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# TRANSFER FUNCTIONS AND RESOLVENT NORM APPROXIMATION OF LARGE MATRICES*

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**Abstract.** A unifying framework for methods employed in the approximation of the resolvent norm of nonnormal matrices is presented. This formulation uses specific transfer functions, and it provides new information about the approximation properties of these methods and their application in computing the pseudospectrum of matrices.

**Key words.** Resolvent norm, transfer function, Arnoldi iteration, pseudospectrum.

**AMS subject classification.** 65F15.

**1. Introduction.** We now know that the analysis of matrix-dependent algorithms is considerably more complicated when nonnormal matrices are involved; see for example [5]. In particular, several studies indicate that the eigenvalues of the matrix in question often provide insufficient or even misleading information [20]. This has been the motivation behind recent research on more reliable indicators as well as on methods for their practical computation. Several studies concur that a better accordance between theory and practice can be achieved by using the resolvent function $R(z) = (A - zI)^{-1}$, for $A \in \mathbb{C}^{n\times n}$ and $z \in \mathcal{C} \subseteq \mathbb{C}$ [7, 19]. The following, well-known, result shows that studying the variation of the resolvent norm corresponds to analyzing how the eigenvalues change under perturbations of $A$:

*For any $\varepsilon > 0$, the locus of points $z \in \mathbb{C}$ for which*[1]

$$\|R(z)\| \geq \varepsilon^{-1} \tag{1.1}$$

*is equivalent to the set of eigenvalues (the $\varepsilon$-pseudoeigenvalues) that solve*

$$(A + \mathcal{E})x = \lambda x, \qquad \|\mathcal{E}\| \leq \varepsilon. \tag{1.2}$$

Since $\|R(z)\| = (\sigma_{\min}(A - zI))^{-1}$, where $\sigma_{\min}(\cdot)$ denotes the smallest singular value, the computation of $\|R(z)\|$ relies on algorithms for singular values or eigenvalues. Standard techniques are adequate when the matrix dimension is small. For instance, the MATLAB function `pscont` [11], plots level curves by first computing the complete singular value decomposition of $A$ using the Golub-Reinsch SVD algorithm. An alternative approach that appears to lend itself to parallel computation is to first block diagonalize $A$ and then approximate its singular values [14]. Many applications of interest, however, lead to matrices that are large, sparse and possibly structured, properties that are not exploited in the aforementioned "dense matrix" approaches. For that reason, projection-type methods for approximating $\|R(z)\|$ that reduce $A$ and reference it only in matrix-vector products have been the subject of recent investigations [3, 4, 10, 15, 16, 18].

In this paper we introduce a unifying framework, based on *transfer functions*, for reduction based approximations of the resolvent norm of nonnormal matrices and apply it on

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[1] In this paper $\|\cdot\|$ denotes the 2-norm for vectors and the induced norm for matrices.

several existing methods. An important benefit of our analysis is that it leads to useful information regarding the quality (or lack thereof) of the approximations constructed by these methods. It also provides the means for obtaining more accurate estimates of the resolvent norm.

In particular, let $D^*$ and $E$ be two tall rectangular, full rank matrices[2] of suitable dimension and let $G_z(A, E, D) := D(A - zI)^{-1}E$ be the projected resolvent function onto the subspaces spanned by the columns of $E$ and $D^*$. In the terminology of automatic control, $G_z(A, E, D)$ is a transfer function. Matrices $E$ and $D$ describe the perturbation structure of the system and can be set a-priori by using the knowledge of system parameters [12]. When perturbations on $A$ are restricted to be so structured as to be of the form $D\Delta E$, where the "disturbance matrix" $\Delta$ has small norm, $\|G_z(A, E, D)\|$ measures the size of the perturbation for $z \in \mathcal{C}$. We show that most projection methods applied to the computation of the resolvent norm reduce to transfer function evaluations corresponding to particular selections of $E$ and $D$. In order to approximate $\|(A - zI)^{-1}\|$, these methods in fact compute $\|G_z(A, E, D)\|$ for specific $E, D$.

MATLAB notation for matrices and vectors will be used. For ease of notation we use $G_z(A)$ to denote the transfer function whenever $D = E = I$ and will write $G_z$ whenever $D, E$ and $A$ are clear from the context. For a rectangular matrix $X$, $\sigma_{\min}(X)$ will denote its smallest nonzero singular value. We use $I_{p_1:p_2}$ to denote the rectangular matrix consisting of columns $p_1, ..., p_2$ of the identity. The notation $e_k$ indicates the $k-$th column and $\widetilde{I}$ a rectangular portion of the identity matrix, whose size will become clear from the context.

For the numerical experiments we use the following nonnormal matrices: $i)$ the pentadiagonal Toeplitz *Grcar matrix* matrix $A = \text{Toeplitz}([-1, \underline{1}, 1, 1, 1])$ [9], where unless indicated otherwise, the Grcar matrix will be of order $n = 100$; $ii)$ the bidiagonal matrix of order $n = 64$ with elements $a_{kk} = -0.3k$ in the diagonal and $a_{k,k+1} = 1$ in the first upper diagonal [18]; $iii)$ the upper triangular *Kahan matrix* of order $n = 50$, with elements $a_{kk} = s^{k-1}$ and $a_{kj} = -s^{k-1}c$ when $j > k$, where $s^{n-1} = 0.1$ and $s^2 + c^2 = 1$ [19]; and $iv)$ the *Tolosa matrix* of order $n = 135$ from the Harwell-Boeing collection [5, 6].

**2. Krylov subspace methods and the transfer function framework.** We next recall some properties of Krylov subspace reduction and show how it naturally induces structured perturbations. We also show that the resolvent norm approximants in the projected space can be written in terms of the norm of specific transfer functions.

**2.1. The Arnoldi method.** Let $A \in \mathbb{C}^{n\times n}$, $v \in \mathbb{C}^n$ and let $m \le n$. Throughout this paper we assume that $m$ is smaller than the degree of the minimum polynomial of $v$ with respect to $A$ so that the Krylov subspace $\mathcal{K}_m(A, v) := \text{span}\{v, Av, \dots, A^{m-1}v\}$ has dimension equal to $m$. A basis $V_m = [v_1, \dots, v_m]$ of $\mathcal{K}_m(A, v)$ with orthonormal columns in $\mathbb{C}$ can be generated one vector at a time using the Arnoldi process, yielding the relation

$$AV_m = V_mH_m + h_{m+1,m}v_{m+1}e_m^* \tag{2.1}$$

or, equivalently, $AV_m = V_{m+1}\widetilde{H}_m$, where $\widetilde{H}_m := [H_m; h_{m+1,m}e_m^*]$. One simple but important observation that will be key to our discussion is the following Lemma:

LEMMA 2.1. *Let $A, H_m, V_m$ be as above. Then*

$$(A + \mathcal{E})V_m = V_mH_m, \qquad \textit{where} \quad \mathcal{E} = -h_{m+1,m}v_{m+1}v_m^*. \tag{2.2}$$

Relation (2.2) implies that the eigenvalues of $H_m$ are also eigenvalues of $A+\mathcal{E}$ for the specific choice of the rank-one matrix $\mathcal{E}$.

[2] Here '*' denotes conjugate transposition.

**2.2. Resolvent norm approximation via the Arnoldi method: A transfer function approach.** The first method that we consider was described by Toh and Trefethen in [18]. The idea is to approximate the norm of the resolvent $\|(A-zI)^{-1}\|$ with $\|(H_m-zI)^{-1}\|$, where $H_m$ is the Hessenberg matrix obtained from the Arnoldi method. The motivation behind that approach is the potential for significant computational savings whenever the resolvent norm is successfully approximated for some $m \ll n$, since then only one matrix $H_m$ need be computed for all $z$'s of interest.

From the characterization of the $\epsilon$-pseudospectrum using singular values, it follows that the values $z$ for which $\|(H_m-zI)^{-1}\| \geq \varepsilon^{-1}$, also solve the perturbed eigenvalue problem

$$(H_m+\Delta)x = \lambda x \tag{2.3}$$

for suitable $\Delta$ that satisfies $\|\Delta\| \leq \varepsilon$. From Lemma 2.1 we obtain the following:

$$(H_m-zI)^{-1} = G_z(A+\mathcal{E}, V_m, V_m^*). \tag{2.4}$$

Note that Equation (2.4) can be written entirely in terms of transfer functions, i.e. $G_z(H_m) = G_z(A+\mathcal{E}, V_m, V_m^*)$. We next note that from Lemma 2.1 it follows that the values $\lambda$ that satisfy relation (2.3) with $\|\Delta\| \leq \varepsilon$ also satisfy

$$(A+\mathcal{E}+V_m\Delta V_m^*)V_m x = \lambda V_m x, \qquad \|\Delta\| \leq \varepsilon,$$

which differs from the desired relation (1.2) above; notice the bound for the term $\|V_m\Delta V_m^*\| \leq \|\Delta\| \leq \varepsilon$ as well. In particular, relation (2.3) does not correspond to a perturbed eigenvalue problem for $A$ but for $A+\mathcal{E}$. Therefore, when $\|\mathcal{E}\|$ is not small, $\|(H_m-zI)^{-1}\|$ would be a poor approximation of $\|(A-zI)^{-1}\|$. In light of unsatisfactory experimental and lack of theoretical evidence of this method, Toh and Trefethen also consider a modification of the above approach, that is based on using the rectangular matrix $\widetilde{H}_m$ instead of $H_m$ [18]. This modification, that for future reference we call "augmented Arnoldi", is supported by theoretical evidence which predicts that ([18, Theorem 1])

$$\sigma_{\min}(\widetilde{H}_1 - z\widetilde{I}) \geq \sigma_{\min}(\widetilde{H}_2 - z\widetilde{I}) \geq \cdots \geq \sigma_{\min}(A-zI), \tag{2.5}$$

where the size of $\widetilde{I}$ in each term conforms with that of $\widetilde{H}_j \in \mathbb{C}^{(j+1)\times j}$. Numerical experiments in [18] show that $\sigma_{\min}^{-1}(\widetilde{H}_m - z\widetilde{I})$ often provides a better approximation to $\|(A-zI)^{-1}\|$ than $\|(H_m-zI)^{-1}\|$.

The next proposition indicates that by using an appropriate transfer function we can improve over the above approximations.

PROPOSITION 2.2. *With the notation above, let $\widetilde{H}_m - z\widetilde{I} = [U,\widetilde{u}][\Sigma;0]W^*$ be the singular value decomposition of $\widetilde{H}_m - z\widetilde{I}$. Then for $z \in \mathcal{C}$*

$$\frac{1}{\sigma_{\min}(\widetilde{H}_m - z\widetilde{I})} \leq \|G_z(A, V_{m+1}, V_m^*)\| \leq \frac{1}{\sigma_{\min}(\widetilde{H}_m - z\widetilde{I})} + \|G_z(A, V_{m+1}, V_m^*)\widetilde{u}\|.$$

*Proof.* Let $G_z := G_z(A, V_{m+1}, V_m^*)$. The relation $(A-zI)V_m = V_{m+1}(\widetilde{H}_m - z\widetilde{I})$ implies

$$G_z \cdot (\widetilde{H}_m - z\widetilde{I}) = I. \tag{2.6}$$

The lower bound is obtained by applying standard inequalities for singular values to $\sigma_{\min}(G_z \cdot (\widetilde{H}_m - z\widetilde{I})) = 1$ [13]. From (2.6) it follows $G_z[U,\widetilde{u}]\widetilde{I} = W\Sigma^{-1}$, therefore, $\|G_z\| = \|W^*G_z[U,\widetilde{u}]\| = \|[\Sigma^{-1}, W^*G_z\widetilde{u}]\| \leq \|\Sigma^{-1}\| + \|G_z\widetilde{u}\|$ and the upper bound follows. $\square$

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TABLE 2.1

*Estimates of $\|R(z)\|$ where the matrix $A$ of size $n = 25$ is generated using the MATLAB function* `rand` *with seed* 378800090 *and the starting vector $v$ is the sum of the columns of $A$.*

| $m$ | $[\sigma_{\min}(H_m - zI)]^{-1}$ | $[\sigma_{\min}(\widetilde{H}_m - z\widetilde{I})]^{-1}$ | $\|G_z(A, V_{m+1}, V_m^*)\|$ |
|---|---|---|---|
| | $(z = 0, [\sigma_{\min}(A - zI)]^{-1} = 32.5097)$ | | |
| 18 | 3.4172 | 2.5423 | 3.1327 |
| 20 | 4.9471 | 4.9469 | 9.8644 |
| 22 | 9.0682 | 5.7861 | 16.5909 |
| 23 | 10.2458 | 9.8563 | 30.6873 |
| 24 | 285.5174 | 16.0862 | 31.4461 |
| | $(z = 0.7023, [\sigma_{\min}(A - zI)]^{-1} = 323295.12)$ | | |
| 15 | 5.30 | 4.79 | 18605.65 |
| 18 | 33.63 | 5.01 | 31276.87 |
| 20 | 23.56 | 22.72 | 110153.21 |
| 22 | 31.98 | 30.74 | 292217.76 |
| 23 | 133.18 | 39.52 | 304784.08 |
| 24 | 165.36 | 65.30 | 323197.02 |

Proposition 2.2 shows that when using $(\sigma_{\min}(\widetilde{H}_m - z\widetilde{I}))^{-1}$ we *underestimate* the reduced resolvent norm corresponding to structured perturbations of the form $V_{m+1}\Delta V_m^*$. In practice, this underestimation can be severe. Relation (2.6) sheds light on what can go wrong when using $\widetilde{H}_m - z\widetilde{I}$. Specifically, it shows that $\widetilde{H}_m - z\widetilde{I}$ is an equation solving inverse of $G_z$, but not a pseudo-inverse, therefore the singular values are not preserved. From the proof we have

$$\|G_z\| = \|[\Sigma^{-1}, W^* G_z \widetilde{u}]\|.$$

Using $\sigma_{\min}(\widetilde{H}_m - z\widetilde{I})$ corresponds to imposing $\|G_z\| \approx \|\Sigma^{-1}\|$, thus excluding the possibly non-negligible component $G_z\widetilde{u}$ of $G_z$ onto the null space of $\widetilde{H}_m - z\widetilde{I}$. Comparing with the inequalities (2.5), the proposition tells us that for every $m < n$, the norm of the transfer-function $G_z(A, V_{m+1}, V_m^*)$ is a better approximation to the norm of the resolvent, in particular

$$\frac{1}{\sigma_{\min}(\widetilde{H}_m - z\widetilde{I})} \le \|G_z(A, V_{m+1}, V_m^*)\| \le \frac{1}{\sigma_{\min}(A - zI)} = \|(A - zI)^{-1}\|.$$

The situation is illustrated for a random matrix in Table 2.1. The entries of the second column of Table 2.1 do not follow any specific pattern, but it happens in this case that they are often better approximations to the sought value than those of the third. On the other hand, the entries of the last column are consistently better approximations than the values of the third column. We also see that the approximation of the third column becomes significantly better when $z = 0.7023$ which is close to an eigenvalue of $A$.

We next illustrate the behavior of our approach when used to approximate the pseudospectrum. The baseline computations of the pseudospectrum are made with the function `pscont`. The first experiment is with the Grcar matrix, whose pseudospectrum is depicted in Figure 2.1.

Figure 2.2 depicts the contour lines of $\sigma_{\min}^{-1}(\widetilde{H}_m - z\widetilde{I})$ for $m = 10$ (left) and $m = 50$ (right). The values and corresponding contours approximated using $m = 10$ are quite far from the exact ones and a much larger subspace dimension appears necessary. Comparing with Figure 2.1, however, shows that even when $m = 50$, the approximation to $\|(A - zI)^{-1}\|$ remains unsatisfactory.

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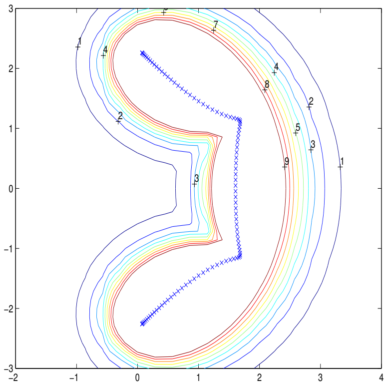

FIG. 2.1. *Contour plot of resolvent function norm of the Grcar matrix.*

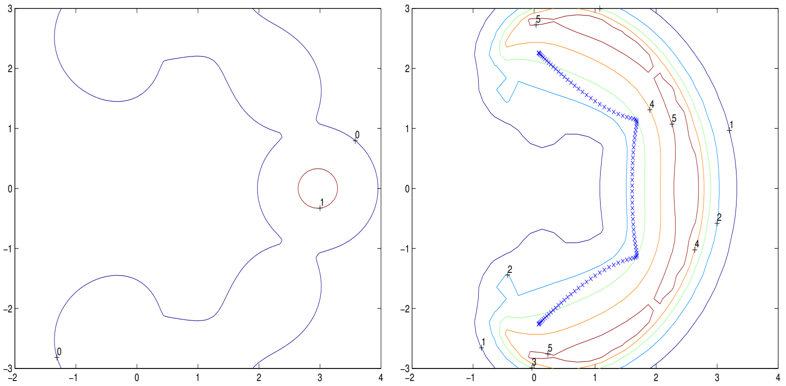

FIG. 2.2. *Contour plot of* $\sigma_m^{-1}(\widetilde{H}_m - z\widetilde{I})$ *for the Grcar matrix. Left:* $m = 10$*; right:* $m = 50$.

Figure 2.3 depicts the contour plot of $\|G_z(A, V_{m+1}, V_m^*)\|$ for $m = 10$ and $m = 30$. We see that there is much better accordance with the contours of Figure 2.1. This improvement is due to the incorporation of the term $G_z\widetilde{u}$ in the computation. Just like Table 2.1, we observe that the approximation becomes less satisfactory as the level curves move away from the spectrum. This will be further discussed in Section 3.

Our next experiments are with the bidiagonal (Fig. 2.4), Kahan (Fig. 2.5), and Tolosa (Fig. 2.6) matrices. For each matrix, the top pair of figures depicts the pseudospectrum (left), and its approximation using the Arnoldi method of [18] (right). The bottom pair depicts approximations to the pseudospectrum using the augmented Arnoldi method of [18] (left), and the transfer function approach (right). All approximations were computed using the same Krylov subspace dimension $m = 20$. The figures demonstrate that the transfer function approach leads to a much more accurate approximation and visualization of the pseudospectrum.

**2.3. Resolvent norm approximation via rational Krylov subspaces: A transfer function analysis.** Methods have been proposed for approximating the norm $\|(A - zI)^{-1}\|$ by means of rational Krylov reduction processes that involves the inverse of $A$. The general approach proposed by Ruhe [16] considers the generalized eigenvalue problem $Ax = \lambda Bx$.

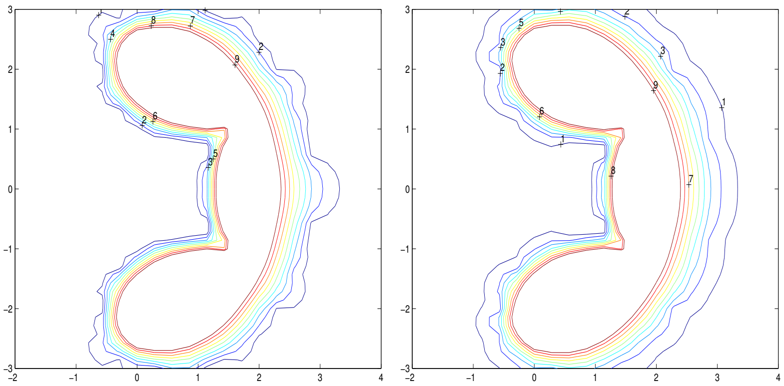

FIG. 2.3. *Contour plot of transfer function norm for the Grcar matrix with* $E = V_{m+1}$ *and* $D = V_m$. *Left:* $m = 10$; *right* $m = 30$.

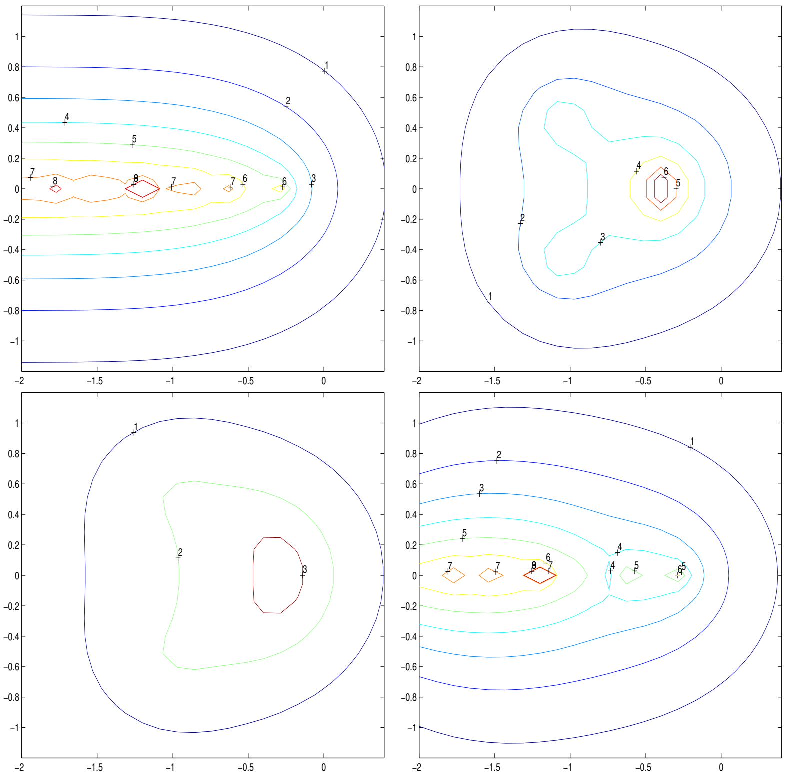

FIG. 2.4. *Bidiagonal matrix. Top: Pseudospectrum (left); Arnoldi (right). Bottom: Augmented Arnoldi (left); projected transfer function (right).*

For $\xi \in \mathbb{C}$ the application of the Arnoldi recurrence to the matrix $(A - \xi B)^{-1}B$ yields

$$(A - \xi B)^{-1} B P_m = P_{m+1} \widetilde{T}_m \tag{2.7}$$

or, equivalently, $BP_m = (A - \xi B)P_{m+1}\widetilde{T}_m$ so that

$$AP_{m+1}\widetilde{T}_m = BP_{m+1}(\widetilde{I} + \xi \widetilde{T}_m). \tag{2.8}$$

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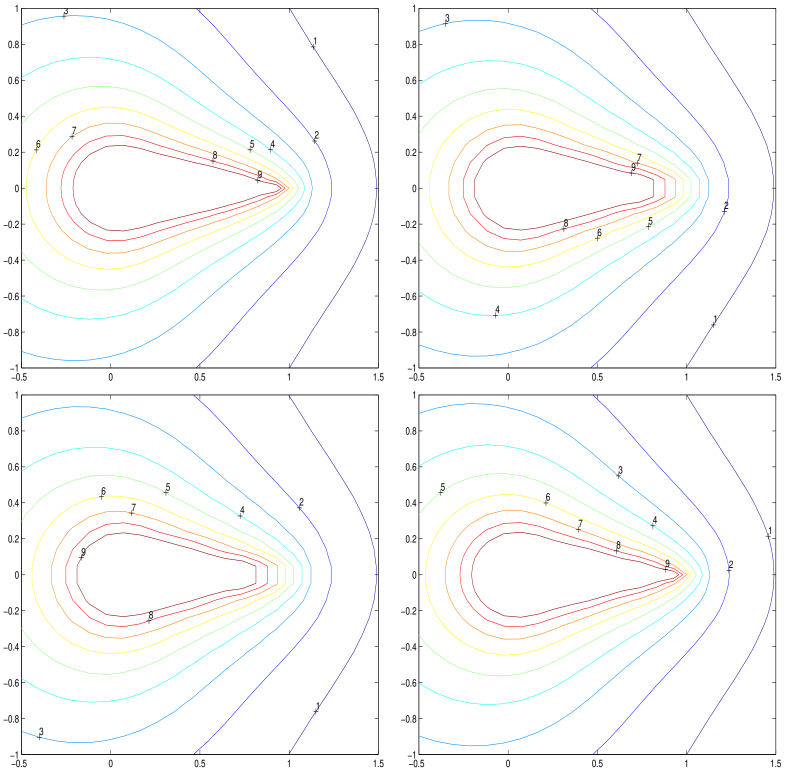

FIG. 2.5. *Kahan matrix. Top: Pseudospectrum (left); Arnoldi (right). Bottom: Augmented Arnoldi (left); projected transfer function (right).*

Letting $K_m = \widetilde{I} + \xi \widetilde{T}_m$, Ruhe showed that

$$\frac{\|\widetilde{T}_m w\|}{\sigma_{\min}(K_m - z\widetilde{T}_m)} \leq \|(A - zB)^{-1}B\|, \tag{2.9}$$

where $w$ is the right singular vector associated with $\sigma_{\min}(K_m - z\widetilde{T}_m)$. In our context, the inequality is of interest for the special case $B = I$. By setting $\xi = 0$ we obtain an Arnoldi recurrence for $A^{-1}$ that was also discussed in [18]. We next present the rational Krylov approach in the transfer function framework. Using (2.8) we can write

$$\begin{aligned}
(B^{-1}A - zI)P_{m+1}\widetilde{T}_m &= P_{m+1}(K_m - z\widetilde{T}_m), \\
T_m &= P_m^*(A - zB)^{-1}BP_{m+1}(K_m - z\widetilde{T}_m), \\
I &= P_m^*(A - zB)^{-1}BP_{m+1}(K_m - z\widetilde{T}_m)T_m^{-1},
\end{aligned}$$

where $T_m$ is the upper $m \times m$ section of $\widetilde{T}_m$. It follows that

$$I = G_z(B^{-1}A, P_{m+1}, P_m^*)(K_m - z\widetilde{T}_m)T_m^{-1}.$$

Setting $\xi = z, B = I$, yields the following equalities:

$$G_z(A, P_m, P_m^*) = T_m \qquad \text{and} \qquad G_z(A, P_m, P_{m+1}^*) = \widetilde{T}_m.$$

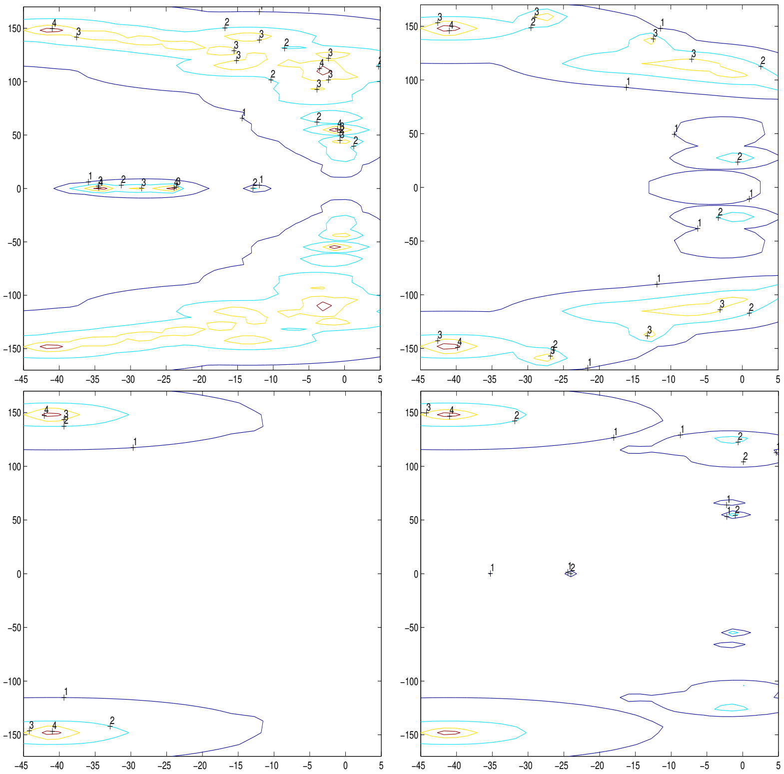

FIG. 2.6. *Tolosa matrix. Top: Pseudospectrum (left); Arnoldi (right). Bottom: Augmented Arnoldi (left); projected transfer function (right).*

In the general case we obtain that the transfer function norm satisfies

$$\frac{1}{\sigma_{\min}((K_m - z\widetilde{T}_m)T_m^{-1})} \le \|G_z(B^{-1}A, P_{m+1}, P_m^*)\| \le \|(A - zB)^{-1}B\|. \tag{2.10}$$

A sharper estimate for the resolvent norm than the one of (2.9) was presented by Toh in [17, Eq. (6.23)]. In our notation it reads

$$\frac{1}{\sigma_{\min}((K_m - z\widetilde{T}_m)R_m^{-1})} \le \|(A - zI)^{-1}\|,$$

where $R_m$ is the $m \times m$ upper triangular matrix in the QR factorization of $\widetilde{T}_m$. The next proposition relates estimates (2.10) and (2.9).

PROPOSITION 2.3. *Let* $(A - zB)^{-1}BP_m = P_{m+1}\widetilde{T}_m$ *with* $K_m = \widetilde{I} + \xi\widetilde{T}_m$. *Let also* $\kappa(T) = \|T\|/\sigma_{\min}(T)$ *and* $\tau = \|\widetilde{T}_m w\|/\sigma_{\min}(K_m - z\widetilde{T}_m)$. *Then*

$$\frac{1}{\kappa(\widetilde{T}_m)}\tau \le \frac{1}{\sigma_{\min}((K_m - z\widetilde{T}_m)T_m^{-1})} \le \kappa(\widetilde{T}_m)\tau. \tag{2.11}$$

*Proof*. Using $\sigma_{\min}((K_m - z\widetilde{T}_m)T_m^{-1}) \le \|T_m^{-1}\|\sigma_{\min}(K_m - z\widetilde{T}_m)$ and also $\|T_m^{-1}\| =$

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$\sigma_{\min}^{-1}(T_m) \le \sigma_{\min}^{-1}(\widetilde{T}_m)$ we have

$$\tau \le \frac{\|T_m^{-1}\| \|\widetilde{T}_m w\|}{\sigma_{\min}((K_m - z\widetilde{T}_m)T_m^{-1})} \le \kappa(\widetilde{T}_m) \frac{1}{\sigma_{\min}((K_m - z\widetilde{T}_m)T_m^{-1})}.$$

From $\sigma_{\min}(K_m - z\widetilde{T}_m) \le \sigma_{\min}((K_m - z\widetilde{T}_m)T_m^{-1})\|T_m\|$ we also have

$$\frac{1}{\sigma_{\min}((K_m - z\widetilde{T}_m)T_m^{-1})} \le \frac{\|T_m\|}{\sigma_{\min}(K_m - z\widetilde{T}_m)} \frac{\|\widetilde{T}_m w\|}{\|\widetilde{T}_m w\|} \le \kappa(\widetilde{T}_m)\tau.$$

□

**2.4. Explicit approximation of the resolvent norm.** Other approaches have been proposed that do not rely directly on reduction, but on some iterative scheme to approximately evaluate $\sigma(z) \approx \sigma_{\min}(A - zI)$ for each $z$, so that $\|R(z)\| \approx \sigma(z)^{-1}$.

In [3] the sought singular value is approximated using a Lanczos-Chebyshev algorithm. We shall focus here on the Lanczos step. The Hermitian version of the Lanczos scheme is used: given a Hermitian matrix $M$ the recurrence is defined, similarly to the Arnoldi case, as

$$MQ_m = Q_m T_m + r e_m^*, \qquad r \perp Q_m, \tag{2.12}$$

where $T_m$ is Hermitian tridiagonal and $Q_m$ has orthogonal columns. Braconnier and Higham in [3] chose $M_z = ((A - zI)(A - zI)^*)^{-1}$ so that for each given $z \in \mathcal{C}$ their approximation was given by $\max_{\lambda \in \Lambda(M_z)} |\lambda|^{\frac{1}{2}} \approx \max_{\lambda \in \Lambda(T_m)} |\lambda|^{\frac{1}{2}} \equiv \sigma^{-1}$.

PROPOSITION 2.4. *Let $M_z Q_m = Q_m T_m + r e_m^*$ with $M_z = ((A - zI)(A - zI)^*)^{-1}$. Then*

$$\|G_z(A, Q_m, I)\|^2 = \max_{\lambda \in \Lambda(T_m)} |\lambda|.$$

*Proof.* The result follows from the equivalence

$$\begin{aligned}
\max_{\lambda \in \Lambda(T_m)} |\lambda| &= \max_{x \in \text{span}\{Q_m\}} \frac{|x^* M_z x|}{x^* x} = \max_{y \in \mathbb{C}^m} \frac{|y^* Q_m^* ((A - zI)^*)^{-1} (A - zI)^{-1} Q_m y|}{y^* y} \\
&= \max_{y \in \mathbb{C}^m} \frac{\|(A - zI)^{-1} Q_m y\|^2}{\|y\|^2} = \|G_z(A, Q_m, I)\|^2.
\end{aligned}$$

□

In [15], Marques and Toumazou used $M_z \in \mathbb{C}^{2n \times 2n}$,

$$M_z = \begin{pmatrix} 0 & (A - zI)^{-1} \\ ((A - zI)^*)^{-1} & 0 \end{pmatrix},$$

so that $\max_{\lambda \in \Lambda(M_z)} |\lambda| \approx \max_{\lambda \in \Lambda(T_m)} |\lambda| \equiv \sigma^{-1}$. By starting the Lanczos recurrence with $q_1 = [\hat{q}_1; 0]$, only half of the elements of the basis $Q_m$ are nonzero. These correspond to the first or second $n$ locations [8]. Hence, by splitting $Q_m$ and $r$ as $Q_m = [U_1; U_2]$ and $r = [r_1; r_2]$, respectively, we obtain $(A - zI)^{-1} U_2 = U_1 T_m + r_1 e_m^*$ with $U_i^* U_i = I$, $i = 1, 2$, so that $G_z(A, U_2, U_1^*) := U_1^* (A - zI)^{-1} U_2 = T_m$ and

$$\|G_z(A, U_2, U_1^*)\| = \max_{\lambda \in \Lambda(T_m)} |\lambda|.$$

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Rearranging the equations so as to eliminate the zero columns of $U_1$ and $U_2$, we can write $(A - zI)^{-1}X_m = Y_m J_m$, where $J_m$ is upper bidiagonal and $X_m, Y_m$ have orthonormal columns [8]. When $m = n$ this equality corresponds to a unitary transformation so that the singular values of $J_n$ coincide with those of $(A-zI)^{-1}$. When $m$ is large enough, $U_1$ and $U_2$ will have large components along the directions of the leading singular vectors of $(A-zI)^{-1}$, in which case a good estimate of its largest singular value could be obtained. We note that the approaches of [15] and [3] are equivalent in exact arithmetic ([8]), while the augmented version appears to deliver more accurate results in finite–precision arithmetic [15].

**3. Accuracy and cost control in the transfer function framework.** We saw that transfer functions provide a useful framework for several recent methods designed for approximating the resolvent norm. Our methodology was the following: given a known method, construct the corresponding transfer function and analyze its properties. Instead, we can start from the general transfer function $G_z(A, E, D)$ and construct $E, D$ in order to obtain useful approximations to the resolvent norm.

We pose the problem as follows: for given $z \in \mathcal{C}$, find $E, D$ that solve the following optimization problem:

$$\max_{\substack{E \in \mathbb{C}^{n\times s}\ D \in \mathbb{C}^{t\times n} \\ E^*E=I,\, DD^*=I}} \|D(A - zI)^{-1}E\|.$$

One natural choice is to choose $E$ and $D$ that have large components along the directions of the right/left singular vector of the leading singular value of $(A - zI)^{-1}$. This was the case with the methods described in Section 2.4, where $E = E(z)$ and $D = D(z)$. Let $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n$ be the singular values of $(A - zI)^{-1}$, with $\sigma_i = \sigma_i(z)$ and $w_i$ be the corresponding right singular vectors. Assume for simplicity that $D = I$. Then

$$\|(A - zI)^{-1}E\| = \|[\sigma_1 w_1^* E; \sigma_2 w_2^* E; \ldots ; \sigma_n w_n^* E]\|.$$

If $\sigma_1 \gg \sigma_i$, for $\sigma_i \neq \sigma_1$, it follows that $\|(A - zI)^{-1}E\| \approx \sigma_1$, unless $\|w_1^* E\|$ is very small. Therefore, when $z$ is close to the spectrum of $A$, a sufficient condition for achieving a good approximation to $\|(A - zI)^{-1}\|$ is that $E$ has a non–negligible component along $w_1$. In this context, continuation may enhance the performance of the method by using the computed singular subspace information for generating $E(z)$ and $D(z)$ for a subsequent $z$ [3].

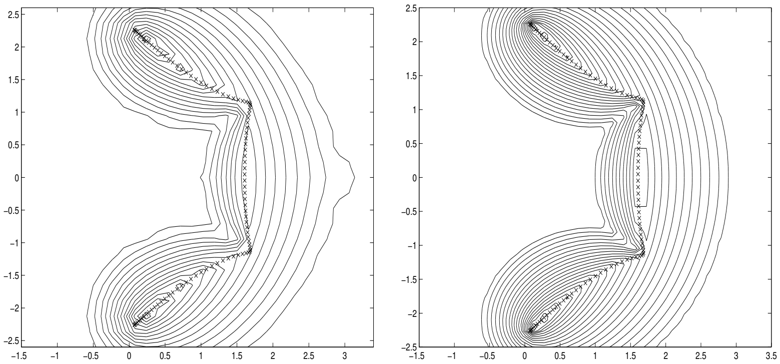


FIG. 3.1. *Contour plot of transfer function norm for the Grcar matrix. Left: For real random perturbations with orthonormal bases $E$ and $D$; Right: For $E, D$ sections of the identity matrix.*

These facts are illustrated in Figure 3.1(left), where $\|G_z\|$ is plotted for $E$ equal to an orthogonal basis of an $n \times (m + 1)$ matrix with real random entries uniformly distributed in the interval $[0, 1]$ and $m = 10$; here $D = [I, 0]E \in \mathbb{R}^{n\times m}$. Note that a less accurate approximation is obtained away from the spectrum, where the largest singular value of $(A - zI)^{-1}$ is less dominant. This property is also common in projection type approximations, which are most successful for $z$ near the spectrum [2].

If $A$ has special structure, $E$ and $D$ could be constructed to focus on parts of $A$ that best capture the nonnormality. One such example is when $A$ is upper triangular with large off–diagonal elements, in which case the resolvent frequently has large elements on the top right corner. Then we can select indices $p, t \ll n$ and $E = I_{n-p:n}$ and $D = I_{1:t}$ so that $\|D^*(A - zI)^{-1}E\| \approx \|R(z)\|$. The Grcar matrix demonstrates a similar behavior even though it is not triangular; see Figure 3.1(right), in which $p = t = 10$.

In choosing $D$ and $E$ we also have to consider computational cost. For instance, the Arnoldi methods described in [18] result in savings since the same $H_m$ is used independently of $z$. In the transfer function framework of Section 2.2, however, we need to compute $G_z(A, V_{m+1}, V_m^*) = V_m^*(A-zI)^{-1}V_{m+1}$. This appears prohibitive. If we observe, however, that

$$(H_m - zI)^{-1} = V_m^*(A - zI)^{-1}V_m + h_{m+1,m}V_m^*(A - zI)^{-1}v_{m+1}e_m^T(H_m - zI)^{-1}$$

and define $\phi(z) := V_m^*(A - zI)^{-1}v_{m+1}$ then

$$G(A, V_{m+1}, V_m^*) = [(I - h_{m+1,m}\phi(z)e_m^T)(H - zI)^{-1}, \phi(z)].$$

Therefore, only one system of size $n$ with right–hand side $v_{m+1}$ need be solved for each $z \in \mathcal{C}$. When computing the pseudospectrum, this observation can be used in order to reduce substantially the cost of the transfer function approach of Section 2.2. This is work in progress and will be reported elsewhere [1].

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