac{3}{4} & \frac{3}{8} & \frac{3}{16} & \frac{3}{32} \\ & 1 & \frac{3}{4} & \frac{3}{8} & \frac{3}{16} \\ & & 1 & \frac{3}{4} & \frac{3}{8} \\ & & & 1 & \frac{3}{4} \\ & & & & 1 \end{pmatrix}, \tag{2.6}$$

$$C = \begin{pmatrix} 1 & 2 & 2 & 2 & 2 \\ & 1 & 2 & 2 & 2 \\ & & 1 & 2 & 2 \\ & & & 1 & 2 \\ & & & & 1 \end{pmatrix},$$

with spectra

$$\Lambda(A) = \{0\}, \qquad \Lambda(B) = \Lambda(C) = \{1\}.$$

Despite appearances, the dimension in each case is N. [Note that A is banded, the entries of B decay geometrically, and the entries of C do not decay at all, which means that it violates our assumption (2.3).] The symbols of these matrices in the limit $N \to \infty$ are

$$f_A(z) = z + z^2,$$

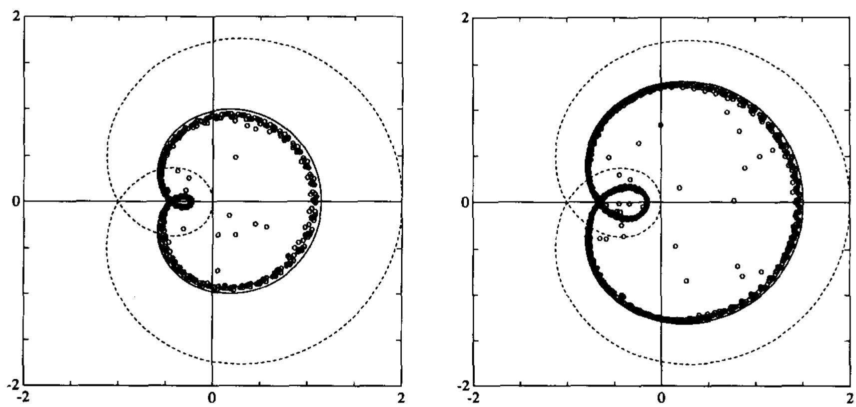
$$f_B(z) = 1 + \tfrac{3}{4}\left(z + \tfrac{1}{2}z^2 + \tfrac{1}{4}z^3 + \cdots\right) = \frac{1 + z/4}{1 - z/2},$$

$$f_C(z) = 1 + 2\left(z + z^2 + z^3 + \cdots\right) = \frac{1 + z}{1 - z},$$

and the corresponding regions $f(\Delta)$ are

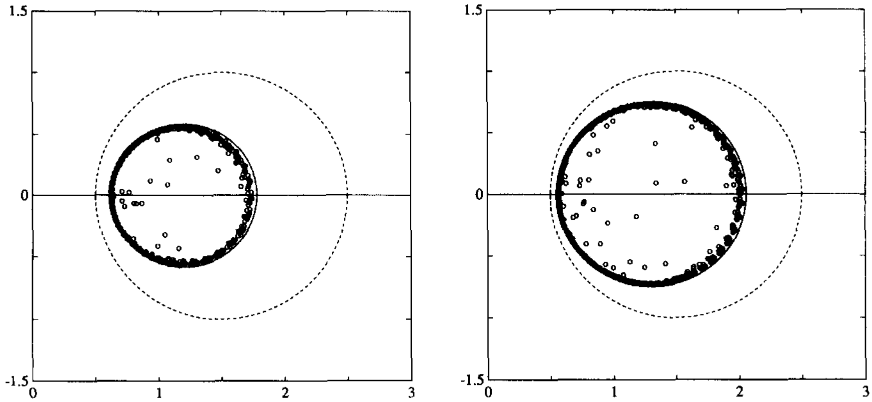
$f_A(\Delta)$: a region bounded by a limaçon,
$f_B(\Delta)$: the closed disk of radius 1 about $\lambda = \frac{3}{2}$,
$f_C(\Delta)$: the closed right half plane.

Figures 3–5 show computed ε-pseudo-eigenvalues for A, B, and C for both $N = 50$ and $N = 100$. In each plot, the eigenvalues of ten random complex



(a) $N = 50$ (b) $N = 100$

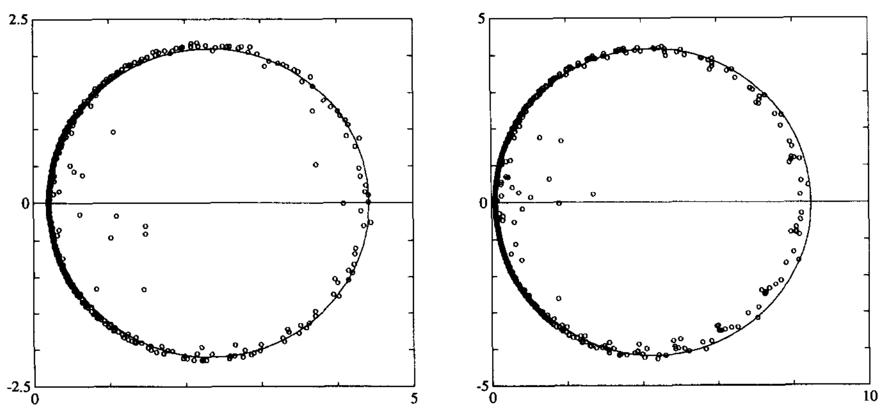
FIG. 3. Eigenvalues of $A + E$ (2.6), $\|E\| \approx \varepsilon = 10^{-8}$; the results from ten random complex perturbations E are superimposed. The eigenvalues of A are all 0. The solid and dashed curves represent $f(S_r)$ with r given by (2.5) and equal to 1, respectively. Thus the outer part of the dashed curve is the boundary of the spectrum of the associated Toeplitz operator of dimension $N = \infty$.



(a) $N = 50$ (b) $N = 100$

FIG. 4. Same as Figure 3, but for the matrix B of (2.6). The eigenvalues of B are all 1.

perturbations $A + E$ with $\|E\| \approx 10^{-8}$ are superimposed, and on top of these are drawn the curves $f(S_r)$ with $r = (\varepsilon / c_N)^{1/N}$ (solid) and $r = 1$ (dashed). In each case most of the computed eigenvalues lie close to the solid curve, in keeping with (2.4).



(a) $N = 50$ (b) $n = 100$

FIG. 5. Same as Figures 3 and 4 but for the matrix C of (2.6). The eigenvalues of C are all 1. Note the different scales in (a) and (b). As $N \to \infty$, the pseudospectra grow linearly to fill the right half plane.

The following two theorems make these observations precise. Although the theorems are stated for upper triangular Toeplitz matrices, the same results are valid in the lower triangular case, and indeed, the identity $\Lambda_\varepsilon(A) = \Lambda_\varepsilon(A^T)$ holds trivially for any matrix A and any ε.

THEOREM 2.2. *Let A_N be an $N \times N$ (nondiagonal) triangular Toeplitz matrix with entries $\{a_k\}$ and symbol $f_N(z)$. If c_N and r are defined by*

$$c_N = \sum_{k=1}^{N-1} |a_k| > 0, \qquad r = \left(\frac{\varepsilon}{c_N}\right)^{1/N}, \tag{2.7}$$

then for any $\varepsilon \geqslant 0$,

$$f_N(\Delta_r) \subseteq \Lambda_\varepsilon(A_N) \subseteq f_N(\Delta) + \Delta_\varepsilon. \tag{2.8}$$

THEOREM 2.3. *Let A be a triangular Toeplitz operator with absolutely summable entries $\{a_k\}$ and symbol $f(z)$, and let A_N denote the $N \times N$ triangular Toeplitz matrix defined by $a_0, \dots, a_{N-1}$. Then*

$$\lim_{N\to\infty} \Lambda_\varepsilon(A_N) = f(\Delta) + \Delta_\varepsilon = \Lambda_\varepsilon(A) \tag{2.9}$$

for each $\varepsilon > 0$, and therefore

$$\lim_{\varepsilon\to 0} \lim_{N\to\infty} \Lambda_\varepsilon(A_N) = f(\Delta) = \Lambda(A). \tag{2.10}$$

Before proving these theorems, let us clarify a few points. In Theorem 2.2, the motivation is problems with $\varepsilon \ll c_N$ and thus $r < 1$, but this is not essential; the theorem holds as stated even if $r > 1$. Numerical experiments like those of Figures 3–5 suggest that the first set inclusion in (2.8) is typically much sharper than the second. In Theorem 2.3, the limit of sets is defined by $\lim_{\nu\to\infty} \Lambda_\nu = \{z \in \mathbb{C} : z_\nu \to z \text{ for some } z_\nu \in \Lambda_\nu\}$. The assumption of absolute summability of the entries $\{a_k\}$ in this theorem can certainly be weakened.

Proof of Theorem 2.2. To prove the first set of inclusion in (2.8), we construct pseudo-eigenvectors as follows. Given $\varepsilon \geqslant 0$, let r be defined by (2.7). Now, given any $\lambda \in f_N(\Delta_r)$, let $\lambda = f_N(z)$ for some $z \in \Delta_r$ and define

$u = (1, z, z^2, \dots, z^{N-1})^T$. Then we readily calculate

$$(\lambda I - A_N)u = z^N \begin{bmatrix} 0 & & & & & \\ a_{N-1} & \cdot & & & & \\ \vdots & \cdot & \cdot & & & \\ a_3 & & \cdot & \cdot & & \\ a_2 & a_3 & & \cdot & \cdot & \\ a_1 & a_2 & a_3 & \cdots & a_{N-1} & 0 \end{bmatrix} u, \tag{2.11}$$

and since the norm of this matrix is bounded by c_N, this implies

$$\frac{\|(\lambda I - A_N)u\|}{\|u\|} \leqslant |z|^N c_N \leqslant \varepsilon. \tag{2.12}$$

In other words, u is an ε-pseudo-eigenvector of A_N, and thus $\lambda \in \Lambda_\varepsilon(A_N)$ by condition (ii) of the definition in the Introduction.

Our proof of the second set inclusion in (2.8) is less elementary; we do not know if it can be simplified.* If $\lambda \in \Lambda_\varepsilon(A_N)$, then by condition (iv) in the Introduction, $\sigma_N(\lambda I - A_N) \leqslant \varepsilon$, or equivalently, with the definition

$$H_N = \begin{bmatrix} a_{N-1} & \cdots & a_2 & a_1 & a_0 - \lambda \\ \vdots & \cdot^{\cdot^{\cdot}} & a_1 & a_0 - \lambda & \\ a_2 & \cdot^{\cdot^{\cdot}} & a_0 - \lambda & & \\ a_1 & \cdot^{\cdot^{\cdot}} & & & \\ a_0 - \lambda & & & & \end{bmatrix}, \tag{2.13}$$

$\sigma_N(H_N) \leqslant \varepsilon$. This matrix H_N is known as a *Hankel matrix*, and by a result in the theory of AAK, or Carathéodory-Fejér (CF), approximation that goes back to Takagi in 1924, $\sigma_N(H_N)$ is equal to the distance in the supremum norm $\|\phi\|_\infty = \sup_{z \in S} |\phi(z)|$ between

$$a_{N-1}z + \cdots + (a_0 - \lambda)z^N$$

and its best approximation $r(z) + g(z)$, where $r(z)$ is a rational function of order at most $N - 1$ with no poles in Δ, and $g(z^{-1})$ is analytic and bounded in Δ [1, 24]. (The order of a rational function is the maximum of the degrees of

* It can; see the Note Added in Proof.

its numerator and denominator.) Therefore,

$$\begin{aligned}
\varepsilon &\geqslant \left\| a_{N-1}z + \cdots + (a_0 - \lambda) z^N - (r + g)(z) \right\|_\infty \\
&= \left\| a_{N-1}z^{-1} + \cdots + (a_0 - \lambda) z^{-N} - (r + g)(z^{-1}) \right\|_\infty \\
&= \left\| (a_0 - \lambda) + \cdots + a_{N-1}z^{N-1} - z^N(r + g)(z^{-1}) \right\|_\infty \\
&= \left\| f_N(z) - \lambda - z^N(r + g)(z^{-1}) \right\|_\infty .
\end{aligned} \tag{2.14}$$

Now the function $(r + g)(z)$ has winding number $\leqslant N - 1$ about the origin when z traverses S, and therefore $z^N(r + g)(z^{-1})$ has winding number $\geqslant 1$. If $\lambda \notin f_N(\Delta)$, on the other hand, then $f_N(z) - \lambda$ is a function with winding number 0 on S and minimum modulus there equal to the distance from λ to $f_N(\Delta)$. As in the proof of Rouché's theorem, these facts are consistent with (2.14) only if that distance is $\leqslant \varepsilon$, or in other words, $\lambda \in f_N(\Delta) + \Delta_\varepsilon$. ■

In Theorem 2.2, the constant c_N entering into the definition of r can be improved by using the ideas of AAK/CF approximation in the first part of the proof as well as the second. The number c_N appeared only as an upper bound on the norm of the matrix in (2.11), and a sharper bound would be the number $\tilde{c}_N$ defined by

$$\tilde{c}_N = \inf_{z_0 \in \mathbb{C}} \| f_N - z_0 \|_\infty, \tag{2.15}$$

that is, the radius of the smallest disk containing $f_N(D)$. As remarked above, however, the improvement will be insignificant in most applications because of the Nth root.

Proof of Theorem 2.3. For any fixed $\varepsilon > 0$, the value r of (2.7) converges to 1 as $N \to \infty$, so by (2.8) we have $f(\Delta) \subseteq \lim_{N\to\infty} \Lambda_\varepsilon(A_N) \subseteq f(\Delta) + \Delta_\varepsilon$. The second inclusion must be an equality, however, since in particular we can always perturb A by a multiple of the identity. This establishes the first equality of (2.9). For the second, see Theorem 3.3 below and also the Note Added in Proof.

Equation (2.10) follows from (2.9). ■

Note that Theorems 2.2 and 2.3 contain a rather intriguing assertion: although triangular Toeplitz matrices and operators have highly sensitive eigenvalues in general, their eigenvalues are completely insensitive *outside* the region $f(\Delta)$.

We close this section by mentioning that the pseudospectra of our matrices A, B, and C, besides showing something of the variety of behavior that may arise even within the narrow class of triangular Toeplitz matrices, also offer some more direct lessons for numerical analysis. The matrix A, which is the simplest nonhermitian example that is not just a Jordan block, illustrates that in general pseudospectra are not just disks. This is an indication that looking at the Jordan canonical form alone, although sufficient for linear perturbation analysis in a theoretical sense [17], is insufficient for perturbation analysis in practice—because a perturbation that is "small" for practical purposes may still lie far outside the linear range. The matrix B, with pseudospectra consisting of disks eccentrically situated with respect to the spectral point 1, provided an example in [25] to illustrate that the convergence of a matrix iteration may be determined in practice by the pseudospectrum rather than the spectrum; similar phenomena and further Toeplitz examples are discussed in [20]. The matrix C, finally, is adapted from a well-known example devised by Kahan to prove that QR decomposition with column pivoting is not a failsafe method for determining the rank of a matrix [16; 11, p. 167]. Kahan's matrix differs slightly from C, having the Toeplitz structure modified by a column scaling, but the essence of it can still be seen in C: though the exact spectrum contains only the point 1, other points in the right half plane—in particular the point $z = 4$—lie well within the pseudospectrum and indeed are ε-pseudo-eigenvalues for values of ε that decrease exponentially as $N \to \infty$.

3. GENERAL TOEPLITZ MATRICES

Now let A be a not necessarily triangular Toeplitz matrix, Toeplitz operator, or Laurent operator,

$$A = \begin{pmatrix} a_0 & a_1 & \cdots & a_{N-2} & a_{N-1} \\ a_{-1} & a_0 & \ddots & \vdots & \vdots \\ a_{-2} & a_{-1} & \ddots & a_1 & a_2 \\ \vdots & \vdots & \ddots & a_0 & a_1 \\ a_{1-N} & a_{2-N} & \cdots & a_{-1} & a_0 \end{pmatrix}, \tag{3.1}$$

and let $f(z)$ denote the symbol

$$f(z) = \sum_{k=-\infty}^{\infty} a_k z^k, \tag{3.2}$$

with

$$\sum_{k=-\infty}^{\infty} |a_k| < \infty. \tag{3.3}$$

In the case of Toeplitz or Laurent operators, the spectrum Λ of A is fully understood:

THEOREM 3.1. *Let A and f be as described above.*

(i) *If A is a Laurent operator*, $\Lambda(A) = f(S)$.
(ii) *If A is a Toeplitz operator*, $\Lambda(A) = f(S) \cup \{\lambda \in \mathbb{C} : I(f(S), \lambda) \neq 0\}$.

Here and in the theorems below, $I(f(S), \lambda)$ denotes the *winding number* or *index* of the continuous curve $f(S)$ about the point $\lambda \in \mathbb{C}$,

$$I\big(f(S), \lambda\big) = \frac{1}{2\pi i}\int_S \frac{f'(z)}{f(z) - \lambda}\,dz, \qquad \lambda \notin f(S).$$

If $\lambda \in f(S)$, then $I(f(S), \lambda)$ is undefined.

Theorem 3.1(ii) asserts that the spectrum of a Toeplitz operator can be divided into three parts, and these can be interpreted as follows:

$$\begin{array}{rl} I(f(S), \lambda) > 0: & \text{geometrically decreasing right eigenvectors,} \\ I(f(S), \lambda) < 0: & \text{geometrically decreasing left eigenvectors,} \\ \lambda \in f(S): & \text{approximate eigenvectors with no geomet-} \\ & \text{ric increase or decrease.} \end{array} \tag{3.4}$$

These interpretations will be the key to our analysis of pseudospectra below.

Proof of Theorem 3.1. As mentioned in the last section, our proof of Theorem 2.1(i) carries over to the present case unchanged. As for (ii), this result was first proved independently around 1958 by Krein [18] and Calderón, Spitzer, and Widom [4], with the regularity assumption (3.3), and generalized to arbitrary continuous symbols by Devinatz in 1964 [7]. For a discussion see [31]. A proof based on (3.3) goes as follows. Without loss of generality consider $\lambda = 0$, and suppose first $\lambda \notin f(S) \cup \{\lambda \in \mathbb{C} : I(f(S), \lambda) \neq 0\}$, that is, $I(f(S), \lambda) = 0$. Then $f(z)$ has a continuous logarithm $L(z)$ on S which is also in the Wiener class, and if we divide the Laurent series of $L(z)$ into analytic and coanalytic parts with respect to S, $L(z) = L_+(z) + L_-(z)$, then $L_+(z)$ and $L_-(z)$ are also in the Wiener class. This gives us a factorization of the symbol,

$$f(z) = e^{L(z)} = e^{L_+(z)}\,e^{L_-(z)} = f_+(z)f_-(z),$$

which corresponds to a factorization $A = A_+A_-$ of the Toeplitz operator into upper and lower triangular Toeplitz operators of the kind considered in Theorem 2.1(ii). Since $f_+(z)$ and $f_-(z^{-1})$ are nonzero in Δ, that theorem implies that A_+ and A_- are both invertible, and therefore the same is true of their product A.

Conversely, suppose $\lambda \in f(S) \cup \{\lambda \in \mathbb{C} : I(f(S), \lambda) \neq 0\}$. If $\lambda \in f(S)$, then as indicated in (3.4), A may have no eigenvectors, but ε-pseudo-eigenvectors can be constructed by multiplying vectors $(1, z, z^2, \dots)^T$ for $z \in S$ by a smooth envelope to reduce edge effects. By making the envelope sufficiently smooth, ε can be made arbitrarily small, and this implies $\lambda \in \Lambda$. On the other hand, suppose $I(f(S), \lambda) \neq 0$, or, without loss of generality (by symmetry), $I(f(S), \lambda) = n > 0$. The arguments below will show that A has geometrically decreasing ε-pseudo-eigenvectors for arbitrarily small ε, so again, $\lambda \in \Lambda$. A more standard proof notes that by the argument of the last paragraph, the Toeplitz operator defined by the symbol $z^{-n}f(z)$ is invertible. If A were invertible too, this would imply the invertibility of the Toeplitz operator defined by the symbol $z^{-n}f(z)/f(z) = z^{-n}$, namely the nth power of a shift operator, which would be a contradiction. ■

Theorem 3.1 omits the case of Toeplitz matrices because their spectra have no simple characterization. Some results are known about the limits of the spectra as $N \to \infty$, however, for a family of Toeplitz matrices $\{A_N\}$ obtained as finite sections of a Toeplitz operator A as in Theorem 2.3. For each N, let $\lambda_{k,N}$, $k = 1, 2, \dots, N$, be the eigenvalues of A_N, and define the measure α_N on Borel sets $E \subset \mathbb{C}$ by

$$\alpha_N(E) = N^{-1} \sum_{\lambda_{k,N} \in E} 1.$$

If A is hermitian, then the measures $\{\alpha_N\}$ converge weakly as $N \to \infty$ to the measure

$$\alpha(E) = \frac{1}{2\pi} \int_{f(e^{i\theta}) \in E} d\theta;$$

see Grenander and Szegö [12]. If A is nonhermitian, it is known that if A is banded, there is a set $G \subset \mathbb{C}$ consisting of a finite union of closed analytic arcs such that α_N converges weakly to a measure α with support G, for which explicit formulas are available [14, 27]. The case of Hessenberg matrices with only two nonvanishing diagonals is particularly simple [14, 22]. Results for Toeplitz matrices whose symbol is a semiinfinite Laurent series are discussed in [28], and other generalizations are considered in [19], [6], and [33]. For analogous results concerning Wiener-Hopf integral operators, the continuous analogues of Toeplitz matrices and operators, see [2].

Now let us turn to pseudospectra. Our understanding here is not as complete as in the triangular case of the last section, but the main features of the answer are apparent, and we are able to prove at least some points.

The fundamental observation is that if N is large and ε is small, then in analogy to (3.4), Λ_ε looks approximately like the union of three sets:

$$\Lambda_\varepsilon \approx \Omega_r \cup \Omega^R \cup (\Lambda + \Delta_\varepsilon). \tag{3.5}$$

We must explain this notation. For any $r < 1$ and $R > 1$, the sets Ω_r and Ω^R are defined by

$$\Omega_r = \{z \in \mathbb{C} : I(f(S_r), z) > 0\}, \qquad \Omega^R = \{z \in \mathbb{C} : I(f(S_R), z) < 0\}. \tag{3.6}$$

In (3.5), appropriate values are

$$r = (\varepsilon/c)^{1/N}, \qquad R = (\varepsilon/C)^{-1/N} \tag{3.7}$$

for some constants c and C analogous to c_N of the last section. (In the figures below, c and C are taken equal to 1.) The sets Ω_r and Ω^R correspond to geometrically decreasing right and left pseudo-eigenvectors of A, respectively. Equivalently, they correspond to geometrically decreasing and increasing right pseudo-eigenvectors. Finally, the set $\Lambda + \Delta_\varepsilon$ in (3.5) consists of the union of the ε-balls about the eigenvalues of A, and corresponds to pseudo-eigenvectors with no geometric increase or decrease.

To illustrate (3.5), let us begin with the tridiagonal matrix

$$A = \begin{pmatrix} 0 & 2 & & & \\ 1 & 0 & 2 & & \\ & 1 & 0 & 2 & \\ & & 1 & 0 & 2 \\ & & & 1 & 0 \end{pmatrix} \tag{3.8}$$

of dimension N. Since A can be symmetrized by a similarity transformation involving the matrix $D = \mathrm{diag}(1, 2^{1/2}, 2^1, \ldots, 2^{N-1/2})$, its eigenvalues are real:

$$\Lambda = \left\{2\sqrt{2}\cos\frac{\pi j}{N+1},\ 1 \leqslant j \leqslant N\right\}. \tag{3.9}$$

The condition number of D is exponentially large as a function of N, however, suggesting that the exact eigenvalues of A are unlikely to be very meaningful. Figure 6 shows that in fact, the ε-pseudo-eigenvalues of A with $\varepsilon = 10^{-4}$ and $N = 100$ lie approximately along an ellipse. To explain this distribution, note

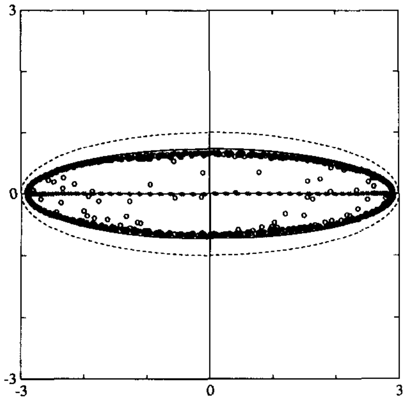


FIG. 6. Eigenvalues of $A + E$ (3.8), $\|E\| \approx \varepsilon = 10^{-4}$, $N = 100$; results from ten random perturbations are superimposed. The eigenvalues of A are real and are marked by asterisks. As in the last section, the dashed curve is $f(S)$, the boundary of the spectrum of the associated Toeplitz operator. The solid curve is the boundary of the set $\Omega_r \cup \Omega^R$ of (3.5), an approximation to the boundary of the ε-pseudospectrum.

that the symbol for this example is

$$f(z) = 2z + z^{-1}. \tag{3.10}$$

The dashed curve in the figure is the ellipse $f(S)$, which is the boundary of the spectrum of the associated Toeplitz operator. The solid curve is $f(S_r)$ with r defined by (3.7). Evidently Λ_ε is closely approximated by the set Ω_r of (3.5). In this example Ω_r is the only term in (3.5) that matters, because Λ is contained in Ω_r, and Ω^R is the empty set.

Obviously the matrix (3.8) is very special. To illustrate (3.5) more fully, consider the more "generic" example

$$B = \begin{pmatrix} 0 & 0 & 1 & 0.7 & & \\ 2i & 0 & 0 & 1 & 0.7 & \\ & 2i & 0 & 0 & 1 & 0.7 \\ & & 2i & 0 & 0 & 1 \\ & & & 2i & 0 & 0 \\ & & & & 2i & 0 \end{pmatrix}, \tag{3.11}$$

again of dimension N. The symbol of this matrix is

$$f(z) = 2iz^{-1} + z^2 + 0.7z^3.$$

The dashed curve in Figure 7 shows that this function maps S onto a rather complicated shape that might be a rendering by Picasso of the head of a bull. The two "horns" are enclosed by $f(S)$ with winding number $+1$, the "face" with winding number -1, and according to Theorem 3.1, the spectrum of the Toeplitz operator is the union of both of these regions together with the dashed boundary curve. The pseudospectrum of the Toeplitz matrix, however, is smaller, and consists of three parts. Within each horn is a region Ω_r enclosed by $f(S_r)$ with winding number $+1$ (solid curve). Within the face is a quite disjoint region Ω^R enclosed by $f(S_R)$ with winding number -1. Connecting these sets are chains of eigenvalues that are evidently insensitive to perturbations.

For a more orderly pair of examples, Figures 8 and 9 are analogous plots for the two 100×100 matrices

$$C_1 = \begin{pmatrix} 0 & 1 & & & \\ 0 & 0 & 1 & & \\ 1 & 0 & 0 & 1 & \\ & 1 & 0 & 0 & 1 \\ & & 1 & 0 & 0 \end{pmatrix}, \qquad C_{0.5} = \begin{pmatrix} 0 & 1 & & & \\ 0 & 0 & 1 & & \\ 0.5 & 0 & 0 & 1 & \\ & 0.5 & 0 & 0 & 1 \\ & & 0.5 & 0 & 0 \end{pmatrix}. \tag{3.12}$$

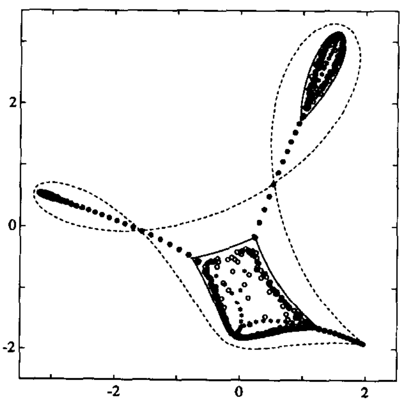


FIG. 7. Same as Figure 6, but for the matrix B of (3.11), $N = 100$. The two regions of pseudo-eigenvalues within the "horns" are enclosed by $f(S_r)$ with winding number $I = +1$, and the region of pseudo-eigenvalues in the "face" is enclosed by $f(S_R)$ with winding number $I = -1$. The dashed curve corresponds to the Toeplitz operator.

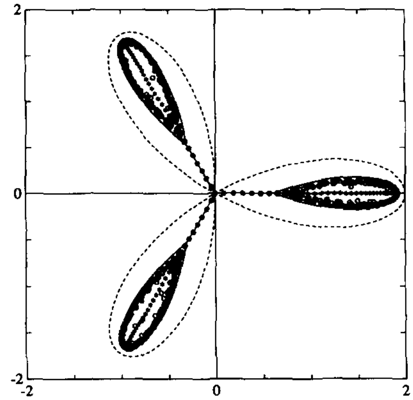


FIG. 8. Same as Figure 6, but for the matrix C_1 of (3.12), $N = 100$. The three lobes of pseudo-eigenvalues are enclosed by $f(S_R)$ with winding number $I = -1$.

In both cases, the ε-pseudospectrum for $\varepsilon = 10^{-4}$ is a three-fold symmetric shape about the origin consisting of the union of three spikes and a region with significant interior. The spikes would have lengths $3/(2^{2/3}) \approx 1.89$ in Figure 8 and $\frac{3}{2}$ in Figure 9 in the limit $N \to \infty$. The regions with interior are the contributions Ω_r and Ω^R. To see where they come from, note that C_1 and $C_{0.5}$

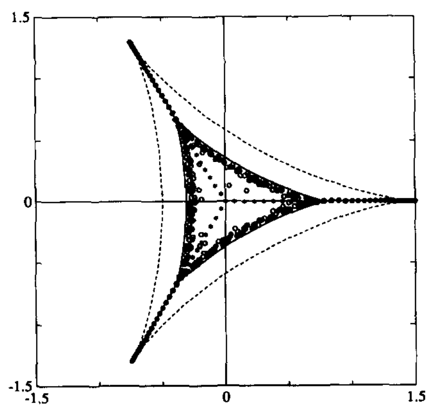


FIG. 9. Same as Figure 6, but for the matrix $C_{0.5}$ of (3.12), $N = 100$. The triangular region of pseudo-eigenvalues is enclosed by $f(S_r)$ with winding number $I = +1$.

are special cases of a matrix C_γ with symbol

$$f(z) = z + \gamma z^{-2}. \tag{3.13}$$

For $|\gamma| \leqslant 0.5$, $f(S)$ has positive or zero index with respect to all points $\gamma \in \mathbb{C} \setminus f(S)$, for $|\gamma| \geqslant 1$ the index is negative or zero, and for $0.5 < |\gamma| < 1$ there are points λ of both positive and negative index. These observations explain the dashed curves in the figures, which bound the spectra of the associated Toeplitz operators. For the pseudo-eigenvalues of the Toeplitz matrices, other curves $f(S_r)$ and $f(S_R)$ become relevant. In Figure 8, with $\gamma = 1$, Ω_r is empty and only Ω^R contributes to the pseudospectrum. In Figure 9, with $\gamma = 0.5$, Ω^R is empty and only Ω_r appears.

Up to this point we have presented an approximate formula (3.5), and examples that suggest it is reasonably close to the truth. This brings us to the question, how much of this can be made precise? Even in the last section, for triangular matrices, there was a sizable gap between the two set inclusions of (2.8). Here, the gap widens.

Our main result is an estimate for banded Toeplitz matrices which is analogous to the left-hand inclusion of Theorem 2.2. The following theorem implies that except when $f(S)$ is a curve with no interior, the sensitivity of the eigenvalues of a banded Toeplitz matrix grows exponentially with the dimension.

THEOREM 3.2. *Let A be a banded Toeplitz operator with bandwidth l, i.e., $a_k = 0$ for $|k| > l$. Let $f(z)$ be the symbol of A, and let A_N denote the $N \times N$ Toeplitz matrix defined by $a_{1-N}, \dots, a_{N-1}$. Then for any $r < 1$ and $\rho > r$ we have*

$$\Omega_r \cup \Omega^{1/r} \cup \big(\Lambda(A) + \Delta_\varepsilon\big) \subseteq \Lambda_\varepsilon(A_N) \qquad \textit{for} \quad \varepsilon = C\rho^N, \tag{3.14}$$

where C is a constant that depends on r, ρ, and $a_{-l}, \dots, a_l$ but not on N.

Proof. First of all we note that the inclusion $\Lambda(A) + \Delta_\varepsilon \subseteq \Lambda_\varepsilon(A_N)$ is a triviality, valid for any matrix or operator. Second, by symmetry, $\Omega^{1/r}$ must satisfy an estimate of the type (3.14) if Ω_r does. Thus all that we really have to prove is $\Omega_r \subseteq \Lambda_\varepsilon(A_N)$.

The idea is to construct geometrically decreasing pseudo-eigenvectors as in the proof of Theorem 2.2. Given any $r < 1$, let $\lambda \in \Omega_r$ be arbitrary. Assume without loss of generality that $a_{-l} \neq 0$. Then $f(z)$ has a pole of order exactly l at $z = 0$, and since $I(f(S_r), \lambda) \geqslant 1$, it follows by the argument principle that the equation $f(z) = \lambda$ has at least $l + 1$ solutions $z \in D_r$, counted with multiplicity. Let $z_0, z_1, \ldots, z_l$ be any $l+1$ of these solutions; if there are more, we do not need them. Assume for the moment that the z_j are distinct. Corresponding to each z_j is a vector $u_j = (1, z_j, z_j^2, \ldots, z_j^{N-1})^T$ that satisfies, in analogy to (2.11),

$$(\lambda I - A_N)u_j = z_j^N \begin{pmatrix} a_l & & & \\ \vdots & \ddots & & \\ a_1 & \cdots & a_l & \\ \end{pmatrix} u_j + v_j, \tag{3.15}$$

where v_j is defined via an $N \times N$ matrix with nonzero entries only in the upper-right $l \times l$ triangle:

$$v_j = z_j^{-N} \begin{pmatrix} & a_{-l} & \cdots & a_{-1} \\ & & \ddots & \vdots \\ & & & a_{-l} \\ & & & \end{pmatrix} u_j.$$

Now let $u = \sum_{j=0}^{l} c_j u_j$ be a nonzero linear combination of these $l+1$ vectors with the property that the last l entries of $\sum_{j=0}^{l} z_j^{-N} c_j u_j$ are 0. Then the contributions involving v_j in (3.15) cancel, and we have

$$(\lambda I - A_N)u = \begin{pmatrix} a_l & & & \\ \vdots & \ddots & & \\ a_1 & \cdots & a_l & \\ \end{pmatrix} \sum_{j=0}^{l} z_j^N c_j u_j. \tag{3.16}$$

We need to relate the norm of the right-hand side of this equation to $\|u\|$. To do this, write $u = Uc$, where U is the $N \times (l+1)$ Vandermonde matrix whose columns are the vectors u_j, and c is an $(l+1)$-vector. Let L be the lower triangular matrix above, and let D be the diagonal matrix with elements $z_0^N, \ldots, z_l^N$. Then we have

$$\|UDc\| = \|UDU^+Uc\| = \|UDU^+u\| \leqslant \kappa(U)\|D\|\,\|u\|,$$

where U^+ denotes the pseudoinverse of U and $\kappa(U) = \sigma_0/\sigma_l$ is its condition number. Since $\|D\| \leqslant r^N$, it follows that (3.16) implies

$$\frac{\|(\lambda I - A_N)u\|}{\|u\|} \leqslant r^N \kappa(U)\|L\|, \tag{3.17}$$

and therefore, by condition (ii) of the definition in the Introduction, $\lambda \in \Lambda_\varepsilon(A_N)$ for $\varepsilon = r^N \kappa(U)\|L\|$.

This completes the proof except for two points: the constant C in (3.14) is required to be independent of $\lambda \in \Omega_r$ and N, and we have assumed that the roots $z_0, \ldots, z_l$ are distinct. These matters can be dealt with as follows. If the roots $z_0, \ldots, z_l$ are distinct for all $\lambda \in \overline{\Omega}_r$, then the function

$$\sup_{N \geqslant 1} \frac{\sigma_N(\lambda I - A_N)}{r^N} = \sup_{N \geqslant 1} \frac{\left\|(\lambda I - A_N)^{-1}\right\|^{-1}}{r^N}$$

is a continuous function of λ on the compact set $\overline{\Omega}_r$; its maximum provides the constant C in (3.14), and we can take $\rho = r$. On the other hand, if some of the roots $z_0, \ldots, z_l$ are confluent at some points $\lambda \in \overline{\Omega}_r$, then an analysis involving confluent Vandermonde matrices yields a bound analogous to (3.17) except with r^N replaced by an algebraically growing factor at worst $N^l r^N$. In this case we need to take $\rho > r$. Doing so yields the conclusion that

$$\sup_{N \geqslant 1} \frac{\sigma_N(\lambda I - A_N)}{\rho^N} = \sup_{N \geqslant 1} \frac{\left\|(\lambda I - A_N)^{-1}\right\|^{-1}}{\rho^N}$$

is bounded at every point $\lambda_\varepsilon \in \overline{\Omega}_r$, and since this supremum is easily shown to be continuous, this establishes (3.14) in the confluent case. ∎

What about an analogue of Theorem 2.3 for the limit $N \to \infty$? We do not know the form of $\Lambda_\varepsilon(A)$ in the nontriangular case, but H. Widom has pointed out to us that the following result is a corollary of Theorem II of [32]:

THEOREM 3.3. *Let A be an arbitrary Toeplitz operator with absolutely summable entries, and let A_N denote its $N \times N$ Toeplitz matrix section. Then*

$$\lim_{N \to \infty} \Lambda_\varepsilon(A_N) = \Lambda_\varepsilon(A) \tag{3.18}$$

for each $\varepsilon > 0$, and therefore

$$\lim_{\varepsilon \to 0} \lim_{N \to \infty} \Lambda_\varepsilon(A_N) = \Lambda(A). \tag{3.19}$$

To close this section, we present a final example from numerical analysis. Let

$$A = L + D + U \tag{3.20}$$

be the symmetric tridiagonal matrix with entries 1, -2, 1, with L, D, and U denoting the subdiagonal, diagonal, and superdiagonal parts. Such a matrix would arise in the discrete solution by finite differences of a one-dimensional constant-coefficient diffusion equation. When a linear system $Ax = b$ is solved iteratively by the Gauss-Seidel iteration, the errors $e^{(n)}$ satisfy $e^{(n)} = G^n e^{(0)}$, where

$$G = -(L+D)^{-1}U$$

is the *Gauss-Seidel iteration matrix*. The spectrum of this matrix has been of interest for many years, because it determines the asymptotic convergence rate of the Gauss-Seidel iteration. Frankel showed in 1950 that all the eigenvalues of G are real and lie in $[0, 1)$, and that $\lceil N/2 \rceil$ of them are equal to zero. The asymptotic convergence factor is the spectral radius $\rho(G)$, which is equal to the largest of these eigenvalues and of size $1 - O(N^{-2})$.

It is readily shown that except for a first column which is zero, G is an upper Hessenberg Toeplitz matrix:

$$G = \begin{pmatrix} 0 & \frac{1}{2} & & & & \\ 0 & \frac{1}{4} & \frac{1}{2} & & & \\ 0 & \frac{1}{8} & \frac{1}{4} & \frac{1}{2} & & \\ 0 & \frac{1}{16} & \frac{1}{8} & \frac{1}{4} & \frac{1}{2} & \\ 0 & \frac{1}{32} & \frac{1}{16} & \frac{1}{8} & \frac{1}{4} & \frac{1}{2} \\ 0 & \frac{1}{64} & \frac{1}{32} & \frac{1}{16} & \frac{1}{8} & \frac{1}{4} \end{pmatrix} \quad (N \times N). \tag{3.21}$$

If one ignores the first column, the symbol of this matrix in the limit $N \to \infty$ is the quotient of the symbols of $-U$ and $L + D$:

$$f(z) = \frac{z}{2 - z^{-1}}.$$

For $N = 100$, the corresponding curve $f(\Omega_r)$ and some computed pseudo-eigenvalues are shown in Figure 10.

Why was the sensitivity to perturbations of the eigenvalues of the Gauss-Seidel iteration matrix not discovered in the 1950s? The reason is that the *largest* eigenvalue of G is insensitive; in fact, one can show that its condition number is asymptotic to 1 as $N \to \infty$. Thus the distinction between eigenvalues and pseudo-eigenvalues has no effect on the observed convergence rate for the Gauss-Seidel iteration applied to the matrix A of (3.18). If A is taken

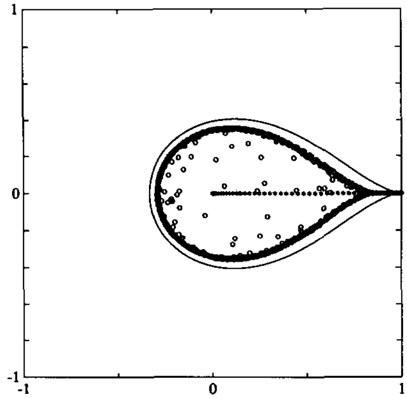


FIG. 10. Eigenvalues of $G + E$, $\|E\| \approx \varepsilon = 10^{-4}$, where G is the Gauss-Seidel iteration matrix of (3.19) with $N = 100$; results from ten random perturbations are superimposed. As shown by Frankel in 1950, the eigenvalues of G are real numbers in $[0, 1)$ (marked by asterisks). The eigenvalues of $G + E$ are very different.

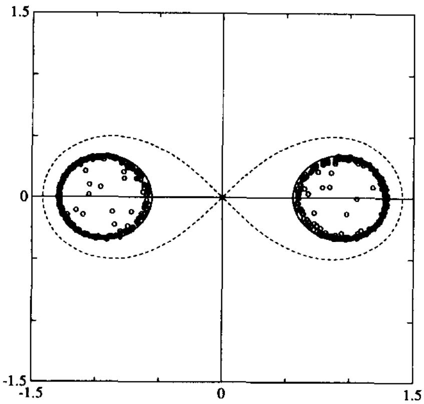
to be nonsymmetric, however, as occurs in the discretization of convection-diffusion problems, the picture changes utterly. The pseudospectral radius of G may be much closer to 1 than the spectral radius, with dramatic effects upon convergence. We shall discuss such matters in a future paper.

4. BLOCK TOEPLITZ MATRICES

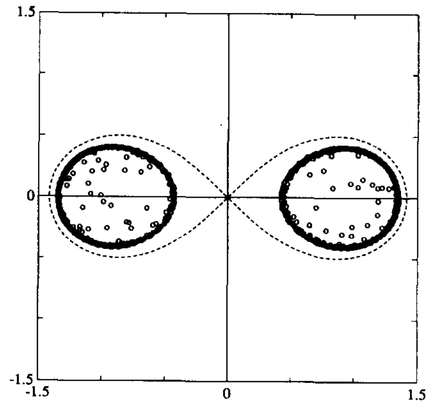
What can be said of the pseudo-eigenvalues of the $N \times N$ bidiagonal matrix

$$A = \begin{pmatrix} 1 & \gamma & & & & \\ & -1 & \gamma & & & \\ & & 1 & \gamma & & \\ & & & -1 & \gamma & \\ & & & & 1 & \gamma \\ & & & & & -1 \end{pmatrix} \qquad (\gamma \in \mathbb{C}), \tag{4.1}$$

whose eigenvalues are obviously $\{-1, 1\}$? This matrix looks like a Jordan block, except that the diagonal elements are not constant but cycle repetitively through a fixed sequence. Figure 11 shows computed eigenvalues corresponding to $\gamma = 1$, $N = 50$ and 100, and ten random complex perturbations $A + E$ with $\|E\| \approx \varepsilon = 10^{-4}$.



(a) $N = 50, \gamma = 1$



(b) $N = 100, \gamma = 1$

FIG. 11. Eigenvalues $A + E$ (4.1), $\|E\| \approx \varepsilon = 10^{-4}$; results from ten complex perturbations are superimposed. The eigenvalues of A are ± 1. The solid and dashed curves represent the lemniscates $\|\lambda^2 - 1\| = \gamma^2 r = r$ with r given by (4.6) and equal to 1, respectively.

Though it may not be obvious to the reader, the pseudo-eigenvalues in each of these pictures lie approximately along a *lemniscate*: the curve or union of curves in the complex plane along which a polynomial $p(\lambda)$ has constant modulus $|p(\lambda)| = C$. For the matrix A of (4.1), the polynomial is $p(\lambda) = \lambda^2 - 1$, and C depends on the choice of γ. By varying γ and the sequence of elements on the diagonal, one can obtain pseudospectra that approximate arbitrary lemniscates of arbitrary polynomials.

The explanation for this behavior is as follows. The matrix A of (4.1) can be viewed as an upper bidiagonal *block Toeplitz matrix* of dimension $N/2$,

$$A = \begin{pmatrix} D & E & \\ & D & E \\ & & D \end{pmatrix}, \tag{4.2}$$

where D and E are the 2×2 matrices

$$D = \begin{pmatrix} 1 & \gamma \\ 0 & -1 \end{pmatrix}, \qquad E = \begin{pmatrix} 0 & 0 \\ \gamma & 0 \end{pmatrix}. \tag{4.3}$$

Just as in Section 2, A will accordingly have approximate pseudo-eigenvectors of the form $u = U \otimes (1, z, z^2, \ldots, z^{(N-1)/2})^T$, where U is a 2-vector and $\otimes$ denotes the tensor product. This 2-vector will be either of the eigenvectors of the symbol of A, which is now the 2×2 matrix function

$$f(z) = D + zE = \begin{pmatrix} 1 & \gamma \\ \gamma z & -1 \end{pmatrix}. \tag{4.4}$$

The ε-pseudo-eigenvalues of A will be the corresponding eigenvalues λ of $f(z)$, namely the roots of the equation

$$\lambda^2 - 1 = \gamma^2 z. \tag{4.5}$$

If z ranges over the disk D_r, these values of λ fill the region bounded approximately by the lemniscate $|\lambda^2 - 1| = \gamma^2 r$. Since the highest power of z present is $z^{(N-1)/2}$, the appropriate value of r will be

$$r \approx \varepsilon^{2/N}. \tag{4.6}$$

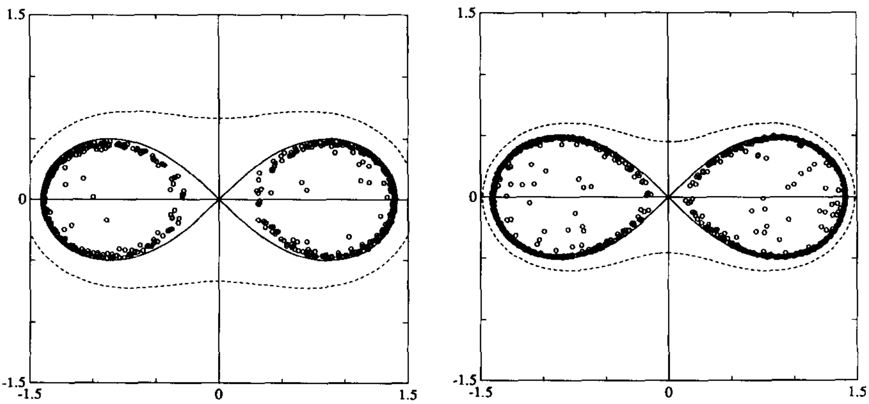
If this explanation of Figure 11 is correct, then a pseudospectrum bounded approximately by the critical lemniscate $|\lambda^2 - 1| = 1$ should be obtained if we pick γ and N to satisfy

$$1 = \gamma^2 r = \gamma^2 \varepsilon^{2/N},$$

that is,

$$\gamma = \varepsilon^{-1/N}. \tag{4.7}$$

Figure 12 shows results of an experiment with this value of γ for $N = 50$ and 100. As predicted, the eigenvalues fall roughly on the critical lemniscate.



(a) $N = 50, \gamma = \varepsilon^{-1/N} \approx 1.202$ (b) $N = 100, \gamma = \epsilon^{-1/N} \approx 1.096$

FIG. 12. Same as Figure 11, but for γ given by (4.7). The solid curve now coincides with the critical lemniscate $|\lambda^2 - 1| = 1$.

These examples give just a hint of the phenomena that may arise in pseudospectra of block Toeplitz matrices. For block Toeplitz matrices with larger blocks and more than two nonzero diagonals, the variety of pseudospectra that can be obtained goes far beyond the class of lemniscates. We have not explored these matters, and will not attempt to give any theorems on the subject here. For the spectra of block Toeplitz operators, results can be found in [10] and [19].

5. VARIABLE COEFFICIENTS

Another variation on the theme of Toeplitz matrices is to let the coefficients vary—usually smoothly. Such problems are related to integral equations with variable kernels, and it is natural to expect the resulting spectra and pseudospectra to be associated with the symbols $f(z)$ obtained by freezing the coefficients at various points. Roughly speaking, the pseudospectra of matrices obtained in this fashion approximate superpositions of pseudospectra of the associated Toeplitz matrices defined by frozen coefficients (though not for the same ε). We shall not attempt to make this statement precise. In the hermitian case for exact spectra, theorems to this effect have been given in a well-known paper of Kac, Murdock, and Szegö [15].

We shall give two examples. First, Figure 13 shows computed pseudo-

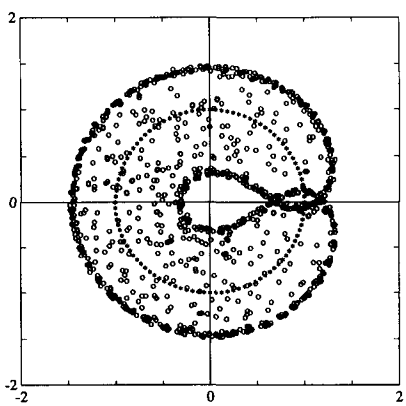


FIG. 13. Eigenvalues of $A + E$ (5.1), $\|E\| \approx \varepsilon = 10^{-4}$, $N = 100$; results from ten random perturbations are superimposed. The eigenvalues of A lie on the unit circle and are marked by asterisks.

eigenvalues of the bidiagonal matrix

$$A = \begin{pmatrix} \omega & 1 & & & \\ & \omega^2 & 1 & & \\ & & \omega^3 & \ddots & \\ & & & \ddots & 1 \\ & & & & \omega^N \end{pmatrix}, \qquad \omega = e^{2\pi i/N}, \tag{5.1}$$

with $N = 100$. For large N, the pseudospectra of A approximate a superposition of pseudospectra of bidiagonal Toeplitz matrices with elements $e^{i\theta}$ on the diagonal and 1 on the superdiagonal. This is a superposition of disks about the points $e^{i\theta}$—in other words, a region in the shape of a ring sausage, as in the figure.

The fact that the sausage has ends may be viewed as accidental. If $a_{N,1}$ is set to 1 instead of 0 in (5.1), giving a "circulant matrix with variable coefficients," the ends of the sausage disappear and we are left with a pseudospectrum in the form of an annulus (not shown).[3]

In our second example, also bidiagonal, we vary the superdiagonal rather than the diagonal elements (Figure 14). The matrix is

$$B = \begin{pmatrix} 0 & 1 & & & & \\ & 0 & \frac{1}{2} & & & \\ & & 0 & \frac{1}{3} & & \\ & & & 0 & \ddots & \\ & & & & \ddots & \dfrac{1}{N-1} \\ & & & & & 0 \end{pmatrix}, \tag{5.2}$$

again of dimension $N = 100$. If the dimension were $N = \infty$, the transpose of this matrix could be interpreted as the map

$$f(z) \mapsto \int_0^z f(w)\, dw \tag{5.3}$$

[3] This alteration of $a_{N,1}$ is an example of a matrix perturbation that is small in rank rather than in norm. The fact that low-rank perturbations may have dramatic effects on spectra is well known, and discussed, for example, in [13]. For a more subtle example of low-rank perturbations see [30], which considers spectra of matrices that are Toeplitz except in a few of the first and last rows.

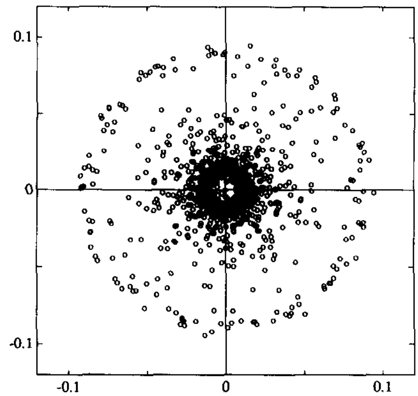


FIG. 14. Same as Figure 13, but for the matrix B of (5.2), $N = 100$. The only eigenvalue of B is 0.

described in the basis of monomials. Very loosely speaking, for each $r \in [0.01, 1]$, it is as if B had a Jordan block with r on the superdiagonal, with the dimension of the block increasing as r decreases. Superimposing the resulting pseudospectra gives a radially symmetric dependence on ε that remains nontrivial even in the limit $N \to \infty$. This further illustrates the point made at the end of Section 1, the basis of our definition of pseudospectra, that to fully understand the behavior of matrices and operators one must sometimes be prepared to consider finite ε.

The examples of this section are extremely simple, being both bidiagonal. For more complicated "Toeplitz matrices" with variable coefficients, the pseudospectral possibilities are extremely varied.

We would like to thank Professor I. C. Gohberg, P. Halmos, and N. Levenberg for discussions and references. We are especially grateful to Professor H. Widom for his remarks on the subject of $\Lambda_\varepsilon(A_N) \to \Lambda_\varepsilon(A)$, which led to fundamental improvements in Sections 2 and 3.

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Note added in proof. Since this manuscript was accepted for publication, several contributions have been made by S. C. Reddy. First, our proof of the second inclusion in (2.8) can be simplified; an elementary proof of this inclusion, as well as of the second equality in (2.9), follows from the fact that for a triangular infinite matrix such as $\lambda I - A$, the $N \times N$ section of the inverse equals the inverse of the $N \times N$ section. Second, our results of Section 2 generalize to constant-coefficient differential operators with boundary conditions at one endpoint; the details are given in Reddy's dissertation [35]. Finally, in work not yet published, Reddy has shown that these results also generalize to triangular Wiener-Hopf integral operators.

Additional examples of pseudospectra of non-normal matrices, both Toeplitz and non-Toeplitz, are presented in [36].

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