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An Inexact Shift-and-Invert Arnoldi Algorithm for Large Non-Hermitian Generalised Toeplitz Eigenproblems

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Abstract. The shift-and-invert Arnoldi method is a most effective approach to compute a few eigenpairs of a large non-Hermitian Toeplitz matrix pencil, where the Gohberg-Semencul formula can be used to obtain the Toeplitz inverse. However, two large non-Hermitian Toeplitz systems must be solved in the first step of this method, and the cost becomes prohibitive if the desired accuracy for this step is high — especially for some ill-conditioned problems. To overcome this difficulty, we establish a relationship between the errors in solving these systems and the residual of the Toeplitz eigenproblem. We consequently present a practical stopping criterion for their numerical solution, and propose an inexact shift-and-invert Arnoldi algorithm for the generalised Toeplitz eigenproblem. Numerical experiments illustrate our theoretical results and demonstrate the efficiency of the new algorithm.

AMS subject classifications: 65F15, 65F10

Key words: Toeplitz matrix, generalised eigenproblem, shift-and-invert Arnoldi method, Gohberg-Semencul formula.

1. Introduction

Toeplitz matrices and operators arise in several areas of mathematics and its applications, including complex and harmonic analysis, probability theory and statistics, signal and image processing, information theory and numerical analysis [4, 5, 14]. The design of fast algorithms for Toeplitz matrices is a wide and active research field in structured numerical linear algebra, bearing in mind that a Toeplitz matrix is constant along its diagonals so only the first column and the first row of a Toeplitz matrix need be stored.

The Hermitian Toeplitz eigenproblem and the generalised Hermitian Toeplitz eigenproblem in particular have received considerable attention over recent decades — cf. [1, 13, 16, 21, 22, 25] and the references therein. Iterative methods such as the preconditioned

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Lanczos method and the shift-and-invert Lanczos method [19] are widely used to solve for the smallest eigenpair or a few extreme eigenpairs of a large Hermitian Toeplitz matrix (pencil). For instance, the sine transform-based preconditioner has been used to speed up the convergence rate of the preconditioned Lanczos method in computing the minimum eigenvalue of a symmetric positive definite Toeplitz matrix [13]. This involves only Toeplitz and sine transform matrix-vector multiplications, and hence can be computed efficiently by fast transform algorithms. Wang & Lu [22] generalised this idea and employed the sine transform-based preconditioner to compute the minimum eigenvalue of a symmetric Toeplitz matrix pencil. Recently, parallel shift-and-invert Lanczos algorithms were investigated for computing a few eigenpairs of a symmetric Toeplitz matrix, based on an efficient implementation of the discrete sine transform [1, 21] and also the Gohberg-Semencul formula [6] for solving the Toeplitz linear systems involved.

Recently, special attention has been paid to the eigenproblems of large scale Toeplitz matrices [1, 3, 8, 10, 13, 21, 22, 25]. There is an extensive literature concerning the Hermitian, the generalised Hermitian, and the non-Hermitian Toeplitz eigenproblem. However, to the best of our knowledge little attention has been paid to large non-Hermitian generalised Toeplitz eigenproblems of interest in signal processing and control theory, and on Toeplitz matrices generated by rational functions [2, 16, 25]. In this article, we focus on computing a few eigenpairs of the following non-Hermitian Toeplitz generalised eigenproblem:

$$A\mathbf{x} = \lambda B\mathbf{x}\,, \tag{1.1}$$

where A and B are large Toeplitz matrices, and the matrix pencil (A, B) is regular [7, 19]. When $B = I$ (the identity matrix), this generalised eigenproblem reduces to the standard Toeplitz eigenproblem.

In particular, we focus on computing a few eigenpairs of a large non-Hermitian Toeplitz matrix pencil, including extreme eigenpairs or those closest to a given shift. As previously mentioned, the shift-and-invert Arnoldi method where the Gohberg-Semencul formula [6] can be used is one of the most effective approaches for this type of problem — but two large non-Hermitian Toeplitz systems must be solved in advance, and if the desired accuracy for solving the Toeplitz linear systems is too high the computational cost becomes prohibitive. In Section 2, we establish a relationship between the errors of the Toeplitz systems and the residual of the Toeplitz eigenproblem. We then give a practical stopping criterion for solving the Toeplitz systems approximately, and propose an inexact shift-and-invert Arnoldi algorithm for the generalised Toeplitz eigenproblem. Numerical experiments discussed in Section 3 illustrate our theoretical results and demonstrate the efficiency of the new algorithm. Some concluding remarks are made in Section 4.

2. An Inexact Shift-and-Invert Arnoldi Method for Generalised Toeplitz Eigenproblems

The shift-and-invert technique [19] has proven a most effective method for large-scale eigenproblems. In this technique, under a shift $\sigma \in \mathbb{C}$ we have from (1.1) that

$$(A - \sigma B)\mathbf{x} = (\lambda - \sigma)B\mathbf{x}\,,$$

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so if $A-\sigma B$ is invertible the generalised eigenproblem (1.1) can be rewritten as the standard eigenproblem

$$(A-\sigma B)^{-1}B\mathbf{x} = \mu\mathbf{x}\,, \tag{2.1}$$

where $\mu = (\lambda-\sigma)^{-1}$. Consequently, we may iterate with the matrix $(A-\sigma B)^{-1}B$ to obtain the solution $\mathbf{x}$; and the matrix $A-\sigma B$ factor is typically introduced only once or a few times (when σ is changed), leading to a solution involving a much smaller number of iterations with $(A-\sigma B)^{-1}B$ than is required for the original problem (1.1) in A and B [19].

In practical computations, the shift-and-invert technique is often combined with some effective projection approach. In particular, the Arnoldi method for large-scale non-Hermitian eigenproblems is widely used to compute a number of eigenvalues closest to a given shift σ, and also the associated eigenvectors of the large non-Hermitian matrices. For computation in exact arithmetic, given a unit vector $\mathbf{v}_1$ we have the m-step shift-and-invert Arnoldi process [19]

$$(A-\sigma B)^{-1}BV_m = V_m H_m + h_{m+1,m}\mathbf{v}_{m+1}\mathbf{e}_m^{\mathrm{T}}\,, \tag{2.2}$$

where $V_m = [\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_m]$ denotes an orthonormal basis for the Krylov subspace $\mathscr{K}_m((A-\sigma B)^{-1}B, \mathbf{v}_1)$, $\mathbf{e}_m$ is the m-th column of the $m\times m$ identity matrix, and H_m is an $m\times m$ upper Hessenberg matrix. If $(\widetilde{\mu}, \widetilde{\mathbf{w}})$ with $\|\widetilde{\mathbf{w}}\|_2 = 1$ denotes an eigenpair of H_m, the shift-and-invert Arnoldi method uses $(\widetilde{\lambda} = 1/\widetilde{\mu}+\sigma,\ \widetilde{\mathbf{x}} = V_m\widetilde{\mathbf{w}})$ as an approximation to $(\lambda, \mathbf{x})$. Writing $\widehat{\mathbf{r}} = A\widetilde{\mathbf{x}} - \widetilde{\lambda}B\widetilde{\mathbf{x}}$ for the residual corresponding to the Ritz pair $(\widetilde{\lambda}, \widetilde{\mathbf{x}})$, we then have [9]

$$\frac{\|\widehat{\mathbf{r}}\|_2}{\|A-\sigma B\|_2} \le h_{m+1,m}|\widetilde{\lambda}-\sigma|\cdot|\mathbf{e}_m^{\mathrm{T}}\widetilde{\mathbf{w}}|\,, \tag{2.3}$$

which can be used as a cheap stopping criterion for the shift-and-invert Arnoldi method.

However, in the shift-and-invert Arnoldi process we need to compute m matrix-vector products $(A-\sigma B)^{-1}B\mathbf{v}_j$, $j = 1, 2, \cdots, m$. The explicit computation of the inverse $(A-\sigma B)^{-1}$ by some direct method, such as LU decomposition say [7], is prohibitive in practice for large dense matrices. One option is to solve m corresponding linear systems with respect to $A-\sigma B$ for a given shift σ, in computing $(A-\sigma B)^{-1}$ once and for all. Fortunately, when $A-\sigma B$ is a Toeplitz matrix we have the Gohberg-Semencul formula (GSF) for the inverse [6], which has the advantage that we need not form and store $(A-\sigma B)^{-1}$ explicitly. Indeed, the inverse of a Toeplitz matrix T can be reconstructed from its first and last columns. Thus if $\mathbf{e}_1$, $\mathbf{e}_n$ respectively denote the first and last columns of the $n\times n$ identity matrix, and $\mathbf{z} = [\xi_0, \xi_1, \cdots, \xi_{n-1}]^{\mathrm{T}}$ and $\mathbf{y} = [\eta_0, \eta_1, \cdots, \eta_{n-1}]^{\mathrm{T}}$ are the solutions of the two Toeplitz systems

$$T\mathbf{z} = \mathbf{e}_1 \quad \text{and} \quad T\mathbf{y} = \mathbf{e}_n\,, \tag{2.4}$$

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then if $\xi_0 \neq 0$ the GSF for the inverse is [6]

$$
\begin{aligned}
&T^{-1} \\
=&\frac{1}{\xi_0}\left\{\begin{bmatrix} \xi_0 & 0 & \cdots & 0 \\ \xi_1 & \xi_0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \xi_{n-1} & \xi_{n-2} & \cdots & \xi_0 \end{bmatrix}\begin{bmatrix} \eta_{n-1} & \eta_{n-2} & \cdots & \eta_0 \\ 0 & \eta_{n-1} & \cdots & \eta_1 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \eta_{n-1} \end{bmatrix} - \begin{bmatrix} 0 & \cdots & 0 & 0 \\ \eta_0 & \cdots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots \\ \eta_{n-2} & \cdots & \eta_0 & 0 \end{bmatrix}\begin{bmatrix} 0 & \xi_{n-1} & \cdots & \xi_1 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \xi_{n-1} \\ 0 & 0 & \cdots & 0 \end{bmatrix}\right\} \\
\equiv&\frac{1}{\xi_0}\left(L_z R_y - L_y^0 R_z^0\right). \qquad (2.5)
\end{aligned}
$$

On solving the two non-Hermitian Toeplitz systems (2.4), the inverse T^{-1} of a Toeplitz matrix is therefore obtained explicitly from the GSF (2.5) in terms of the four triangular Toeplitz matrices L_z, R_y, L_y^0 and R_z^0, and all the matrix-vector products can be derived directly. Indeed, for any Toeplitz matrix-vector product we can first embed the Toeplitz matrix into a $2n \times 2n$ circulant matrix, and carry it out with $O(n\log n)$ complexity [4, 5]. Nevertheless, under the GSF (2.5) the four Toeplitz matrix-vector products require about sixteen FFT of size n, to compute the matrix-vector product with respect to T^{-1}. To relieve this burden, one can factor the right-hand side of Eq. (2.5) into two circulant matrices and two skew-circulant matrices — viz.

$$
T^{-1} = \frac{1}{2\xi_0}\left[(L_z + R_z^0)(R_y - L_y^0) + (R_y + L_y^0)(L_z - R_z^0)\right],
$$

such that the Toeplitz matrix-vector product can be realised in six FFT of size n [11, 17].

In the shift-and-invert Arnoldi algorithm, one has to solve the two large scale non-Hermitian Toeplitz linear systems (2.4) in some desired precision, theoretically as accurately as possible. However, if the desired accuracy is too high the cost in solving the linear systems becomes prohibitive, especially for some ill-conditioned problems. In order to reduce this computational cost, it is interesting to consider how the Toeplitz systems may be solved approximately [11, 17]. Since the Toeplitz linear systems are to be solved once and for all, this can be understood as an "inexact" inverse technology. Let $\widetilde{\mathbf{z}} = [\widetilde{\xi}_0, \widetilde{\xi}_1, \cdots, \widetilde{\xi}_{n-1}]^{\mathrm{T}}$ and $\widetilde{\mathbf{y}} = [\widetilde{\eta}_0, \widetilde{\eta}_1, \cdots, \widetilde{\eta}_{n-1}]^{\mathrm{T}}$ be the numerical solutions of the two Toeplitz systems $T\mathbf{z} = \mathbf{e}_1$ and $T\mathbf{y} = \mathbf{e}_n$, respectively. If $\widetilde{\xi}_0 \neq 0$, we denote

$$
\begin{aligned}
&\widetilde{T}^{-1} \\
=&\frac{1}{\widetilde{\xi}_0}\left\{\begin{bmatrix} \widetilde{\xi}_0 & 0 & \cdots & 0 \\ \widetilde{\xi}_1 & \widetilde{\xi}_0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \widetilde{\xi}_{n-1} & \widetilde{\xi}_{n-2} & \cdots & \widetilde{\xi}_0 \end{bmatrix}\begin{bmatrix} \widetilde{\eta}_{n-1} & \widetilde{\eta}_{n-2} & \cdots & \widetilde{\eta}_0 \\ 0 & \widetilde{\eta}_{n-1} & \cdots & \widetilde{\eta}_1 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \widetilde{\eta}_{n-1} \end{bmatrix} - \begin{bmatrix} 0 & \cdots & 0 & 0 \\ \widetilde{\eta}_0 & \cdots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots \\ \widetilde{\eta}_{n-2} & \cdots & \widetilde{\eta}_0 & 0 \end{bmatrix}\begin{bmatrix} 0 & \widetilde{\xi}_{n-1} & \cdots & \widetilde{\xi}_1 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \widetilde{\xi}_{n-1} \\ 0 & 0 & \cdots & 0 \end{bmatrix}\right\} \\
\equiv&\frac{1}{\widetilde{\xi}_0}\left(\widetilde{L}_z \widetilde{R}_y - \widetilde{L}_y^0 \widetilde{R}_z^0\right), \qquad (2.6)
\end{aligned}
$$

which can be viewed as a perturbation to the Toeplitz inverse T^{-1}. The following theorem gives an error analysis on the Gohberg-Semencul formula in terms of ∞-norm, where a proof similar to that for Theorem 3.1 in [23] is given here for completeness.

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Theorem 2.1. *Let $\varepsilon > 0$. If $\xi_0 \neq 0$, $\widetilde{\xi}_0 \neq 0$ and*

$$\frac{\|\widetilde{\mathbf{z}}-\mathbf{z}\|_1}{\|\mathbf{z}\|_1} \leq \varepsilon \quad \text{and} \quad \frac{\|\widetilde{\mathbf{y}}-\mathbf{y}\|_1}{\|\mathbf{y}\|_1} \leq \varepsilon\,, \tag{2.7}$$

then

$$\|T^{-1}-\widetilde{T}^{-1}\|_\infty \leq \left|\frac{2}{\xi_0}\right| \cdot \left[\varepsilon + \left(\varepsilon + (1+\varepsilon)\widetilde{\varepsilon}\right)(1+\varepsilon)\right] \cdot \|\mathbf{z}\|_1 \|\mathbf{y}\|_1\,, \tag{2.8}$$

where $\widetilde{\varepsilon} = |1/\xi_0 - 1/\widetilde{\xi}_0|/|1/\xi_0|$ is the relative error of $1/\widetilde{\xi}_0$ with respect to $1/\xi_0$.

Proof. It follows from inequalities (2.5) and (2.6) that

$$\begin{aligned}
&\left\|T^{-1}-\widetilde{T}^{-1}\right\|_\infty \\
&= \left\| \frac{1}{\xi_0}\left(L_z R_y - L_y^0 R_z^0\right) - \frac{1}{\widetilde{\xi}_0}\left(\widetilde{L}_z \widetilde{R}_y - \widetilde{L}_y^0 \widetilde{R}_z^0\right) \right\|_\infty \\
&= \left\| \left(\frac{1}{\xi_0}L_z\right)R_y - L_y^0\left(\frac{1}{\xi_0}R_z^0\right) - \left(\frac{1}{\widetilde{\xi}_0}\widetilde{L}_z\right)\widetilde{R}_y + \widetilde{L}_y^0\left(\frac{1}{\widetilde{\xi}_0}\widetilde{R}_z^0\right) \right\|_\infty \\
&\leq \left\| \left(\frac{1}{\xi_0}L_z\right)R_y - \left(\frac{1}{\widetilde{\xi}_0}\widetilde{L}_z\right)\widetilde{R}_y \right\|_\infty + \left\| \widetilde{L}_y^0\left(\frac{1}{\widetilde{\xi}_0}\widetilde{R}_z^0\right) - L_y^0\left(\frac{1}{\xi_0}R_z^0\right) \right\|_\infty .
\end{aligned} \tag{2.9}$$

Moreover,

$$\begin{aligned}
&\left\| \left(\frac{1}{\xi_0}L_z\right)R_y - \left(\frac{1}{\widetilde{\xi}_0}\widetilde{L}_z\right)\widetilde{R}_y \right\|_\infty \\
&= \left\| \left(\frac{1}{\xi_0}L_z\right)R_y - \left(\frac{1}{\xi_0}L_z\right)\widetilde{R}_y + \left(\frac{1}{\xi_0}L_z\right)\widetilde{R}_y - \left(\frac{1}{\widetilde{\xi}_0}\widetilde{L}_z\right)\widetilde{R}_y \right\|_\infty \\
&= \left\| \left(\frac{1}{\xi_0}L_z\right)(R_y - \widetilde{R}_y) + \left(\frac{1}{\xi_0}L_z - \frac{1}{\widetilde{\xi}_0}\widetilde{L}_z\right)\widetilde{R}_y \right\|_\infty \\
&\leq \left|\frac{1}{\xi_0}\right| \cdot \|L_z\|_\infty \left\|R_y - \widetilde{R}_y\right\|_\infty + \left\| \frac{1}{\xi_0}L_z - \frac{1}{\widetilde{\xi}_0}\widetilde{L}_z \right\|_\infty \left\|\widetilde{R}_y\right\|_\infty .
\end{aligned} \tag{2.10}$$

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Denoting $\widetilde{\varepsilon} = |1/\xi_0 - 1/\widetilde{\xi}_0|/|1/\xi_0|$, we obtain from inequality (2.7) that

$$\begin{aligned}\left\| \frac{1}{\xi_0} L_z - \frac{1}{\widetilde{\xi}_0} \widetilde{L}_z \right\|_\infty &= \left\| \frac{1}{\xi_0}\mathbf{z} - \frac{1}{\widetilde{\xi}_0}\widetilde{\mathbf{z}} \right\|_1 \\ &= \left| \frac{1}{\xi_0} \right| \cdot \left\| \mathbf{z} - \widetilde{\mathbf{z}} + \left(1 - \frac{\xi_0}{\widetilde{\xi}_0}\right)\widetilde{\mathbf{z}} \right\|_1 \\ &\le \left| \frac{1}{\xi_0} \right| \cdot \left[\|\mathbf{z} - \widetilde{\mathbf{z}}\|_1 + \widetilde{\varepsilon}\|\widetilde{\mathbf{z}}\|_1 \right] \\ &\le \left| \frac{1}{\xi_0} \right| \cdot \left[\varepsilon + (1+\varepsilon)\widetilde{\varepsilon} \right] \cdot \|\mathbf{z}\|_1 \,. \end{aligned} \tag{2.11}$$

Furthermore, from Eqs. (2.5) and (2.6) and the inequalities in (2.7) we have

$$\|L_z\|_\infty = \|\mathbf{z}\|_1 \,, \quad \left\|\widetilde{R}_y\right\|_\infty = \|\widetilde{\mathbf{y}}\|_1 \le (1+\varepsilon)\,\|\mathbf{y}\|_1 \,, \tag{2.12}$$

$$\text{and} \qquad \left\|R_y - \widetilde{R}_y\right\|_\infty = \|\mathbf{y} - \widetilde{\mathbf{y}}\|_1 \le \varepsilon \|\mathbf{y}\|_1 \,. \tag{2.13}$$

From inequalities (2.10)–(2.13), we obtain

$$\begin{aligned} &\left\| \left(\frac{1}{\xi_0} L_z \right) R_y - \left(\frac{1}{\widetilde{\xi}_0} \widetilde{L}_z \right) \widetilde{R}_y \right\|_\infty \\ \le\ & \left| \frac{1}{\xi_0} \right| \varepsilon \cdot \|\mathbf{z}\|_1 \|\mathbf{y}\|_1 + \left| \frac{1}{\xi_0} \right| (1+\varepsilon)\Big(\varepsilon + (1+\varepsilon)\widetilde{\varepsilon}\Big) \cdot \|\mathbf{z}\|_1 \|\mathbf{y}\|_1 \\ =\ & \left| \frac{1}{\xi_0} \right| \Big[\varepsilon + (1+\varepsilon)\Big(\varepsilon + (1+\varepsilon)\widetilde{\varepsilon}\Big) \Big] \cdot \|\mathbf{z}\|_1 \|\mathbf{y}\|_1 \,. \end{aligned} \tag{2.14}$$

Similarly, for the second part of the right-hand side of (2.9) we obtain

$$\left\| \widetilde{L}_y^0 \left(\frac{1}{\widetilde{\xi}_0} \widetilde{R}_z^0 \right) - L_y^0 \left(\frac{1}{\xi_0} R_z^0 \right) \right\|_\infty \le \left| \frac{1}{\xi_0} \right| \cdot \Big[\varepsilon + (1+\varepsilon)\Big(\varepsilon + (1+\varepsilon)\widetilde{\varepsilon}\Big) \Big] \cdot \|\mathbf{z}\|_1 \|\mathbf{y}\|_1 \,, \tag{2.15}$$

and hence inequality (2.8) on combining inequalities (2.9), (2.14) and (2.15). □

Henceforth we use T to denote $A - \sigma B$ whenever convenient. If the Toeplitz systems are solved approximately, the errors for the matrix-vector products can be expressed as $\mathbf{f}_j = \widetilde{T}^{-1} B\mathbf{v}_j - T^{-1} B\mathbf{v}_j$, $j = 1, 2, \cdots, m$. Writing $F_m = [\mathbf{f}_1, \mathbf{f}_2, \cdots, \mathbf{f}_m]$, we get the following relation for the m-step "inexact" shift-and-invert Arnoldi procedure:

$$(A - \sigma B)^{-1} B V_m + F_m = \Big((A - \sigma B)^{-1} B + E\Big) V_m = V_m H_m + h_{m+1,m} \mathbf{v}_{m+1} \mathbf{e}_m^{\mathrm{T}} \,, \tag{2.16}$$

where $V_m = [\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_m]$ is an $n \times m$ orthonormal matrix, $E = F_m V_m^{\mathrm{T}}$, and H_m is an $m \times m$ upper Hessenberg matrix. Note that neither V_m nor H_m are are the same as in Eq. (2.2). Let $(\widetilde{\mu}, \widetilde{\mathbf{w}})$ be an eigenpair of H_m, and let $\widetilde{\lambda} = 1/\widetilde{\mu} + \sigma$. Let us write

$$\widehat{\mathbf{r}}^{\,real} = A V_m \widetilde{\mathbf{w}} - \widetilde{\lambda} B V_m \widetilde{\mathbf{w}} \tag{2.17}$$

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for the "real" residual with respect to the approximate eigenpair $(\widetilde{\lambda}, V_m\widetilde{\mathbf{w}})$ of the matrix pencil (A,B), and

$$\mathbf{r}^{real} = (A-\sigma B)^{-1}BV_m\widetilde{\mathbf{w}} - \widetilde{\mu}V_m\widetilde{\mathbf{w}} \tag{2.18}$$

and

$$\mathbf{r}^{comp} = \left[(A-\sigma B)^{-1}B + E\right]V_m\widetilde{\mathbf{w}} - \widetilde{\mu}V_m\widetilde{\mathbf{w}} = h_{m+1,m}(\mathbf{e}_m^{\mathrm{T}}\widetilde{\mathbf{w}})\cdot\mathbf{v}_{m+1}$$

for the "real" and the "computed" residuals for the approximate eigenpair $(\widetilde{\mu}, V_m\widetilde{\mathbf{w}})$ of $(A-\sigma B)^{-1}B$, respectively. Multiplying Eq. (2.18) by $(\widetilde{\lambda}-\sigma)(A-\sigma B)$ yields

$$\begin{aligned}(\widetilde{\lambda}-\sigma)(A-\sigma B)\mathbf{r}^{real} &= (\widetilde{\lambda}-\sigma)BV_m\widetilde{\mathbf{w}} - (A-\sigma B)V_m\widetilde{\mathbf{w}}\\ &= \widetilde{\lambda}BV_m\widetilde{\mathbf{w}} - AV_m\widetilde{\mathbf{w}} = -\widehat{\mathbf{r}}^{real},\end{aligned}$$

hence

$$\|\widehat{\mathbf{r}}^{real}\| \le |\widetilde{\lambda}-\sigma|\cdot\|A-\sigma B\|\cdot\|\mathbf{r}^{real}\|. \tag{2.19}$$

Consequently, it is interesting to investigate the gap between $\mathbf{r}^{real}$ and $\mathbf{r}^{comp}$ in the "inexact" Toeplitz eigensolver. Given a convergence threshold $\widetilde{tol}$ for the Toeplitz eigenproblem (1.1), the following theorem investigates how to choose the stopping threshold ε for solving the Toeplitz systems (2.4).

Theorem 2.2. *In the notation mentioned above, if* $\widetilde{\varepsilon} \le \varepsilon \ll 1$ *and*

$$\varepsilon \le \frac{|\xi_0|\cdot\widetilde{tol}}{6\sqrt{m}\cdot\|\mathbf{z}\|_1\|\mathbf{y}\|_1\cdot\|B\|_\infty} \tag{2.20}$$

then

$$\|\mathbf{r}^{real} - \mathbf{r}^{comp}\|_\infty \lesssim \widetilde{tol}, \tag{2.21}$$

for the m-th step of the shift-and-invert Arnoldi process.

Proof. From inequality (2.8), we have

$$\begin{aligned}\|\mathbf{f}_j\|_\infty &= \|\widetilde{T}^{-1}B\mathbf{v}_j - T^{-1}B\mathbf{v}_j\|_\infty\\ &\le \|T^{-1}-\widetilde{T}^{-1}\|_\infty\cdot\|B\mathbf{v}_j\|_\infty\\ &\le \left|\frac{2}{\xi_0}\right|\cdot\left[\varepsilon + \left(\varepsilon + (1+\varepsilon)\widetilde{\varepsilon}\right)(1+\varepsilon)\right]\cdot\|\mathbf{z}\|_1\|\mathbf{y}\|_1\|B\mathbf{v}_j\|_\infty.\end{aligned}$$

If $\widetilde{\varepsilon} \le \varepsilon \ll 1$, then $\varepsilon + (\varepsilon + (1+\varepsilon)\widetilde{\varepsilon})(1+\varepsilon) \le 3\varepsilon + \mathcal{O}(\varepsilon^2)$ and

$$\begin{aligned}&\left|\frac{2}{\xi_0}\right|\cdot\left[\varepsilon + \left(\varepsilon + (1+\varepsilon)\widetilde{\varepsilon}\right)(1+\varepsilon)\right]\cdot\|\mathbf{z}\|_1\|\mathbf{y}\|_1\|B\mathbf{v}_j\|_\infty\\ \lesssim &\left|\frac{2}{\xi_0}\right|\cdot 3\varepsilon\cdot\|\mathbf{z}\|_1\|\mathbf{y}\|_1\|B\|_\infty\cdot\|\mathbf{v}_j\|_\infty\\ \le &\left|\frac{6}{\xi_0}\right|\cdot\|\mathbf{z}\|_1\|\mathbf{y}\|_1\|B\|_\infty\cdot\varepsilon,\end{aligned} \tag{2.22}$$

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where we have omitted the $\mathcal{O}(\varepsilon^2)$ term and used the relation $\|\mathbf{v}_j\|_\infty \le \|\mathbf{v}_j\|_2 = 1$. Hence if

$$\varepsilon \le \frac{|\xi_0| \cdot \widetilde{tol}}{6\sqrt{m} \cdot \|\mathbf{z}\|_1 \|\mathbf{y}\|_1 \cdot \|B\|_\infty},$$

i.e. if

$$\|\mathbf{f}_j\|_\infty \lesssim \left|\frac{6}{\xi_0}\right| \cdot \|\mathbf{z}\|_1 \|\mathbf{y}\|_1 \|B\|_\infty \cdot \varepsilon \le \frac{\widetilde{tol}}{\sqrt{m}}, \quad j = 1, 2, \cdots, m, \tag{2.23}$$

then from Eqs. (2.18) and (2.19) and inequality (2.23) we have that

$$\begin{aligned}\|\mathbf{r}^{real} - \mathbf{r}^{comp}\|_\infty = \|EV_m\widetilde{\mathbf{w}}\|_\infty = \left\|\sum_{j=1}^{m} \mathbf{f}_j \widetilde{w}_j\right\|_\infty \le \sum_{j=1}^{m} \|\mathbf{f}_j\|_\infty \cdot |\widetilde{w}_j| \\ \le \max_{1\le j\le m} \|\mathbf{f}_j\|_\infty \cdot \sqrt{m}\|\widetilde{\mathbf{w}}\|_2 \lesssim \widetilde{tol},\end{aligned}$$

where $\widetilde{\mathbf{w}} = [\widetilde{\overline{w}}_1, \cdots, \widetilde{\overline{w}}_m]^{\mathrm{H}}$ and we used the inequality $\|\widetilde{\mathbf{w}}\|_1 \le \sqrt{m}\|\widetilde{\mathbf{w}}\|_2 = \sqrt{m}$. □

Since V_m is orthonormal, it is preferable to use the 2-norm in practice, and we next give a practical stopping criterion for the approximate solution of the Toeplitz systems (2.4). From inequality (2.3), we obtain the following inequality as the stopping criterion for the Toeplitz eigen-computation:

$$\frac{\|A\widetilde{\mathbf{x}}_i - \widetilde{\lambda}_i B\widetilde{\mathbf{x}}_i\|_2}{\|A - \sigma B\|_2} \le h_{m+1,m}|\widetilde{\lambda}_i - \sigma| \cdot |\mathbf{e}_m^{\mathrm{T}}\widetilde{\mathbf{w}}_i| \le tol, \quad i = 1, 2, \cdots, \ell, \tag{2.24}$$

where *tol* is a user-prescribed tolerance for the Toeplitz eigenproblem and ℓ is the number of desired eigenpairs. Noting inequalities (2.19) and (2.24), we let

$$\widetilde{tol} = \|A - \sigma B\|_2 \cdot tol,$$

where it follows from Theorem 2.2 that if

$$\varepsilon \le \frac{|\xi_0| \cdot \|A - \sigma B\|_2}{6\sqrt{m} \cdot \|\mathbf{z}\|_1 \|\mathbf{y}\|_1 \cdot \|B\|_\infty} \cdot tol \tag{2.25}$$

then

$$\frac{\|\mathbf{r}^{real} - \mathbf{r}^{comp}\|_\infty}{\|A - \sigma B\|_2} \lesssim tol. \tag{2.26}$$

Remark 2.1. Given a convergence threshold tol for the Toeplitz eigenproblem (1.1), inequality (2.25) indicates that if the product of

$$\xi \equiv \frac{|\xi_0|}{\|\mathbf{z}\|_1 \|\mathbf{y}\|_1} \quad \text{and} \quad \eta \equiv \frac{\|A - \sigma B\|_2}{6\sqrt{m} \cdot \|B\|_\infty}$$

is small then we have to solve the Toeplitz linear systems (2.4) to a (relatively) high accuracy, but otherwise we can solve to a (relatively) low accuracy. However, there are some

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Algorithm 2.1: An inexact shift-and-invert Arnoldi algorithm for generalised Toeplitz eigenproblems.

Step 1. Given a shift σ, a convergence threshold tol for the eigenproblem, and four vectors **Acol**, **Arow** and **Bcol**, **Brow**, which are respectively the first column and first row of A and B, compute the inverse of $A-\sigma B$. Solve the Toeplitz linear systems (2.4) approximately, with the stopping criterion provided in (2.27).

Step 2. Compute the desired eigenpairs, using a restarted shift-and-invert Krylov subspace algorithm – e.g. the implicitly restarted shift-and-invert Arnoldi algorithm [20] or the thick-restarted Arnoldi algorithm [12, 24].

unavailable parameters such as $|\xi_0|, \|\mathbf{z}\|_1$ and $\|\mathbf{y}\|_1$ appearing in inequality (2.25). If ξ is not too small, we suggest using

$$\left\{\|\mathbf{r}_z\|_2, \|\mathbf{r}_y\|_2\right\} \leq \frac{\max(\|\mathbf{fcol}\|_2, \|\mathbf{frow}\|_2)}{6\sqrt{m}\cdot\max(\|\mathbf{Bcol}\|_2, \|\mathbf{Brow}\|_2)}\cdot tol \tag{2.27}$$

as the stopping criterion for solving the Toeplitz systems, where $\mathbf{r}_z = \mathbf{e}_1 - T\widetilde{\mathbf{z}}$ and $\mathbf{r}_y = \mathbf{e}_n - T\widetilde{\mathbf{y}}$ are the residuals of the Toeplitz systems, **fcol** and **frow** are the first column and first row of $A-\sigma B$, and **Bcol** and **Brow** are the first column and first row of B, respectively. We find that this scheme is very efficient in practice — cf. the results of our numerical experiments given in Section 3.

In practical calculations, the implementation of the shift-and-invert Arnoldi procedure is limited by heavy storage requirements and computational complexities as the Arnoldi step m increases. One way to offset this is to use some restarting strategy [12, 19, 20, 24]. In this article, we focus on the famous implicit restarting strategy [20]. In summary, in the main algorithm is listed as follows. The key is to compute the inverses approximately, and then quickly apply the inverse during the Arnoldi iterations.

Some further remarks are in order. Firstly, in practical calculations the shift σ is user-described and problem-dependent — cf. [19] for more detail on the choice. When both A and B are real but the shift σ is complex, [18, 19] discuss how to deal with complex arithmetic in the shift-and-invert Arnoldi process. Secondly, it is unnecessary to form explicitly or store the matrices $A, B, A-\sigma B$ and $(A-\sigma B)^{-1}$ in practice. Indeed, each matrix-vector product $(A-\sigma B)^{-1}(B\mathbf{v}_j)$ can be realised in ten FFT of size n, 4 for $\mathbf{u} \equiv B\mathbf{v}_j$ and another 6 for $(A-\sigma B)^{-1}\mathbf{u}$. Thirdly, we mention that the assumption $\xi_0 \neq 0$ is not stringent in practice (2.5). Indeed, we have $\xi_0 = \mathbf{z}^{\mathrm{T}}\mathbf{e}_1 = \mathbf{z}^{\mathrm{T}}(A-\sigma B)\mathbf{z}$, and $\xi_0 \neq 0$ if and only if $\sigma\cdot\mathbf{z}^T B\mathbf{z} \neq \mathbf{z}^T A\mathbf{z}$.

3. Numerical Experiments

In this section, we present the results of some numerical experiments illustrating our theoretical results and demonstrating the efficiency of our new algorithm. All the numer-

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ical experiments were run on an Intel(R) Core(TM)i3-2350 processor with 2.30 GHz CPU and 2GB RAM, under the Windows 7 operating system, using a MATLAB 7.11.0 (R2010b) implementation with machine precision $\epsilon \approx 2.22 \times 10^{-16}$. We used the MATLAB built-in function **eigs.m** (the implicitly restarted shift-and-invert Arnoldi algorithm) to solve the generalised Toeplitz eigenproblem, where the default values are used and the matrix-vector product is redefined via solving the Toeplitz systems (2.4).

The algorithms we used are as follows:

• **Inexact-eigs (Algorithm 2.1)** denotes the "inexact" shift-and-invert Arnoldi algorithm using the (unrestarted) GMRES algorithm with T. Chan's preconditioner [4, 14] as the solver for (2.4). Given a convergence threshold *tol* for the eigenproblem, by (2.27), we used the stopping criterion for the Toeplitz systems

$$\|\mathscr{M}^{-1}\mathbf{b} - \mathscr{M}^{-1}(A-\sigma B)\widetilde{\mathbf{q}}\|_2 \le \frac{\max(\|\mathbf{fcol}\|_2, \|\mathbf{frow}\|_2)}{6\sqrt{20}\cdot \max(\|\mathbf{Bcol}\|_2, \|\mathbf{Brow}\|_2)} \cdot tol\ , \tag{3.1}$$

where $\mathscr{M}$ stands for T. Chan's preconditioner, $\widetilde{\mathbf{q}} = \widetilde{\mathbf{y}}$ (or $\widetilde{\mathbf{z}}$) the approximate solution, and $\mathbf{b} = \mathbf{e}_1$ (or $\mathbf{e}_n$) represents the right-hand side. This algorithm mimics solving the Toeplitz systems "approximately" with an iterative solver.

• **Exact-eigs** denotes the "exact" shift-and-invert Arnoldi algorithm using the (unrestarted) GMRES algorithm with T. Chan's preconditioner for the Toeplitz systems (2.4). The stopping criterion for the Toeplitz linear systems was

$$\|\mathscr{M}^{-1}\mathbf{b} - \mathscr{M}^{-1}(A-\sigma B)\widetilde{\mathbf{q}}\|_2 \le 10^{-14}\ . \tag{3.2}$$

This algorithm mimics solving the two Toeplitz systems "exactly" with an iterative solver. In both of these algorithms (Inexact-eigs and Exact-eigs), we chose the zero vector as the initial guess for GMRES.

In the tables below, n denotes the size of the Toeplitz matrix, (3.1) the value of the right-hand side of (3.1), CPU(sec.) the CPU time used in seconds, and the additional "–" denotes that the algorithm suffers from "out of memory". We recall that the Toeplitz systems (2.4) are solved inexactly in our new algorithm. In order to show efficiency of the inexact strategy, we list the value of the maximal "real" residual norm — cf. (2.17):

$$\|\widehat{\mathbf{r}}^{real}\|_2 = \max_{i=1,\cdots,\ell} \|A(V_m\widetilde{\mathbf{w}}_i) - \widetilde{\lambda}_i B(V_m\widetilde{\mathbf{w}}_i)\|_2\ , \tag{3.3}$$

where ℓ is the number of desired eigenpairs and $(\widetilde{\lambda}_i, V_m\widetilde{\mathbf{w}}_i), i = 1, 2, \cdots, \ell$ are Ritz pairs obtained from running Inexact-eigs. The CPU time of Inexact-eigs and Exact-eigs includes the time to solve the Toeplitz systems and the time to calculate the eigenpairs.

In some practical problems from science and engineering, we are usually given the generating function f rather than the Toeplitz matrix T itself [4, 14]. For example, the function f is called the generating function of T if the diagonals $\{t_k\}_{k=-n+1}^{n-1}$ of T are the Fourier coefficients of a function f [4] — i.e.

$$t_k = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(x)e^{-\mathbf{i}kx}dx, \quad \mathbf{i}^2 = -1\ .$$

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We also note the following contexts:

- Numerical differential equations: the equation gives f;
- Integral equations: the kernel gives f;
- Time series: the spectral density function gives f;
- Filter design: the transfer function gives f;
- Image restoration: the blurring function gives f.

Example 3.1. In this example, we show the efficiency of the inexact strategy (3.1) for large non-Hermitian generalised Toeplitz eigenproblems. The test matrices were taken from [11]. The matrix A is a non-Hermitian Toeplitz matrix generated by the function

$$f(\theta) = \theta^2 + t \cdot \mathbf{i}\theta^3, \quad \theta \in [-\pi, \pi],$$

and B a non-Hermitian Toeplitz matrix generated by the function

$$f(\theta) = \theta^2 + t \cdot \mathbf{i}\,\mathrm{sgn}(\theta), \quad \theta \in [-\pi, \pi],$$

where $t > 0$ is a scalar and $\mathrm{sgn}(\theta)$ is the sign function defined as

$$\mathrm{sgn}(\theta) = \begin{cases} 1, & 0 < \theta \le \pi, \\ 0, & \theta = 0, \\ -1, & -\pi \le \theta < 0. \end{cases}$$

We computed the 10 smallest magnitude eigenpairs of the matrix pencil (A, B) with $t = 1, 10, 100$, respectively. The shift was set to zero ($\sigma = 0$).

Tables 1–3 list the numerical results, and Table 4 reports the 10 smallest eigenvalues computed using the MATLAB built-in function eig(A, B), as well as the approximations obtained from Inexact-eigs and Exact-eigs at $t = 1$. Tables 1–3 demonstrate that the scheme (3.1) is very effective in practice; and Inexact-eigs outperforms Exact-eigs considerably on CPU time, as the the stopping criterion involves 10^{-14} in Exact-eigs whereas it is $\mathcal{O}(10^{-8})$ in Inexact-eigs. From Table 4, we note that the approximate eigenpairs from Inexact-eigs are accurate enough. Further, we observe that Exact-eigs fails when $n > 9000$ due to the preconditioned and unrestarted GMRES algorithm used to solve the Toeplitz systems, because the GMRES algorithm often suffers from large storage requirements if the desired accuracy is too high.

Example 3.2. We now explore the efficiency of our inexact algorithm for a large Hermitian generalised Toeplitz eigenproblem. In this case, the implicitly restarted shift-and-invert Arnoldi method reduces to the implicitly restarted shift-and-invert Lanczos method [20], and we only need to solve one Toeplitz system for the Toeplitz inverse [17]. The test problem is taken from [13, 22]. The matrix A is a Hermitian Toeplitz matrix generated by the even function θ^2 defined on $[0, \pi]$. A symmetric positive definite Toeplitz matrix $B = [b_{jk}]$ is given by

$$b_{jk} = \begin{cases} 1 + \frac{\pi^4}{5}, & \text{if } j = k, \\ (-1)^{|j-k|}\left(\frac{4\pi^2}{|j-k|^2} - \frac{24}{|j-k|^4}\right), & \text{otherwise}, \end{cases} \tag{3.4}$$

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Table 1: Example 3.1. Numerical results for the 10 smallest eigenpairs in magnitude with $\sigma = 0$ and $tol = 10^{-6}$, $t = 1$, where "–" denotes "out of memory".

n	**(3.1)**	$\|\widehat{\mathbf{r}}^{real}\|_2$	**CPU(sec.)**	**CPU(sec.)**
			Inexact-eigs	**Exact-eigs**
3000	8.978×10^{-8}	1.845×10^{-9}	0.780	4.524
6000	8.978×10^{-8}	1.107×10^{-9}	1.623	12.667
9000	8.978×10^{-8}	5.354×10^{-11}	2.668	1.870×10^{2}
12000	8.978×10^{-8}	3.748×10^{-11}	3.776	–
15000	8.978×10^{-8}	4.936×10^{-11}	4.997	–

Table 2: Example 3.1. Numerical results for the 10 smallest eigenpairs in magnitude with $\sigma = 0$ and $tol = 10^{-6}$, $t = 10$. where "–" denotes "out of memory".

n	**(3.1)**	$\|\widehat{\mathbf{r}}^{real}\|_2$	**CPU(sec.)**	**CPU(sec.)**
			Inexact-eigs	**Exact-eigs**
3000	3.276×10^{-7}	5.566×10^{-8}	0.686	1.560
6000	3.276×10^{-7}	1.413×10^{-8}	1.700	14.025
9000	3.276×10^{-7}	7.929×10^{-9}	2.776	6.787×10^{2}
12000	3.276×10^{-7}	4.632×10^{-9}	3.713	–
15000	3.276×10^{-7}	4.715×10^{-9}	5.195	–

Table 3: Example 3.1. Numerical results for the 10 smallest eigenpairs in magnitude with $\sigma = 0$ and $tol = 10^{-6}$, $t = 100$, where "–" demotes "out of memory".

n	**(3.1)**	$\|\widehat{\mathbf{r}}^{real}\|_2$	**CPU(sec.)**	**CPU(sec.)**
			Inexact-eigs	**Exact-eigs**
3000	4.255×10^{-7}	7.674×10^{-6}	0.678	1.872
6000	4.255×10^{-7}	3.127×10^{-6}	1.529	10.421
9000	4.255×10^{-7}	9.841×10^{-7}	2.589	1.205×10^{2}
12000	4.255×10^{-7}	8.098×10^{-7}	3.728	–
15000	4.255×10^{-7}	2.426×10^{-7}	4.805	–

Table 4: Example 3.1. The 10 smallest eigenvalues in magnitude, computed using eig(A,B) and the approximations obtained from Inexact-eig and Exact-eig, $n = 3000$, $t = 1$.

eig: λ_i, $i = 1, 2, \cdots, 10$	**Inexact-eig**	**Exact-eig**
$5.42135345 \times 10^{-9} \pm$	$5.42135001 \times 10^{-9} \pm$	$5.42135075 \times 10^{-9} \pm$
$3.00211667 \times 10^{-6}\mathbf{i}$	$3.00211670 \times 10^{-6}\mathbf{i}$	$3.00211667 \times 10^{-6}\mathbf{i}$
$5.64830112 \times 10^{-8} \pm$	$5.64829957 \times 10^{-8} \pm$	$5.64830061 \times 10^{-8} \pm$
$1.45117763 \times 10^{-5}\mathbf{i}$	$1.45117765 \times 10^{-5}\mathbf{i}$	$1.45117763 \times 10^{-5}\mathbf{i}$
$2.08752894 \times 10^{-7} \pm$	$2.08752850 \times 10^{-7} \pm$	$2.08752891 \times 10^{-7} \pm$
$3.47985781 \times 10^{-5}\mathbf{i}$	$3.47985784 \times 10^{-5}\mathbf{i}$	$3.47985781 \times 10^{-5}\mathbf{i}$
$5.18404012 \times 10^{-7} \pm$	$5.18403803 \times 10^{-7} \pm$	$5.18404088 \times 10^{-7} \pm$
$6.38568356 \times 10^{-5}\mathbf{i}$	$6.38568363 \times 10^{-5}\mathbf{i}$	$6.38568356 \times 10^{-5}\mathbf{i}$
$1.04205274 \times 10^{-6} \pm$	$1.04205202 \times 10^{-6} \pm$	$1.04205223 \times 10^{-6} \pm$
$1.01686715 \times 10^{-4}\mathbf{i}$	$1.01686715 \times 10^{-4}\mathbf{i}$	$1.01686712 \times 10^{-4}\mathbf{i}$

which is derived from the even function $\theta^4 + 1$ defined on $[-\pi, \pi]$. For this test problem, we are interested in the 10 smallest eigenpairs closest to $\sigma = 0$ and the 8 eigenpairs closet

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Table 5: Example 3.2. Numerical results for the 10 smallest magnitude eigenpairs with $\sigma = 0$ and $tol = 10^{-6}$; where "–" denotes "out of memory".

n	(3.1)	$\|\widehat{\mathbf{r}}^{real}\|_2$	CPU(sec.) Inexact-eigs	CPU(sec.) Exact-eigs
3000	5.273×10^{-9}	9.812×10^{-10}	0.764	1.170
6000	5.273×10^{-9}	1.185×10^{-9}	1.809	5.382
9000	5.273×10^{-9}	3.877×10^{-10}	2.808	73.476
12000	5.273×10^{-9}	9.330×10^{-8}	3.853	–
15000	5.273×10^{-9}	1.008×10^{-10}	4.973	–

Table 6: Example 3.2. Numerical results for the 8 eigenpairs closest to $\sigma = 0.5$ and $tol = 10^{-6}$; where "–" denotes "out of memory".

n	(3.1)	$\|\widehat{\mathbf{r}}^{real}\|_2$	CPU(sec.) Inexact-eigs	CPU(sec.) Exact-eigs
3000	1.357×10^{-8}	3.679×10^{-9}	1.404	2.886
6000	1.357×10^{-8}	2.911×10^{-9}	3.229	9.048
9000	1.357×10^{-8}	6.479×10^{-9}	5.304	6.186×10^{2}
12000	1.357×10^{-8}	5.662×10^{-9}	8.346	–
15000	1.357×10^{-8}	5.791×10^{-10}	11.872	–

to $\sigma = 0.5$.

Tables 5–6 report the numerical results. Again, we observe that Inexact-eigs performs much better than Exact-eigs on CPU time, and we benefit from the GSF formula and by solving the Toeplitz systems inaccurately. A stopping criterion of 10^{-14} is required for Exact-eigs, whereas for Inexact-eig we only need a stopping criterion $\mathcal{O}(10^{-8})$ or $\mathcal{O}(10^{-9})$, providing a significant improvement.

Example 3.3. In this example, we explore the effectiveness of Theorem 2.2 and the inexact strategy (2.27) for solving generalised Toeplitz eigenproblems. The test matrices were derived from the MATLAB built-in function "gallery". The matrix A generated by the MATLAB command `gallery('parter',n)` is a non-Hermitian Cauchy and Toeplitz matrix such that $A(i,j) = 1/(i-j+0.5)$. The matrix B was generated from the MATLAB command `gallery('toeppd',n,p,w,theta)`, where we used the default values `p = n`, `w = rand(p,1)`, and `theta = rand(p,1)`. The resulting matrix is an n-by-n symmetric, positive semi-definite Toeplitz matrix composed of the sum of p rank 2 (or, for certain `theta`, rank 1) SPD Toeplitz matrix.

In order to evaluate $\mathbf{r}^{comp}$ and $\mathbf{r}^{real}$ explicitly and illustrate our theoretical results, we ran the thick-restarted shift-and-invert Arnoldi algorithm [12, 24] instead of the implicitly restarted shift-and-invert Arnoldi algorithm. This thick-restarted Arnoldi method is mathematically equivalent to the famous implicitly restarted Arnoldi method due to Sorensen [20], and the thick-restarting strategy is less complicated than the implicit-restarting strategy — cf. [12, 24] for details. We ran Algorithm 2.1 with $tol = 10^{-6}$ to solve the smallest eigenpair of the large generalised Toeplitz eigenproblem. The Toeplitz systems (2.4) were solved with different tolerances $\mathbf{tol}_{sys} = 10^{-6}, 10^{-8}, 10^{-10}, 10^{-12}$, as well as those obtained from inequalities (2.25) and (2.27). In (2.25), the values of $|\xi_0|, \|\mathbf{z}\|_1$ and

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Table 7: Example 3.3. Solving non-Hermitian generalised Toeplitz eigenproblem with different tolerance tol_{sys} for the Toeplitz systems (2.4), $\sigma = 0$, $m = 20$, $tol = 10^{-6}$.

n	$\mathbf{tol}_{sys}$	$\|\mathbf{r}^{real}\|_2$	$\|\mathbf{r}^{comp}\|_2$	$\frac{\|\mathbf{r}^{real}-\mathbf{r}^{comp}\|_2}{\|A-\sigma B\|_2}$	$\|\widehat{\mathbf{r}}^{real}\|_2$
4000	10^{-6}	3.421×10^{-4}	3.826×10^{-8}	3.417×10^{-3}	8.424×10^{-6}
	10^{-8}	5.671×10^{-7}	3.827×10^{-8}	7.623×10^{-6}	2.494×10^{-8}
	10^{-10}	4.155×10^{-8}	3.827×10^{-8}	1.001×10^{-7}	8.554×10^{-10}
	10^{-12}	3.820×10^{-8}	3.827×10^{-8}	1.942×10^{-9}	7.760×10^{-10}
	(2.27): 4.258×10^{-11}	4.155×10^{-8}	3.827×10^{-8}	1.001×10^{-7}	8.554×10^{-10}
	(2.25): 7.771×10^{-13}	3.820×10^{-8}	3.827×10^{-8}	1.942×10^{-9}	7.760×10^{-10}
6000	10^{-6}	3.954×10^{-4}	2.584×10^{-8}	4.016×10^{-3}	8.348×10^{-6}
	10^{-8}	2.972×10^{-7}	2.591×10^{-8}	3.475×10^{-6}	7.559×10^{-9}
	10^{-10}	2.704×10^{-8}	2.591×10^{-8}	1.208×10^{-7}	4.480×10^{-10}
	10^{-12}	2.587×10^{-8}	2.591×10^{-8}	3.628×10^{-9}	3.880×10^{-10}
	(2.27): 2.862×10^{-11}	2.704×10^{-8}	2.594×10^{-8}	1.208×10^{-7}	4.480×10^{-10}
	(2.25): 4.256×10^{-13}	2.590×10^{-8}	2.591×10^{-8}	2.008×10^{-10}	3.877×10^{-10}
8000	10^{-6}	1.416×10^{-4}	3.816×10^{-8}	1.971×10^{-3}	2.474×10^{-6}
	10^{-8}	1.721×10^{-6}	3.819×10^{-8}	2.403×10^{-5}	3.112×10^{-8}
	10^{-10}	5.270×10^{-8}	3.819×10^{-8}	6.400×10^{-7}	8.211×10^{-10}
	10^{-12}	3.820×10^{-8}	3.819×10^{-8}	2.001×10^{-8}	9.979×10^{-11}
	(2.27): 5.150×10^{-11}	3.647×10^{-8}	3.819×10^{-8}	6.396×10^{-8}	1.266×10^{-10}
	(2.25): 2.768×10^{-13}	3.820×10^{-8}	3.819×10^{-8}	3.897×10^{-10}	9.645×10^{-13}

$\|\mathbf{y}\|_1$ were evaluated on solving the Toeplitz systems (2.4) to an accuracy of 10^{-14}, and $\|A-\sigma B\|_2, \|B\|_\infty$ was approximated using $\max(\|\mathbf{fcol}\|_2, \|\mathbf{frow}\|_2)$ and $\max(\|\mathbf{Bcol}\|_\infty, \|\mathbf{Brow}\|_\infty)$, respectively. Table 7 lists the numerical results, showing that the Toeplitz systems should be solved with an accuracy of $tol_{\mathbf{sys}} = 10^{-10}$ if it is required that $\|\mathbf{r}^{real} - \mathbf{r}^{comp}\|_2 / \|A - \sigma B\|_2 \leq tol = 10^{-6}$. In regard to the "practical" bound from (2.27) and the "theoretical" bound from (2.25), the convergence thresholds $tol_{\mathbf{sys}}$ are about $\mathcal{O}(10^{-11})$ and $\mathcal{O}(10^{-13})$, respectively. Thus Theorem 2.2 is effective and our inexact strategy under (2.27) is very efficient in practice. We mention that the value of ξ is $\mathcal{O}(10^{-3})$ for this problem, which is not very small — cf. Remark 2.1.

4. Conclusion

This article discusses the development of efficient algorithms for calculating a few eigenpairs of a large non-Hermitian Toeplitz matrix pencil, and in particular an inexact shift-and-invert Arnoldi algorithm to solve non-Hermitian generalised Toeplitz eigenproblems. In the first step of the shift-and-invert Arnoldi method, two large non-Hermitian Toeplitz systems are to be solved — and if the desired accuracy to do so is high the cost can be prohibitive, especially for some ill-conditioned problems. To deal with this problem, we first established a relationship between the errors of the Toeplitz systems and the residual of the Toeplitz eigenproblem, and then proposed a practical stopping criterion for solving the Toeplitz systems approximately. When the Toeplitz systems are difficult to solve in practice, our numerical results demonstrate that an "inexact" algorithm often considerably outperforms the "exact" algorithm.

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