

The Projection Methods for Computing the Pseudospectra of Large Scale Matrices

Zhengsheng Wang, Xiangyong Ji, Yong Du

Abstract—The projection methods, usually viewed as the methods for computing eigenvalues, can also be used to estimate pseudospectra. This paper proposes a kind of projection methods for computing the pseudospectra of large scale matrices, including orthogonalization projection method and oblique projection method respectively. This possibility may be of practical importance in applications involving large scale highly nonnormal matrices. Numerical algorithms are given and some numerical experiments illustrate the efficiency of the new algorithms.

Keywords—Pseudospectra, eigenvalue, projection method, Arnoldi, IOM(q)

I. INTRODUCTION

The concept of pseudospectra was introduced by Trefethen to explain the behavior of nonnormal matrices^[1,2]. The pseudospectra of a square matrix is the set of all eigenvalues of complex matrices within a given distance. It is a useful tool for understanding the behavior of various matrix processes. Many phenomena (for example, hydrodynamic instability and convergence of iterative methods for linear systems) can not be accounted for by eigenvalue analysis but are more understandable by examining the pseudospectra^[1,2,10,15,16].

Let $\|\cdot\|$ be a matrix norm induced by a vector norm. The following definitions of pseudospectra are equivalent.

- (I) $\Lambda_\varepsilon(A) = \{z \in \mathbb{C} : \|(zI - A)^{-1}\| \geq \varepsilon^{-1}\}$;
- (II) $\Lambda_\varepsilon(A) = \{z \in \mathbb{C} : z \in \Lambda(A + E) \text{ for some } E \text{ with } \|E\| \leq \varepsilon\}$;
- (III) $\Lambda_\varepsilon(A) = \{z \in \mathbb{C} : \text{there exists } v \in \mathbb{C}^N \text{ with } \|v\| = 1 \text{ such that } \|(A - zI)v\| \leq \varepsilon\}$;
- (IV) If $\|\cdot\|$ is the 2-norm, the following definition is also equivalent:

$$\Lambda_\varepsilon(A) = \{z \in \mathbb{C} : \sigma_{\min}(zI - A) \leq \varepsilon\};$$

Note that if $zI - A$ is singular, we denote $\|(A - zI)^{-1}\| = \infty$ and $\sigma_{\min}(\cdot)$ denotes the minimum singular value. From these definitions, it immediately follows that for any $\varepsilon_1 >$

ε_2 , $\Lambda_{\varepsilon_1}(A) \supseteq \Lambda_{\varepsilon_2}(A)$. Furthermore, $\Lambda_0(A)$ coincides with the eigenvalues of A . Especially, if matrix A is normal, the $\Lambda_\varepsilon(A)$ is just the closed ε -neighborhood of $\Lambda(A)$.

In order for the pseudospectra to become a useful and practical tool, we need efficient methods for its computation and visualization. The straightforward way to compute pseudospectra involves many applications of the singular value decomposition (SVD)^[1-3]. Definition (IV) motivates the simplest algorithm for estimating $\Lambda_\varepsilon(A)$, typically referred to as Grid-SVD, which is the most popular method for pseudospectra computing, consisting of two major steps as the following.

Algorithm 1.1 The Grid-SVD Method

- 1) Construct a mesh Ω over a region of the complex plane that includes $\Lambda_\varepsilon(A)$;
- 2) Compute $\sigma_{\min}(zI - A)$ for every node z of Ω .

Subsequently, the values can be processed, e.g. by contour plotting software, to visualize the pseudospectra by plotting contours, denoted here by $\partial\Lambda_\varepsilon(A)$, for specific values of ε .

Another way for computing pseudospectra is called poor man's pseudospectrum method according to the definition (II) of the pseudospectra based on the distribution of the random perturbations^[1].

Algorithm 1.2 The Poor Man's Pseudospectrum Method

- 1) Select random matrices E with $\|E\| < \varepsilon$;
- 2) Superimpose plots of $\Lambda(A + E)$, Computing using standard dense matrix eigenvalue algorithms.

It is a cloudy of eigenvalues surrounding the spectrum whose density depends upon the number of perturbations taken and the probability distribution of the random perturbations. And if E is generated as a full-rank random matrix, the cost of normalizing this matrix is $O(N^3)$ operations, whereas rank-1 matrix can be constructed and normalized in $O(N^2)$ operations. Such perturbation plots have intuitive appeal.

The computation of pseudospectra of matrix is only a decade old. Remarkable progress has been made in the 1990s. Most of the references date from this decade. The literature on the numerical computation of pseudospectra is growing, and is cited and reviewed by Trefethen^[1]. There are the inverse iteration, preliminary triangular algorithm, Lanczos iteration, continuation algorithm and even the parallel implementation^[1-10,17-22]. The total cost of grid can be approximated reliably by the sum of the cost of computing

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$\sigma_{\min}(zI - A)$ at all grid mesh points in Ω . Clearly, as the size of the matrix and/or the number of mesh points increase the cost of grid becomes prohibitive. Research efforts designed to speed-up the computation of pseudospectra have been aiming.

Since calculation of pseudospectra is much more expensive, this suggests that it may be desirable to develop methods for determining them iteratively. Large nonsymmetric matrix eigenvalue problems are commonly solved by the projection methods such as Krylov subspace method and its variants^[11–14]. In this paper, we explore the possibility that the projection methods can also be used to estimate pseudospectra. The idea investigated here is that the pseudospectra of a matrix can be approximated by those of the projection matrices constructed by projection methods. In details, The motivation in projection method is the following: Since the eigenvalues of the much smaller matrix on a lower-dimensional projection subspace are used as approximation of the eigenvalues of the original matrix, it is hoped that in the proximity of the approximated eigenvalues, one can also construct useful approximations to the pseudospectra of A . For example, the eigenvalues of Hessenberg matrix produced by Arnoldi iteration are used as Ritz value approximations of the eigenvalues of the original matrix. One can computing the pseudospectra of large matrix by Arnoldi iteration^[5].

The outline of this paper is as follows. In Section 2, we describe the orthogonalization projection method (Arnoldi) for computing the pseudospectra of large matrix. In Section 3, the oblique projection method (IOM(q): Incomplete Orthogonalization Method) for computing pseudospectra is proposed. In Section 4, some numerical experiments and comparisons are given which show that this kind of methods are powerful and cost effective scheme for computing pseudospectra of large matrices. Finally, we make some concluding remarks.

Throughout the paper, let $\|\cdot\|$ denote the 2-norm, $C^{N \times N}$ and $R^{N \times N}$ denote the $N \times N$ complex and real matrix, C denote the complex number, and A^H denote the conjugate transpose matrix of A .

II. THE ORTHOGONALIZATION PROJECTION METHOD

Let $A \in C^{N \times N}$ (or $R^{N \times N}$). The Arnoldi iteration process gives a complete unitary reduction of A to upper-Hessenberg matrix $Q^H A Q = H$ or $A Q = A H$, starting from the condition that the first column of Q is a prescribed unit vector.

Let Q_n be the $N \times n$ matrix whose columns are the first n columns of Q and let \tilde{H}_n be the $(n+1) \times n$ upper-left section of H ,

$$\tilde{H}_n = \begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1n} \\ h_{21} & h_{22} & \cdots & h_{2n} \\ & \ddots & \ddots & \vdots \\ & & h_{n,n-1} & h_{nn} \\ & & & h_{n+1,n} \end{bmatrix}_{(n+1) \times n} \quad (1)$$

Then we have

$$A Q_n = Q_{n+1} \tilde{H}_n$$

The Arnoldi process realizes the orthogonalization Projection onto the Krylov subspace, which is the modified Gram-Schmidt process that implements the $(n+1) \times n$ -term recurrence relation. We briefly describe the Arnoldi algorithm as follows.

Algorithm 2.1 The Arnoldi Iteration

- 1) Start: Choose an initial unit vector v .
- 2) For $i = 1, 2, 3, \dots$, do the full orthogonalization process

- $w := A v_i - \sum_{j=1}^i h_{ji} v_j$ with $h_{ji} := v_j^H A v_i$
- $h_{i+1,i} := \|w\|$, $v_{i+1} = w/h_{i+1,i}$

The $Q_n Q_{n+1}^H$ is the $n \times (n+1)$ identity, i.e., the $n \times (n+1)$ matrix with 1 on the main diagonal and 0 elsewhere. Therefore, $Q_n^H Q_{n+1} \tilde{H}_n$ is the $n \times n$ Hessenberg matrix obtained by removing the last row of \tilde{H}_n

$$H_n = \begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1n} \\ h_{21} & h_{22} & \cdots & h_{2n} \\ & \ddots & \ddots & \vdots \\ & & h_{n,n-1} & h_{nn} \end{bmatrix}_{n \times n}$$

Then we can accordingly derive the formula

$$H_n = Q_n^H A Q_n$$

For sufficiently large n , some of the pseudospectra of A can be reasonably approximated by the corresponding pseudospectra of H_n or \tilde{H}_n

$$\Lambda_\varepsilon(A) \approx \Lambda_\varepsilon(H_n) \approx \Lambda_\varepsilon(\tilde{H}_n)$$

For $n \ll N$, the computation of $\Lambda_\varepsilon(H_n)$ or $\Lambda_\varepsilon(\tilde{H}_n)$ will be $O((n/N)^3)$ times faster than that of $\Lambda_\varepsilon(A)$. Note that in considering $\Lambda_\varepsilon(\tilde{H}_n)$, we are dealing with the ε -pseudospectra of a rectangular matrix^[22].

We are not aware of very satisfactory theorems to justify the approximation $\Lambda_\varepsilon(A) \approx \Lambda_\varepsilon(H_n)$. However, there are the following results^[5].

Theorem 2.1 Let an $N \times N$ matrix A be unitary similar to a Hessenberg matrix H , and let \tilde{H}_n denote the $(n+1) \times n$ section (1). Then for any z we have

$$\sigma_{\min}(zI - \tilde{H}_1) \geq \sigma_{\min}(zI - \tilde{H}_2) \geq \sigma_{\min}(zI - \tilde{H}_3) \geq \cdots \geq \sigma_{\min}(A) \quad (2)$$

and, consequently, for any $\varepsilon \geq 0$

$$\Lambda_\varepsilon(\tilde{H}_1) \subseteq \Lambda_\varepsilon(\tilde{H}_2) \subseteq \Lambda_\varepsilon(\tilde{H}_3) \subseteq \cdots \subseteq \Lambda_\varepsilon(A) \quad (3)$$

Note that in Theorem 2.1, there is no Ritz values. Just like eigenvalue problems, we can give a the definition of Ritz values as the points z at which $\sigma_{\min}(zI - H_n)$ achieves a local minimum (namely, zero). And analogue for the rectangular case would be to consider the points at which $\sigma_{\min}(zI - \tilde{H}_n)$ achieves a local minimum. It follows from (2) that this minimum value will be equal to zero if and only if z is an eigenvalue of A corresponding to an eigenvector that lies in the Krylov subspace.

Besides pseudospectra, it is well known that the Arnoldi iteration also may provide estimates of the *numerical range* (namely, *field of values*)^[7] of A , which is denoted by $W(A) = \{x^H A x : \|x\| = 1\}$. Now it is H_n that we most naturally make use of

$$W(A) \approx W(H_n)$$

Theorem 2.2 Let a A and H be as in Theorem 2.1, and matrix H_n is the $n \times n$ matrix produced by Arnoldi iteration. Then

$$W(H_1) \subseteq W(H_2) \subseteq W(H_3) \subseteq \cdots \subseteq W(A)$$

We briefly describe the Arnoldi method for pseudospectra computing as follows.

Algorithm 2.2 The Arnoldi Method for Pseudospectra

- 1) Compute the Hessenberg matrix by Arnoldi iteration;
- 2) Compute the pseudospectra of the Hessenberg matrix using the small dense matrix methods;
- 3) Use a visualisation tool to display the computed Pseudospectra.

III. THE OBLIQUE PROJECTION METHOD

IOM(q) proposed by Saad is formally similar to Arnoldi's method except for a generation of V_n . In it, Av_i is only orthogonalized against the previous q vectors v_{i-q+1}, \dots, v_i , where $2 \leq q \leq N$, so it is less computational cost than Arnoldi iteration. IOM(q) realizes an oblique projection process over Krylov subspace and is more attractive, valuable and interesting both in theory and in practice.

Algorithm 3.1 The IOM(q)(Incomplete Orthogonalization Method) Iteration

- 1) Start: Choose the parameter q satisfying $2 \leq q \leq N$ and an initial vector v .
- 2) For $i = 1, 2, 3, \dots$, do
 - the incomplete orthogonalization process:
 - $i_0 := \max\{1, i - q + 1\}$
 - $w := Av_i - \sum_{j=i_0}^i h_{ji} v_j$ with $h_{ji} := v_j^H Av_i$
 - $h_{i+1,i} := \|w\|, v_{i+1} = w/h_{i+1,i}$

To describe the algorithm we start by noticing that after n steps of IOM(q) we have an not l_2 -orthonormal system V_{n+1} and a $(n+1) \times n$ banded upper-Hessenberg matrix \hat{H}_n whose only nonzero entries are the elements h_{ij} generated by the method. Thus \hat{H}_n is the same as H_n generated by IOM(q) except for an additional row whose only nonzero element is $h_{n+1,n}$ in the $(n+1, n)$ position. From the Step 2 of IOM(q) iteration,

$$AV_n = V_n H_n + h_{n+1,n} v_{n+1} e_n^H$$

and

$$AV_n = V_{n+1} \hat{H}_n$$

where the banded upper-Hessenberg matrices H_n and \hat{H}_n with the following form

$$H_n = \begin{bmatrix} * & * & * & * & & \\ & * & * & * & * & \\ & & * & * & * & * \\ & & & * & * & * \\ & & & & * & * \\ & & & & & * & * \end{bmatrix}_{n \times n}$$

$$\hat{H}_n = \begin{bmatrix} * & * & * & * & & \\ * & * & * & * & * & \\ & * & * & * & * & * \\ & & * & * & * & * \\ & & & * & * & * \\ & & & & * & * \\ 0 & . & . & . & . & * \end{bmatrix}_{(n+1) \times n}$$

We consider $\|V_{n+1}\|$, where V_{n+1} is an $N \times (n+1)$ matrix. Then

$$\|V_{n+1}\| = \sqrt{\lambda_{\max}[V_{n+1}^\top V_{n+1}]}$$

Let $V_{n+1} = (v_1, v_2, \dots, v_k, v_{n+1})$, then $V_{n+1}^\top = (v_1^\top, v_2^\top, \dots, v_n^\top, v_{n+1}^\top)^\top$. Then,

$$V_{n+1}^\top V_{n+1} = \begin{bmatrix} v_1^\top v_1 & v_1^\top v_2 & \cdots & v_1^\top v_n & v_1^\top v_{n+1} \\ v_2^\top v_1 & v_2^\top v_2 & \cdots & v_2^\top v_n & v_2^\top v_{n+1} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ v_n^\top v_1 & v_n^\top v_2 & \cdots & v_n^\top v_n & v_n^\top v_{n+1} \\ v_{n+1}^\top v_1 & v_{n+1}^\top v_2 & \cdots & v_{n+1}^\top v_n & v_{n+1}^\top v_{n+1} \end{bmatrix}$$

which is a $(n+1) \times (n+1)$ symmetric matrix.

From the Gerschgorin disk theory, the eigenvalues of $V_{n+1}^\top V_{n+1}$ lie in the disks whose centers are 1 and radiuses are the sum of the moduli of the entries in each line except for the elements on the diagonal line.

It is easy to prove that

$$1 \leq \lambda_{\max}[V_{n+1}^\top V_{n+1}] \leq R_{\max} + 1$$

where R_{\max} stands for the biggest radius of the disks.

Now we analyze the maximal radius of these disks. From the incomplete orthogonormality

$$(v_i, v_j) = \delta_{ij}, |i - j| \leq q + 1$$

it also is easy to prove that

$$\|v_i^\top v_j\| \leq 1$$

Then, we have $R_{max} \leq n - q$. Therefore,

$$1 \leq \lambda_{max}[V_{n+1}^\top V_{n+1}] \leq n - q + 1$$

From the previous analysis, we finally have

$$1 \leq \|V_{n+1}\| \leq \sqrt{n - q + 1}$$

which gives an upper bound of $\|V_{n+1}\|$. Especially, if $q = n$, then $\|V_{n+1}\| = 1$. This is the Arnoldi iteration.

Therefore, for $n \ll N$, some of the pseudospectra of A can be reasonably approximated by the corresponding pseudospectra of H_n or \hat{H}_n

$$\Lambda_\varepsilon(A) \approx \Lambda_\varepsilon(H_n) \approx \Lambda_\varepsilon(\hat{H}_n) \quad (4)$$

For $n \ll N$, the computation of $\Lambda_\varepsilon(H_n)$ or $\Lambda_\varepsilon(\hat{H}_n)$ will be $O((n/N)^3)$ times faster than that of $\Lambda_\varepsilon(A)$. Also, the computation of the IOM iteration is less than that of Arnoldi iteration, especially when N is very large. Note that in considering $\Lambda_\varepsilon(\hat{H}_n)$, we are dealing with the ε -pseudospectra of a rectangular matrix.

We are not aware of very satisfactory theorems to justify the approximation $\Lambda_\varepsilon(A) \approx \Lambda_\varepsilon(H_n)$. Also, we have no results like Theorem 2.1 and Theorem 2.2, because $zI - A$ and $zI - H_n$ are not unitarily similar, i.e., they have different singular values. However, in fact, the IOM(q) is the Arnoldi method in the extreme case $q = 0$. In another word, $zI - A$ and $zI - H_n$ are approximately unitarily similar. Therefore, we still can use the IOM(q) to estimate the pseudospectra of the large matrix approximately in (4) which is very effective when A is very large banded structured matrix. And the following numerical experiments in the next section show that it is more attractive, valuable and interesting both in theory and in practice.

Algorithm 3.2 The IOM(q) Method for Pseudospectra

- 1) Compute the banded Hessenberg matrix by IOM(q) iteration;
- 2) Compute the pseudospectra of the banded Hessenberg matrix using the small dense matrix methods;
- 3) Use a visualisation tool to display the computed pseudospectra.

IV. NUMERICAL EXPERIMENTS

In this section, we apply our results to some matrices to show their applications in practice. Because of the very long CPUtime, here we take some moderate (not very large)

matrices which are taken from Gallery Higham test matrices in MATLAB as examples and we hope to investigate more large problems in the future. Here, all the computations are finished with MATLAB 6.5 on PC (Intel(R) Pentium(R), Processor 1500MHz 1.50GHz, Memory 256MB).

In Algorithm 2.2 and Algorithm 3.2, the smaller dense matrix method is the Algorithm 1.2, which is denoted RANDPS. The maximum number of choosing the random matrix E with $\|E\| \leq \varepsilon$ is taken as 100. Note that the smaller dense matrix method in Algorithm 2.2 and Algorithm 3.2 may also be chosen as the Grid-SVD method here.

Example 1 Consider the 100×100 ($N = 100$) Grcar matrix, a Toeplitz matrix with -1 on the subdiagonal and 1 on the main diagonal and on the first three superdiagonals. Arnoldi method approximation at step $n = 30, 50, 70$ and 90 are plotted. The axis limits are $-2 \leq Re \leq 4, -4 \leq Im \leq 4$.

Table 1 and Figure 1 show the results.

Table 1: The CPUtime comparison

Methods	CPUtime
RANDPS	137.5480
Arnoldi(n=30)	12.6680
Arnoldi(n=50)	31.6350
Arnoldi(n=70)	62.0690
Arnoldi(n=90)	97.2340

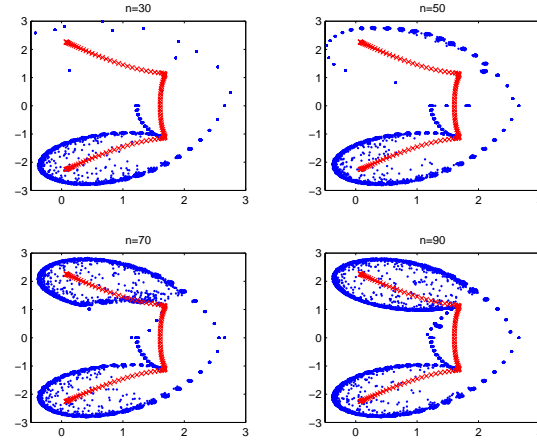


Fig. 1. pseudospectra of the 100×100 Grcar matrix compared with those of four Arnoldi approximations ($\varepsilon=0.01$, $n = 30, 50, 70$ and 90). The upper half of each plot corresponds to lower-dimensional projection matrix, and the lower half to origin matrix A ; the axis limits in each case are $-0.5 \leq Re \leq 3, -3 \leq Im \leq 3$. The red 'x' are the eigenvalue of A in the whole plane.

Example 2 Consider the 200×200 ($N = 200$) Toeppen matrix with 0.5 on the subdiagonal and 1 on the main diagonal and on the first two superdiagonals. The approximation by Arnoldi iteration which is denoted ARNRANDPS with $n = 100$

and IOM(q) iteration which is denoted IOMRANDPS with $n = 100$, $q = 30$ and $q = 60$ are plotted. Figure 2 shows the results. Obviously, seen from the figure 2, the approximation

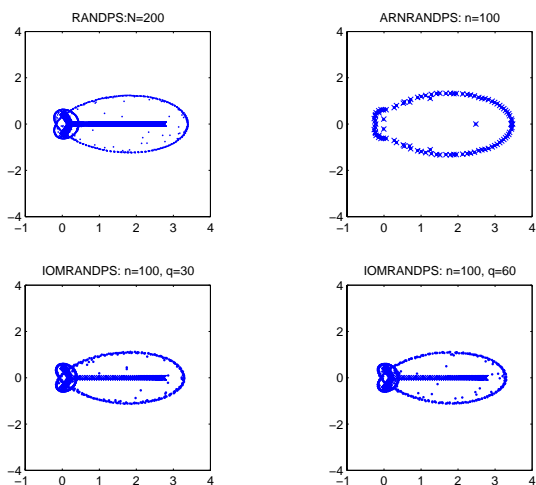


Fig. 2. pseudospectra of the 200×200 Teplitz matrix compared with those of Arnoldi approximations ($\varepsilon=0.001$, $n = 100$) and IOM(q) approximations ($\varepsilon=0.001$, $n = 100$, $q = 30$ and $q = 60$). The axis limits in each case are $-1 \leq Re \leq 4$, $-4 \leq Im \leq 4$.

by IOM(q) is better than that by Arnoldi method. The reason is that the origin Teplitz matrix is band structured matrix and the projection matrix by IOM(q) process is also band structure.

V. CONCLUSION AND REMARKS

Perhaps pseudospectra will play a role tool in breaking down walls between the theorists of functional analysis and the engineers of scientific computing[1]. To improve the efficiency of computing pseudospectra, there are two main ways: (1) The first way to speed up the calculation of pseudospectra is the simplest: avoid computing singular values in uninteresting regions of the complex plane, where the resolvent norm is small and there are no boundaries of the pseudospectra of interest; (2) The second way to speed up the calculation of pseudospectra, independent of the first, is to reduce the dimension of the $N \times N$ matrix A by projection onto an subspace, such as Krylov subspace and invariant subspace of dimension $n < N$.

The idea in this paper is the latter. We have proposed a kind of projection methods for computing pseudospectra of large matrices. The first way is the version of the Arnoldi iteration method (an orthogonal projection method) on a low-dimensional subspace. The second way is the version of the IOM(q) iteration method (an oblique projection method) on a low-dimensional subspace. The numerical algorithms are given. Numerical experiments show that this kind of

methods are powerful and cost effective scheme for computing pseudospectra of large matrices.

Furthermore, the idea in this paper can be generalized to the pseudospectra of the rectangular matrices. Also, the idea in this paper may provide some insights for the pseudospectra in other norms.

ACKNOWLEDGMENT

This research was supported by the Aviation Science Foundation of China (No.2009ZH52069) and the NUAU Research Funding (No.NS2010202).

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