Inexact Shift-and-Invert Arnoldi for Toeplitz Matrix Exponential

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Abstract

We revisit the shift-and-invert Arnoldi method proposed in [S. Lee, H. Pang, and H. Sun. Shift-invert Arnoldi approximation to the Toeplitz matrix exponential, SIAM J. Sci. Comput., 32: 774–792, 2010] for numerical approximation to the product of Toeplitz matrix exponential with a vector. In this approach, one has to solve two large scale Toeplitz linear systems in advance. However, if the desired accuracy is high, the cost will be prohibitive. Therefore, it is interesting to investigate how to solve the Toeplitz systems inexactly in this method. The contribution of this paper is in three regards. First, we give a new stability analysis on the Gohberg-Semencul formula (GSF) and define the GSF condition number of a Toeplitz matrix. It is shown that, when the size of the Toeplitz matrix is large, our result is sharper than the one given in [M. Gutknecht and M. Hochbruck. The stability of inversion formulas for Toeplitz matrices, Linear Algebra Appl., 223/224: 307–324, 1995]. Second, we establish a relation between the error of Toeplitz systems and the residual of Toeplitz matrix exponential. We show that if the GSF condition number of the Toeplitz matrix is medium sized, the Toeplitz systems can be solved in a low accuracy. Third, based on this relationship, we present a practical stopping criterion for relaxing the accuracy of the Toeplitz systems, and propose an inexact shift-and-invert Arnoldi algorithm for the Toeplitz matrix exponential problem. Numerical experiments illustrate the numerical behavior of the new algorithm, and show the effectiveness of our theoretical results.

Keywords: Toeplitz matrix, Matrix exponential, Shift-and-invert Arnoldi, Gohberg-Semencul formula (GSF), GSF condition number.

1 Introduction

Toeplitz matrices occur in a variety of applications in mathematics and engineering such as complex and harmonic analysis, statistics, signal and image processing, information theory, numerical analysis, see [3, 4, 20] and the references therein. In this paper, we are interested in numerical approximation to the product of Toeplitz matrix exponential with a vector

\[ y(t) = \exp(-tA)v, \]  

where \( t \) is a scalar, \( v \) is a given vector, and \(-tA\) is a real \( n \times n \) large Toeplitz matrix whose spectrum is located in the left half plane. This problem plays an important role in various application fields such as computational finance [15, 25], numerical solution of Volterra-Wiener-Hopf equations [1], calculating the Wiener-Hopf integral equations [10], and so on.

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The Krylov subspace method is an efficient approach to approximate the matrix exponential with a vector, especially when the matrix is very large [13, 18, 23]. Indeed, it is the twentieth dubious way to compute the matrix exponential [18]. In this type of method, the matrix is first projected into a much smaller subspace, then the exponential is applied to the projected matrix, and finally the approximation is projected back to the original large space [13, 18, 23]. This procedure can be achieved by using the Lanczos process for symmetric matrices or by the Arnoldi process for non-symmetric matrices, while both procedures require only matrix-vector multiplications.

The shift-and-invert Arnoldi and Lanczos methods were widely investigated to speed up the Arnoldi and the Lanczos methods for matrix exponential [19, 26]. Recently, by making use of the shift-and-invert Arnoldi technique, Toeplitz structure and the famous Golberg-Semencul formula (GSF) [9], Pang et al. proposed a shift-and-invert Arnoldi method for Toeplitz matrix exponential [15, 21]. An advantage of this approach is that it is unnecessary to explicitly form or store the Toeplitz matrix and its inverse, and each matrix-vector product can be realized in several Fast Fourier Transformations (FFTs) [15, 21]. In the first step of this approach, one has to solve two large scale (non-Hermitian) Toeplitz linear systems in a desired accuracy. However, if the desired accuracy is very high, the cost for solving the Toeplitz linear systems will be very large, especially for some ill-conditioned problems. Thus, it is interesting to investigate how to solve the Toeplitz linear systems inexactly in the shift-and-invert Arnoldi method for matrix exponential.

In this paper, we first give a new stability analysis on the Golberg-Semencul formula in terms of 1-norm and 2-norm, and define the “GSF condition number” of a Toeplitz matrix. It is shown that our results are sharper than the one given in [12] when the Toeplitz matrix is large. We then establish a relation between the error of Toeplitz systems and the residual of Toeplitz matrix exponential. Based on the relationship, we present a practical stopping criterion for solving the Toeplitz systems inexactly.

This paper is organized as follows. In Section 2, we briefly introduce the shift-and-invert Arnoldi method for Toeplitz matrix exponential [15]. In Section 3, we give a stability analysis on the Golberg-Semencul formula and propose an inexact shift-and-invert Arnoldi algorithm. Numerical results given in Section 4 show the efficiency of our new algorithm and the effectiveness of the theoretical results.

2 The shift-and-invert Arnoldi method for Toeplitz matrix exponential

In the shift-and-invert Arnoldi/Lanczos method [2, 15, 19, 21, 26], the Krylov subspace is constructed by using the matrix \((I + \gamma A)^{-1}\), where \(\gamma\) is a user-prescribed parameter and \(I\) is the identity matrix whose order is clear from context. Let \(v_1 = v/\|v\|_2\), the \(m\)-step shift-and-invert Arnoldi process leads to the following relation

\[
(I + \gamma A)^{-1}V_m = V_m H_m + h_{m+1} v_{m+1} e_m^T, \tag{2.1}
\]

where \(V_m = [v_1, v_2, \ldots, v_m]\) is an \(n \times m\) orthonormal matrix, \(n\) is the size of the Toeplitz matrix, \(H_m = V_m^T (I + \gamma A)^{-1} V_m\) is an \(m\)-by-\(m\) upper Hessenberg matrix, and \(e_m\) is the \(m\)-th column of the \(m\)-by-\(m\) identity matrix.

Let \(\beta = \|v\|_2\), if \(H_m\) is invertible, then the shift-and-invert Arnoldi method exploits

\[
y_m(t) = V_m \left[ \exp\left(-\frac{t}{\gamma} \cdot (H^{-1} - I)\right) \cdot \beta e_1 \right] \equiv V_m u_m(t)
\]
as an approximation to \( y(t) \), where \( u_m(t) = \exp\left(- (t/\gamma) \cdot (H_m^{-1} - I)\right) \cdot \beta e_1 \). The residual is
\[
    r_m(t) = -Ay_m(t) - y'_m(t) = -AV_mu_m(t) - V_mu_m(t) = \frac{h_{m+1,m}}{\gamma} \text{e}_m^T H_m^{-1} u_m(t) \cdot (I + \gamma A)v_{m+1},
\]
and
\[
    \|r_m(t)\|_2 = \frac{h_{m+1,m}}{\gamma} \text{e}_m^T H_m^{-1} u_m(t) \cdot \| (I + \gamma A)v_{m+1} \|_2, \tag{2.2}
\]
which can be used as a cheap stopping criterion in practice.

In the \( m \)-step shift-and-invert Arnoldi method, we have to compute \( m \) Toeplitz matrix-vector products \( (I + \gamma A)^{-1} v_i, \quad i = 1, 2, \ldots, m \). Since \( \gamma \) is a given shift, we are interested in computing \( (I + \gamma A)^{-1} \) once for all. One option is to compute the inverse by some direct methods such as the LU decomposition \([11]\). However, Toeplitz matrix is often dense, and the computation of the inverse of a large dense matrix is prohibitive, especially when the matrix is large. Fortunately, as \( I + \gamma A \) is also a Toeplitz matrix, we have the Gohberg-Semencul formula (GSF) \([9]\) for its inverse. Indeed, the inverse of a Toeplitz matrix can be reconstructed from its first and last columns. More precisely, denote by \( e_1, e_n \) the first and the last column of the \( n \)-by-\( n \) identity matrix, and let \( x = [\xi_0, \xi_1, \ldots, \xi_{n-1}]^T \) and \( y = [\eta_0, \eta_1, \ldots, \eta_{n-1}]^T \) be the solutions of the following two Toeplitz systems
\[
    Tx = e_1 \quad \text{and} \quad Ty = e_n. \tag{2.3}
\]
If \( \xi_0 \neq 0 \), then the Gohberg-Semencul formula can be expressed as
\[
    T^{-1} = \frac{1}{\xi_0} \begin{bmatrix}
        \xi_0 & 0 & \cdots & 0 & \eta_{n-1} & \eta_{n-2} & \cdots & \eta_0 \\
        \xi_1 & \xi_0 & \cdots & 0 & 0 & \eta_{n-1} & \cdots & \eta_1 \\
        \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
        \xi_{n-1} & \xi_{n-2} & \cdots & \xi_0 & 0 & 0 & \cdots & \eta_{n-1} \\
    \end{bmatrix} - \begin{bmatrix}
        0 & \cdots & 0 & 0 & \eta_{n-1} & \cdots & \xi_1 \\
        \eta_0 & \cdots & 0 & 0 & \vdots & \vdots & \ddots & \vdots \\
        \vdots & \vdots & \ddots & \vdots & 0 & 0 & \cdots & \eta_{n-1} \\
        \eta_{n-2} & \cdots & \eta_0 & 0 & 0 & \cdots & 0 \\
    \end{bmatrix} \equiv \frac{1}{\xi_0} \left( L_z R_y - L_y^0 R_z^0 \right), \tag{2.4}
\]
where \( L_z, L_y^0 \) are lower Toeplitz matrices, and \( R_y, R_z^0 \) are upper Toeplitz matrices. Consequently, the Toeplitz matrix-vector product \( (I + \gamma A)^{-1} v_i \) can be realized in several FFTs of length \( n \) \([15, 21]\). We are in a position to present the following algorithm for the Toeplitz matrix exponential; for more details, refer to \([15]\).

**Algorithm 1.** An shift-and-invert Arnoldi algorithm for product of Toeplitz matrix exponential with a vector

**Step 1.** Solve the Toeplitz systems \((I + \gamma A)x = e_1\) and \((I + \gamma A)y = e_n;\)

**Step 2.** Choose a convergence tolerance \( \text{tol}_{\text{exp}} \) and the starting vector \( v_1 = v/\|v\|_2;\)

\[
\text{for } i = 1, 2, \ldots \text{ do }
\]

Perform the shift-and-invert Arnoldi process in which the Toeplitz matrix vector products \((I + \gamma A)^{-1} v_i \) are realized through FFTs.

If \( \| r_i(t) \|_2 \leq \text{tol}_{\text{exp}} \), then form the approximation \( y_i(t) = V_i u_i(t) \) and Stop, else Continue;

end for
In Step 1 of this algorithm, we have to solve two large scale non-Hermitian Toeplitz linear systems \([23]\). If the desired accuracy is too high, then we have to pay a large amount of computational cost for solving the Toeplitz linear systems, especially for some ill-conditioned problems. It is interesting to investigate how to solve the Toeplitz systems inexactly \([15, 21]\).

### 3 An inexact shift-and-invert Arnoldi algorithm for Toeplitz matrix exponential

In this section, we consider how to solve the Toeplitz systems inexact by the shift-and-invert Arnoldi method. As we solve the Toeplitz linear systems once for all, it can be understood as an “inexact” inverse technology. We first give a new stability analysis on the Gohberg-Semencul formula with respect to 1-norm and 2-norm, and then establish a relation between the error of Toeplitz systems and the residual of Toeplitz matrix exponential. Based on these theoretical results, we propose an inexact shift-and-invert Arnoldi algorithm for Toeplitz matrix exponential.

#### 3.1 A new stability analysis on the Gohberg-Semencul formula and the GSF condition number

In this subsection, we give a stability analysis on the Gohberg-Semencul formula and define the “GSF condition number” of a Toeplitz matrix. Let \(\tilde{x} = [\tilde{\xi}_0, \tilde{\xi}_1, \ldots, \tilde{\xi}_{n-1}]^T\) and \(\tilde{y} = [\tilde{\eta}_0, \tilde{\eta}_1, \ldots, \tilde{\eta}_{n-1}]^T\) be the numerical solutions of \(Tx = e_1\) and \(Ty = e_n\), respectively. If \(\tilde{\xi}_0 \neq 0\), we denote

\[
\tilde{T}^{-1} = \frac{1}{\xi_0} \left\{ \begin{bmatrix}
  \tilde{\xi}_0 & 0 & \cdots & 0 \\
  \tilde{\xi}_1 & \tilde{\xi}_0 & \cdots & 0 \\
  \vdots & \vdots & \ddots & \vdots \\
  \tilde{\xi}_{n-1} & \tilde{\xi}_{n-2} & \cdots & \tilde{\xi}_0 \\
 \end{bmatrix} \begin{bmatrix}
  \tilde{\eta}_{n-1} & \tilde{\eta}_{n-2} & \cdots & \tilde{\eta}_0 \\
  0 & \tilde{\eta}_{n-1} & \cdots & \tilde{\eta}_1 \\
  \vdots & \vdots & \ddots & \vdots \\
  0 & 0 & \cdots & \tilde{\eta}_{n-1} \\
 \end{bmatrix} \right\}
\]

which is a perturbation to the Toeplitz inverse \(T^{-1}\). The following theorem gives an error analysis on the Gohberg-Semencul formula in terms of 1-norm.

**Theorem 3.1.** Given \(\varepsilon > 0\), if \(\xi_0 \neq 0, \tilde{\xi}_0 \neq 0\), let \(\tilde{\varepsilon} = \frac{|1/\xi_0 - 1/\tilde{\xi}_0|}{|1/\xi_0|}\) be the relative error of \(1/\tilde{\xi}_0\) with respect to \(1/\xi_0\), and

\[
\frac{\|\tilde{x} - x\|_1}{\|x\|_1} \leq \varepsilon \quad \text{and} \quad \frac{\|\tilde{y} - y\|_1}{\|y\|_1} \leq \varepsilon,
\]

then we have

\[
\left\| T^{-1} - \tilde{T}^{-1} \right\|_1 \leq \frac{2}{\xi_0} \cdot \left[ \varepsilon + (1 + \varepsilon) \tilde{\varepsilon} \right] \left( 1 + \varepsilon \right) \cdot \left\| x \right\|_1 \cdot \left\| y \right\|_1,
\]

and

\[
\left\| T^{-1} - \tilde{T}^{-1} \right\|_1 \leq \frac{2}{\xi_0} \left[ \varepsilon + (1 + \varepsilon) \tilde{\varepsilon} \right] \left( 1 + \varepsilon \right) \cdot \min \left\{ \|x\|_1, \|y\|_1 \right\}.
\]
Proof. It follows from (2.4) and (3.1) that
\[ \|T^{-1} - \tilde{T}^{-1}\|_1 = \|\frac{1}{\xi_0} (L_x R_y - L_y^0 \tilde{R}_y) - \frac{1}{\xi_0} (\tilde{L}_x R_y - \tilde{L}_y^0 \tilde{R}_y)\|_1 \]
\[ = \|\left( \frac{1}{\xi_0} L_x \right) R_y - L_y^0 \left( \frac{1}{\xi_0} R_y^0 \right) - \left( \frac{1}{\xi_0} \tilde{L}_y^0 \right) \tilde{R}_y + L_y^0 \left( \frac{1}{\xi_0} \tilde{R}_y^0 \right) \|_1 \]
\[ \leq \|\left( \frac{1}{\xi_0} L_x \right) R_y - \left( \frac{1}{\xi_0} \tilde{L}_x \right) \tilde{R}_y\|_1 + \|L_y^0 \left( \frac{1}{\xi_0} \tilde{R}_y^0 \right) - L_y^0 \left( \frac{1}{\xi_0} R_y^0 \right)\|_1. \] (3.5)

Moreover, we have that
\[ \|\left( \frac{1}{\xi_0} L_x \right) R_y - \left( \frac{1}{\xi_0} \tilde{L}_x \right) \tilde{R}_y\|_1 = \|\left( \frac{1}{\xi_0} L_x \right) R_y - \left( \frac{1}{\xi_0} L_x \right) \tilde{R}_y + \left( \frac{1}{\xi_0} L_x \right) \tilde{R}_y - \left( \frac{1}{\xi_0} \tilde{L}_x \right) \tilde{R}_y\|_1 \]
\[ \leq \left| \frac{1}{\xi_0} \right| \|L_x\|_1 \|R_y - \tilde{R}_y\|_1 + \left| \frac{1}{\xi_0} \right| \|L_x\|_1 \|\tilde{R}_y\|_1. \] (3.6)

On the one hand, we obtain from (3.2) that
\[ \left| \frac{1}{\xi_0} - \frac{1}{\xi_0} \tilde{L}_x \right|_1 = \left| \frac{1}{\xi_0} x - \frac{1}{\xi_0} \tilde{x} \right|_1 \]
\[ = \left| \frac{1}{\xi_0} \right| \|x - \tilde{x} + (1 - \frac{\xi_0}{\xi_0}) \tilde{x}\|_1 \]
\[ \leq \left| \frac{1}{\xi_0} \right| \|x - \tilde{x}\|_1 + \tilde{\varepsilon} \|\tilde{x}\|_1 \]
\[ \leq \left| \frac{1}{\xi_0} \right| \left[ \varepsilon + (1 + \varepsilon) \tilde{\varepsilon} \right] \|x\|_1, \] (3.7)
where \( \varepsilon = \frac{|\xi_0 - 1|}{|\xi_0|} \) is the relative error of \( 1/\xi_0 \). On the other hand, we note from (2.4) and (3.1) that
\[ \|L_x\|_1 = \|x\|_1, \|\tilde{R}_y\|_1 = \|\tilde{y}\|_1 \leq (1 + \varepsilon) \|y\|_1, \] (3.8)
and
\[ \|R_y - \tilde{R}_y\|_1 = \|y - \tilde{y}\|_1 \leq \varepsilon \|y\|_1. \] (3.9)

From (3.6)–(3.9), we obtain
\[ \|\left( \frac{1}{\xi_0} L_x \right) R_y - \left( \frac{1}{\xi_0} \tilde{L}_x \right) \tilde{R}_y\|_1 \leq \left| \frac{1}{\xi_0} \right| \|x\|_1 \|y\|_1 \varepsilon + \left| \frac{1}{\xi_0} \right| \left[ \varepsilon + (1 + \varepsilon) \tilde{\varepsilon} \right] \|x\|_1 \|y\|_1 \cdot (1 + \varepsilon) \]
\[ = \left| \frac{1}{\xi_0} \right| \left[ \varepsilon + (1 + \varepsilon) \tilde{\varepsilon} \right] (1 + \varepsilon) \] \|x\|_1 \|y\|_1. \] (3.10)

Similarly, for the second part of (3.5), we can prove that
\[ \|L_y^0 \left( \frac{1}{\xi_0} \tilde{R}_y^0 \right) - L_y^0 \left( \frac{1}{\xi_0} R_y^0 \right)\|_1 \leq \left| \frac{1}{\xi_0} \right| \left[ \varepsilon + (1 + \varepsilon) \tilde{\varepsilon} \right] (1 + \varepsilon) \] \|x\|_1 \|y\|_1. \] (3.11)

Combining (3.5), (3.10) and (3.11), we arrive at
\[ \|T^{-1} - \tilde{T}^{-1}\|_1 \leq \left| \frac{2}{\xi_0} \right| \left[ \varepsilon + (1 + \varepsilon) \tilde{\varepsilon} \right] (1 + \varepsilon) \] \|x\|_1 \|y\|_1. \]
By (2.3), we have that \( \| \mathbf{x} \|_1 \leq \| T^{-1} \|_1 \) and \( \| \mathbf{y} \|_1 \leq \| T^{-1} \|_1 \). Thus,
\[
\left\| T^{-1} - \tilde{T}^{-1} \right\|_1 \leq \frac{2}{\xi_0} \cdot \left[ \varepsilon + (\varepsilon + (1 + \varepsilon)\tilde{c})(1 + \varepsilon) \right] \cdot \| \mathbf{x} \|_1 \cdot \| T^{-1} \|_1,
\]
and
\[
\left\| T^{-1} - \tilde{T}^{-1} \right\|_1 \leq \frac{2}{\xi_0} \cdot \left[ \varepsilon + (\varepsilon + (1 + \varepsilon)\tilde{c})(1 + \varepsilon) \right] \cdot \| \mathbf{y} \|_1 \cdot \| T^{-1} \|_1,
\]
a combination of which yields (3.3).

Furthermore, we have the following corollary on the relative error of Toeplitz inverse.

**Corollary 3.1.** Under the above notations, there holds

\[
\frac{\left\| T^{-1} - \tilde{T}^{-1} \right\|_1}{\| T^{-1} \|_1} \leq \frac{\| T \|_1 \| \mathbf{y} \|_1}{\| \xi_0 \| / \| \mathbf{x} \|_1} \cdot 2 [\varepsilon + (\varepsilon + (1 + \varepsilon)\tilde{c})(1 + \varepsilon)].
\]

**Proof.** We note that \( \| T \|_1 \| \mathbf{y} \|_1 \geq \| T \mathbf{y} \|_1 = 1 \) and \( \| T \|_1 \| \mathbf{x} \|_1 \geq 1 \). It follows from Theorem 3.1 that

\[
\frac{\left\| T^{-1} - \tilde{T}^{-1} \right\|_1}{\| T^{-1} \|_1} \leq \frac{2}{\xi_0} \cdot \left[ \varepsilon + (\varepsilon + (1 + \varepsilon)\tilde{c})(1 + \varepsilon) \right] \cdot \min \{\| \mathbf{x} \|_1, \| \mathbf{y} \|_1\}
\]
\[
\leq \frac{\| T \|_1 \| \mathbf{y} \|_1}{\| \xi_0 \| / \| \mathbf{x} \|_1} \cdot 2 [\varepsilon + (\varepsilon + (1 + \varepsilon)\tilde{c})(1 + \varepsilon)]
\]
\[
= \frac{\| T \|_1 \| \mathbf{y} \|_1}{\| \xi_0 \| / \| \mathbf{x} \|_1} \cdot 2 [\varepsilon + (\varepsilon + (1 + \varepsilon)\tilde{c})(1 + \varepsilon)].
\]

By (3.12), \( \| T \|_1 \| \mathbf{y} \|_1 / (\| \xi_0 \| / \| \mathbf{x} \|_1) \) is an enlarge factor of the solution of \( T^{-1} \) over the vector error \( \varepsilon \). So we can give the following definition on the condition number of a Toeplitz matrix.

**Definition 3.1.** We define

\[
\kappa^{GFS}_1(T) = \frac{\| T \|_1 \| \mathbf{y} \|_1}{\| \xi_0 \| / \| \mathbf{x} \|_1}
\]

as the 1-norm “GFS condition number” of a Toeplitz matrix.

Note that \( \| \xi_0 \| / \| \mathbf{x} \|_1 \) is the “proportion” of \( \| \xi_0 \| \) with respect to \( \| \mathbf{x} \|_1 \), and

\[
\kappa^{I}_{\text{eff}}(T) = \frac{\| T \|_1 \| \mathbf{y} \|_1}{\| \mathbf{e}_n \|_1} = \| T \|_1 \| \mathbf{y} \|_1
\]
is the “effective” 1-norm condition number of \( T \mathbf{y} = \mathbf{e}_n \) defined in [6]. Moreover, we notice that

\[
\kappa^{II}_{\text{eff}}(T) = \frac{\| T^{-1} \|_1 \| \mathbf{e}_n \|_1}{\| \mathbf{y} \|_1}
\]

the “effective” 1-norm condition number of \( T \mathbf{y} = \mathbf{e}_n \) defined in [16] [22], and we have that

\[
\kappa_1(T) = \kappa^{I}_{\text{eff}}(T) \cdot \kappa^{II}_{\text{eff}}(T),
\]

(3.14)

where \( \kappa_1(T) = \| T \|_1 \| T^{-1} \|_1 \) is the “classical” 1-norm condition number [11] of the matrix \( T \).

**Remark 3.1.** In terms of Corollary 3.1, \( \kappa^{GFS}_1(T) \) is an estimation to \( \kappa_1(T) \). By (3.14), \( \| \mathbf{x} \|_1 / \| \xi_0 \| \) can be used as an approximation to \( \kappa^{I}_{\text{eff}}(T) \). Thus, an advantage of (3.13) is that one can evaluate the “classical” condition number \( \kappa_1(T) \) of a Toeplitz matrix, and the “effective” condition numbers \( \kappa^{I}_{\text{eff}}(T), \kappa^{II}_{\text{eff}}(T) \) via solving Toeplitz systems, with no need to form the Toeplitz inverse explicitly.
Similarly, we can prove that

$$\left\| T^{-1} - \tilde{T}^{-1} \right\|_2 \leq \frac{2}{\xi_0} \left[ \epsilon + (1 + \epsilon \delta^2)(1 + \epsilon) \right] \cdot \|x\|_1 \cdot \|y\|_1,$$

(3.15)

and

$$\frac{\left\| T^{-1} - \tilde{T}^{-1} \right\|_2}{\|T^{-1}\|_2} \leq \frac{2 \sqrt{\eta}}{\xi_0} \left[ \epsilon + (1 + \epsilon \delta^2)(1 + \epsilon) \right] \cdot \min\{\|x\|_1, \|y\|_1\}.$$

(3.16)

Proof. Recall that

$$\left\| T^{-1} - \tilde{T}^{-1} \right\|_2 \leq \left\| T^{-1} - \tilde{T}^{-1} \right\|_1 \cdot \left\| T^{-1} - \tilde{T}^{-1} \right\|_\infty.$$

(3.17)

On the one hand, we have from (3.3) that

$$\left\| T^{-1} - \tilde{T}^{-1} \right\|_1 \leq \frac{2}{\xi_0} \left[ \epsilon + (1 + \epsilon)(1 + \epsilon \delta^2) \right] \cdot \|x\|_1 \cdot \|y\|_1.$$

On the other hand, we can give an upper bound on $$\left\| T^{-1} - \tilde{T}^{-1} \right\|_\infty$$:

$$\left\| T^{-1} - \tilde{T}^{-1} \right\|_\infty \leq \frac{2}{\xi_0} \left[ \epsilon + (1 + \epsilon)(1 + \epsilon \delta^2) \right] \cdot \|x\|_1 \cdot \|y\|_1,$$

(3.18)

whose proof is similar to that of Theorem 3.1, see [7]. So we have from (3.17), (3.3) and (3.18) that

$$\frac{\left\| T^{-1} - \tilde{T}^{-1} \right\|_2}{\|T^{-1}\|_2} \leq \frac{2}{\xi_0} \left[ \epsilon + (1 + \epsilon)(1 + \epsilon \delta^2) \right] \cdot \|x\|_1 \cdot \|y\|_1.$$

For (3.10), we notice that

$$\|x\|_1 \leq \sqrt{n} \|x\|_2 = \sqrt{n} \left\| T^{-1}e_1 \right\|_2 \leq \sqrt{n} \left\| T^{-1} \right\|_2 \|e_1\|_2 = \sqrt{n} \left\| T^{-1} \right\|_2.$$

(3.19)

Combining (3.15) and (3.19), we drive

$$\frac{\left\| T^{-1} - \tilde{T}^{-1} \right\|_2}{\|T^{-1}\|_2} \leq \frac{2}{\xi_0} \left[ \epsilon + (1 + \epsilon)(1 + \epsilon \delta^2) \right] \cdot \sqrt{n} \cdot \|y\|_1.$$

Similarly, we can prove that

$$\frac{\left\| T^{-1} - \tilde{T}^{-1} \right\|_2}{\|T^{-1}\|_2} \leq \frac{2}{\xi_0} \left[ \epsilon + (1 + \epsilon)(1 + \epsilon \delta^2) \right] \cdot \sqrt{n} \cdot \|x\|_1,$$

a combination of the above two inequalities yields (3.16). \( \square \)

**Remark 3.2.** In [73, p.321], Gutknecht and Hochbruck analyzed the stability of the Gohberg-Semencul formula, and gave the following two upper bounds for the absolute and relative errors with respect to $$T^{-1}$$:

$$\left\| T^{-1} - \tilde{T}^{-1} \right\|_2 \leq \frac{1}{\xi_0} \left( \|x\|_2 \|y\|_2 \left( 4n\varepsilon + 2n^2\varepsilon + 2n\varepsilon \right) + \sqrt{n} \left\| T^{-1} \right\|_2 \right),$$

(3.20)

and

$$\frac{\left\| T^{-1} - \tilde{T}^{-1} \right\|_2}{\|T^{-1}\|_2} \leq \frac{1}{\xi_0} \left( 2n \left\| T^{-1} \right\|_2 \left( 2\varepsilon + (n + 1)\varepsilon \right) + \sqrt{n} \right).$$

(3.21)
that is, Lemma 3.1. spanned by $V \times m$ systems (2.3) are solved inexactly, the errors of the matrix-vector products can be expressed as

$$\| \mathbf{x} \|_2 \leq \| \mathbf{y} \|_2 \cdot (1 + \varepsilon).$$

By setting $\varepsilon = 0$, (3.20) and (3.21) reduce to

$$\| T^{-1} - \tilde{T}^{-1} \|_2 \leq \frac{4n}{\xi_0} \cdot \| \mathbf{x} \|_2 \| \mathbf{y} \|_2 \cdot \varepsilon,$$

and

$$\| T^{-1} - \tilde{T}^{-1} \|_2 \leq \frac{4n}{\xi_0} \| T^{-1} \|_2 \cdot \varepsilon,$$

respectively.

Compared with (3.22) and (3.23), the new bounds given in (3.24) and (3.25) are independent of $n$, while (3.10) relies on $\sqrt{n}$ instead of $n$. Thus, our new upper bounds can be sharper than (3.22) and (3.23) when $n$ is large and $\tilde{\varepsilon} = O(\varepsilon)$. See Example 3 of Section 4 for a comparison of these upper bounds.

### 3.2 Relationship between the error of Toeplitz systems and the residual of Toeplitz matrix exponential

In this subsection, we establish a relationship between the error of Toeplitz systems and the residual of Toeplitz matrix exponential, and propose an inexact shift-and-invert Arnoldi method for product of a Toeplitz matrix exponential, and the residual of Toeplitz matrix exponential with a vector. It is shown that if the GSF condition number of the Toeplitz matrix is medium sized, we can solve the Toeplitz systems in a relatively low accuracy.

For simplicity, in the following we denote $T = I + \gamma A$ whenever necessary. Indeed, if the Toeplitz systems (2.3) are solved inexactly, the errors of the matrix-vector products can be expressed as $f_i = \tilde{T}^{-1}v_i - T^{-1}v_i$, $i = 1, 2, \ldots, m$. Let $F_m = [f_1, f_2, \ldots, f_m]$, we get the following relation for the $m$-step “inexact” shift-and-invert Arnoldi procedure

$$(I + \gamma A)^{-1}V_m + F_m = V_m \tilde{H}_m + \tilde{h}_{m+1, m}v_{m+1}e_m^T,$$

where $V_m = [v_1, v_2, \ldots, v_m]$ is an $n \times m$ orthonormal matrix, and $\tilde{H}_m = V_m^T[(I + \gamma A)^{-1} + F_mV_m^T]V_m$ is an $m \times m$ upper Hessenberg matrix. Note that $V_m$ is different from the one given in (2.4), and the subspace spanned by $V_m$ is not a Krylov subspace any more.

**Lemma 3.1.** If $\tilde{H}_m$ is invertible, denote $G = -\frac{1}{\gamma}(I + \gamma A)F_m\tilde{H}_m^{-1}V_m^T$, then the “inexact” shift-and-invert Arnoldi relation (3.24) can be rewritten as

$$(A + G)V_m = V_m (\frac{1}{\gamma}(\tilde{H}_m^{-1} - I)) - \frac{\tilde{h}_{m+1, m}}{\gamma}(I + \gamma A)v_{m+1}e_m^T\tilde{H}_m^{-1}.$$

**Proof.** Multiplying $I + \gamma A$ on both sides of (3.24) yields

$$V_m + (I + \gamma A)F_m = (I + \gamma A)V_m \tilde{H}_m + \tilde{h}_{m+1, m}(I + \gamma A)v_{m+1}e_m^T,$$

that is,

$$AV_m - \frac{1}{\gamma}(I + \gamma A)F_m\tilde{H}_m^{-1} = \frac{1}{\gamma}V_m (I - \tilde{H}_m)\tilde{H}_m^{-1} - \frac{\tilde{h}_{m+1, m}}{\gamma}(I + \gamma A)v_{m+1}e_m^T\tilde{H}_m^{-1}
\begin{align*}
&= \frac{1}{\gamma}V_m (\tilde{H}_m^{-1} - I) - \frac{\tilde{h}_{m+1, m}}{\gamma}(I + \gamma A)v_{m+1}e_m^T\tilde{H}_m^{-1} \\
&= V_m \left( \frac{1}{\gamma}(\tilde{H}_m^{-1} - I) \right) - \frac{\tilde{h}_{m+1, m}}{\gamma}(I + \gamma A)v_{m+1}e_m^T\tilde{H}_m^{-1}.
\end{align*}$$
The above equation can be rewritten as

\[
(\mathbf{A} - \frac{1}{\gamma}(I + \gamma \mathbf{A}) \mathbf{F}_m \mathbf{H}_m^{-1} \mathbf{V}_m^T) \mathbf{V}_m = (\mathbf{A} + \mathbf{G}) \mathbf{V}_m = \mathbf{V}_m \left( \frac{1}{\gamma} (\mathbf{H}_m^{-1} - I) \right) - \frac{\mathbf{h}_{m+1,m}}{\gamma} (I + \gamma \mathbf{A}) \mathbf{v}_{m+1} \mathbf{e}_m^T \mathbf{H}_m^{-1}.
\]

Let \( \mathbf{u}_m(t) = \exp(- (t/\gamma) \cdot (\mathbf{H}_m^{-1} - I)) \cdot \beta \mathbf{e}_1 \), then we can use \( \mathbf{y}_m(t) = \mathbf{V}_m \mathbf{u}_m(t) \) as an approximation to \( \mathbf{y}(t) \). The “real” residual is defined as [2]

\[
\mathbf{r}^{\text{real}} = -\mathbf{A} \mathbf{V}_m \mathbf{u}_m(t) - \mathbf{V}_m \mathbf{u}'_m(t).
\]

However, it is not computable since \( \mathbf{AV}_m \) is unavailable in practice. Thus, we define

\[
\mathbf{r}^{\text{comp}} = -(\mathbf{A} + \mathbf{G}) \mathbf{V}_m \mathbf{u}_m(t) - \mathbf{V}_m \mathbf{u}'_m(t) = -\mathbf{V}_m \frac{(\mathbf{H}_m^{-1} - I)}{\gamma} \mathbf{u}_m(t) + \mathbf{h}_{m+1,m} \exp(\mathbf{t} \mathbf{H}_m^{-1} \mathbf{u}_m(t)) + \mathbf{V}_m \frac{(\mathbf{H}_m^{-1} - I)}{\gamma} \mathbf{u}_m(t)
\]

as the “computed” residual. Moreover,

\[
\|\mathbf{r}^{\text{comp}}\|_2 = \frac{\mathbf{h}_{m+1,m} \mathbf{e}_m^T \mathbf{H}_m^{-1} \mathbf{u}_m(t)}{\gamma} \cdot \|I + \gamma \mathbf{A}\| \mathbf{v}_{m+1} \|_2,
\]

which can be used as a cheap stopping criterion in the “inexact” shift-and-invert Arnoldi method for Toeplitz matrix exponential.

We are ready to provide a practical stopping criterion for solving the Toeplitz systems inexactly. The key is how to investigate the distance between \( \mathbf{r}^{\text{real}} \) and \( \mathbf{r}^{\text{comp}} \). It is seen that

\[
\|\mathbf{r}^{\text{real}} - \mathbf{r}^{\text{comp}}\|_2 = \|\mathbf{G} \mathbf{V}_m \mathbf{u}_m(t)\|_2
\]

\[
= \frac{1}{\gamma} \|I + \gamma \mathbf{A}\| \mathbf{F}_m \mathbf{H}_m^{-1} \mathbf{u}_m(t)\|_2
\]

\[
\leq \frac{1}{\gamma} \cdot \|I + \gamma \mathbf{A}\|_2 \cdot \|\mathbf{F}_m \mathbf{H}_m^{-1} \mathbf{u}_m(t)\|_2.
\]

From (3.15), we obtain

\[
\|\mathbf{f}_i\|_2 = \|\mathbf{T}^{-1} \mathbf{v}_i - \mathbf{T}^{-1} \mathbf{v}_i\|_2 \leq \|\mathbf{T}^{-1} - \mathbf{T}^{-1}\|_2 \|\mathbf{v}_i\|_2
\]

\[
= \|\mathbf{T}^{-1} - \mathbf{T}^{-1}\|_2 \leq \left| \frac{2}{\xi_0} \right| \cdot \left[ \varepsilon + (\varepsilon + (1 + \varepsilon) \bar{\varepsilon})(1 + \varepsilon) \right] \cdot \|\mathbf{x}||\mathbf{y}|, \quad i = 1, 2, \ldots, m.
\]

If \( \varepsilon \ll 1 \), then \( \varepsilon + (\varepsilon + (1 + \varepsilon) \bar{\varepsilon})(1 + \varepsilon) \leq 3\varepsilon + \mathcal{O}(\varepsilon^2) \), and

\[
\|\mathbf{f}_i\|_2 \leq \left| \frac{2}{\xi_0} \right| \cdot \left[ \varepsilon + (\varepsilon + (1 + \varepsilon) \bar{\varepsilon})(1 + \varepsilon) \right] \cdot \|\mathbf{x}||\mathbf{y}|, \quad i = 1, 2, \ldots, m,
\]

where we omit the high order term \( \mathcal{O}(\varepsilon^2) \).
Denote \( \tilde{H}_m^{-1}u_m(t) = [\alpha_1, \alpha_2, \ldots, \alpha_m]^T \), then

\[
\left\| F_m \tilde{H}_m^{-1}u_m(t) \right\|_2 = \left\| \sum_{i=1}^{m} f_i \alpha_i \right\|_2 \leq \max_{1 \leq i \leq m} \left\| f_i \right\|_2 \cdot \left\| \tilde{H}_m^{-1}u_m(t) \right\|_2 \\
\leq \max_{1 \leq i \leq m} \left\| f_i \right\|_2 \cdot \sqrt{m} \left\| \tilde{H}_m^{-1}u_m(t) \right\|_2.
\]

(3.31)

Combining (3.29), (3.30) and (3.31), we have that

\[
\left\| r^{\text{real}} - r^{\text{comp}} \right\|_2 \leq \frac{1}{\gamma} \left\| I + \gamma A \right\|_2 \cdot \max_{1 \leq i \leq m} \left\| f_i \right\|_2 \cdot \sqrt{m} \left\| \tilde{H}_m^{-1} \right\|_2 \left\| u_m(t) \right\|_2 \\
\leq \frac{1}{\gamma} \left\| I + \gamma A \right\|_2 \cdot \frac{6}{\gamma} \left\| x \right\|_1 \left\| y \right\|_1 \cdot \sqrt{m} \left\| \tilde{H}_m^{-1} \right\|_2 \left\| u_m(t) \right\|_2.
\]

Let \( \text{tol}_\text{exp} \) be the convergence threshold for the shift-and-invert Arnoldi method for solving (1.1). If

\[
\varepsilon \leq \frac{\left| \gamma \zeta_0 \right| \cdot \text{tol}_\text{exp}}{6\sqrt{m} \left\| I + \gamma A \right\|_2 \cdot \left\| x \right\|_1 \left\| y \right\|_1 \cdot \left\| \tilde{H}_m^{-1} \right\|_2 \left\| u_m(t) \right\|_2},
\]

then we have that

\[
\left\| r^{\text{real}} - r^{\text{comp}} \right\|_2 \lesssim \text{tol}_\text{exp}.
\]

In conclusion, we have the following theorem.

**Theorem 3.3.** Under the above notations and assumptions, if

\[
\varepsilon \leq \frac{\left| \zeta_0 \right| \left\| x \right\|_1}{\left\| I + \gamma A \right\|_2 \left\| y \right\|_1} \cdot \frac{\left| \gamma \right| \cdot \text{tol}_\text{exp}}{6\sqrt{m} \left\| \tilde{H}_m^{-1} \right\|_2 \left\| u_m(t) \right\|_2} \\
= \frac{\left| \zeta_0 \right| \left\| x \right\|_1}{\left\| I + \gamma A \right\|_1 \left\| y \right\|_1} \cdot \frac{\left| \gamma \right| \cdot \left\| I + \gamma A \right\|_1 \cdot \text{tol}_\text{exp}}{6\sqrt{m} \left\| I + \gamma A \right\|_2 \cdot \left\| \tilde{H}_m^{-1} \right\|_2 \left\| u_m(t) \right\|_2}.
\]

(3.32)

then

\[
\left\| r^{\text{real}} - r^{\text{comp}} \right\|_2 \lesssim \text{tol}_\text{exp}.
\]

**Remark 3.3.** We notice that

\[
\kappa_1^{\text{GSF}}(I + \gamma A) = \frac{\left\| I + \gamma A \right\|_1 \left\| y \right\|_1}{\left| \zeta_0 \right| \left\| x \right\|_1}
\]

is just the 1-norm “GSF condition number” defined in Definition 3.1, which can be utilized as an estimation to the 1-norm condition number of \( I + \gamma A \). Furthermore, (3.32) can be reformulated as

\[
\varepsilon \leq \frac{1}{\kappa_1^{\text{GSF}}(I + \gamma A)} \cdot \frac{\left| \gamma \right| \cdot \left\| I + \gamma A \right\|_1 \cdot \text{tol}_\text{exp}}{6\sqrt{m} \left\| I + \gamma A \right\|_2 \cdot \left\| \tilde{H}_m^{-1} \right\|_2 \left\| u_m(t) \right\|_2}.
\]

(3.33)

This implies that if the GSF condition number of the Toeplitz matrix is medium sized, we can solve the Toeplitz systems in a (relatively) low accuracy. Otherwise, we have to solve the Toeplitz systems in a (relatively) high accuracy.

**Remark 3.4.** Unfortunately, the parameters \( \left\| \tilde{H}_m^{-1} \right\|_2 \), \( \left\| u_m(t) \right\|_2 \), and \( \kappa_1^{\text{GSF}}(I + \gamma A) \) are unavailable a priori.

We notice that \( \left\| \tilde{H}_m^{-1} \right\|_2 \) is uniformly bounded and \( \left\| u_m(t) \right\|_2 = O(\left\| y(t) \right\|_2) \) as the shift-and-invert Arnoldi
method converges. Therefore, if $\kappa_1^{G SF}(I + \gamma A)$ is medium sized and $\| I + \gamma A \|_1 = O \left( \| \tilde{H}^{-1}_m \|_2 \| u_m(t) \|_2 \right)$, we suggest using

$$\| r_x \|_2, \| r_y \|_2 \leq \frac{|\gamma|}{6\sqrt{m} \cdot \max\{\| fcol \|_2, \| frow \|_2 \}} \cdot tol_{exp}$$

(3.34)

as the stopping criterion for solving the Toeplitz systems, where $r_x = e_1 - T\tilde{x}$ and $r_y = e_n - T\tilde{y}$ are the residuals of the Toeplitz systems, and $fcol, frow$ are the first column and first row of $I + \gamma A$, respectively.

In summary, we propose the following “inexact” shift-and-invert Arnoldi algorithm for solving the Toeplitz matrix exponential problem (1.1).

**Algorithm 2. An inexact shift-and-invert Arnoldi algorithm for product of Toeplitz matrix exponential with a vector**

This algorithm is similar to Algorithm 1, except for the Toeplitz linear systems (2.3) are solved inexactly in Step 1, with the stopping criterion described in (3.34).

We point out that several results on computing matrix functions using inexact Krylov methods have been developed in other contexts, where 2-norm estimates are given. In [8], Frommer et al. considered how to cheaply recover a secondary Lanczos process starting at an arbitrary Lanczos vector. This secondary process is then used to efficiently obtain computable error estimates and error bounds for the Lanczos approximations to the action of a rational matrix function on a vector, e.g., the matrix sign function.

**4 Numerical experiments**

In this section, we perform some numerical examples to show the efficiency of Algorithm 2 and the effectiveness of our theoretical results. All the numerical experiments were run on two core Intel(R) Core(TM)2 E7400 processor with CPU 2.8 GHz and RAM 1.99 GB, under the Windows 7 operating system. The experimental results were obtained by using a MATLAB 7.7 implementation with machine precision $\epsilon \approx 2.22 \times 10^{-16}$.

As was done in [15], we use the (unrestarted) GMRES algorithm [24] with T. Chan’s optimal (circulant) preconditioner [3, 6, 20] for solving the Toeplitz systems in Algorithm 1 and Algorithm 2. Let $tol_{exp}, tol_{sys}$ be the tolerance for computing the Toeplitz matrix exponential-vector product, and that for solving the Toeplitz systems, respectively. Denote by $M$ the optimal preconditioner due to T. Chan, by $\tilde{q} = \tilde{x}$ (or $\tilde{y}$) the approximate solution of the Toeplitz system, and by $b = e_1$ (or $e_n$) the right-hand side. In Algorithm 2 we use

$$\| M^{-1}b - M^{-1}(I + \gamma A)\tilde{q} \|_2 \leq \frac{|\gamma|}{6\sqrt{100} \cdot \max\{\| fcol \|_2, \| frow \|_2 \}} \cdot tol_{exp} \equiv tol_{sys}$$

(4.1)

as the stopping criterion for the Toeplitz systems, where $fcol$ and $frow$ denote the first column and the first row of $I + \gamma A$, respectively. This algorithm mimics solving the two Toeplitz systems “inexactly” with an iterative solver.

In Algorithm 1, we use

$$\| M^{-1}b - M^{-1}(I + \gamma A)\tilde{q} \|_2 \leq 10^{-14} \equiv tol_{sys}$$

(4.2)

as the stopping criterion for the Toeplitz systems. This algorithm mimics solving the Toeplitz systems “exactly” via an iterative solver. Let $y(t)$ be the “exact” solution and $y_m(t)$ be the approximate solutions obtained from Algorithm 1 or Algorithm 2, then we define

$$\text{Error} = \frac{\| y(t) - y_m(t) \|_2}{\| y(t) \|_2}$$

(4.3)
as the relative error of the approximation \( y_m(t) \). Except for Example 1, the “exact” solution \( y(t) \) is calculated by using the MATLAB built-in function \( \expm.m \). In the tables below, we denote by CPU the CPU time in seconds. We choose the vector \( v = [1, 1, \ldots, 1]^T \) for all the numerical experiments in this section.

**Example 1.** In this example, we aim to show the effectiveness of our inexact strategy (3.34), as well as the superiority of Algorithm 2 over Algorithm 1. The Toeplitz matrix \( A \) is generated by the even function \( \theta^2 \) defined on \([−π, π]\). We want to compute \( y(t) = \exp(−tA)v \) with \( t = 1, \text{tol}_\exp = 10^{-6} \) and \( n = 1 \times 10^5, 2 \times 10^5, \ldots, 5 \times 10^5 \), respectively. Since the size \( n \) of the Toeplitz matrix is very large, the MATLAB built-in function \( \expm.m \) is infeasible for this problem. As a compromise, we run Algorithm 1 with the convergence tolerance \( \text{tol}_\exp = 10^{-14} \) for the “exact” solution \( y(t) \). Table 1 lists the numerical results.

We see from Table 1 that Algorithm 2 converges much faster than Algorithm 1 in practical calculations, and the inexact strategy is both efficient and reliable. Thanks to (3.34), it is only necessary to solve the Toeplitz system in the accuracy of \( O(10^{-9}) \) instead of \( 10^{-14} \). Furthermore, the approximate solutions computed from the two methods have the same accuracy in terms of Error.

| \( n \)       | Algorithm 1 | \( \text{tol}_\text{sys} \) | Error        | CPU        |
|--------------|-------------|-----------------------------|--------------|------------|
| \( 1 \times 10^5 \) | Algorithm 1 | \( 1.000 \times 10^{-14} \) | \( 4.615 \times 10^{-7} \) | 2.531 |
|              | Algorithm 2 | \( 1.239 \times 10^{-9} \)  | \( 4.615 \times 10^{-7} \) | 1.297 |
| \( 2 \times 10^5 \) | Algorithm 1 | \( 1.000 \times 10^{-14} \) | \( 3.263 \times 10^{-7} \) | 7.360 |
|              | Algorithm 2 | \( 1.239 \times 10^{-9} \)  | \( 3.263 \times 10^{-7} \) | 3.422 |
| \( 3 \times 10^5 \) | Algorithm 1 | \( 1.000 \times 10^{-14} \) | \( 2.664 \times 10^{-7} \) | 13.375 |
|              | Algorithm 2 | \( 1.239 \times 10^{-9} \)  | \( 2.664 \times 10^{-7} \) | 6.031 |
| \( 4 \times 10^5 \) | Algorithm 1 | \( 1.000 \times 10^{-14} \) | \( 2.307 \times 10^{-7} \) | 20.313 |
|              | Algorithm 2 | \( 1.239 \times 10^{-9} \)  | \( 2.307 \times 10^{-7} \) | 9.125 |
| \( 5 \times 10^5 \) | Algorithm 1 | \( 1.000 \times 10^{-14} \) | \( 2.064 \times 10^{-7} \) | 27.719 |
|              | Algorithm 2 | \( 1.239 \times 10^{-9} \)  | \( 2.064 \times 10^{-7} \) | 10.187 |

Table 1, Example 1: A comparison of Algorithm 1 and Algorithm 2, \( t = 1, γ = 1/10 \) and \( \text{tol}_\exp = 10^{-6} \).

**Example 2.** The aim of this example is two-fold. First, we show the effectiveness of Theorem 3.3. Second, we illustrate that our proposed 1-norm “GSF condition number” (3.13) is a good estimation to the 1-norm “classical condition number” of a Toeplitz matrix. For the first aim, we run Algorithm 2 with the stopping criterion \( \text{tol}_\exp \) chosen as \( 10^{-2}, 10^{-4}, \ldots, 10^{-10} \), and try to show that

\[
||\mathbf{r}^{\text{real}} - \mathbf{r}^{\text{comp}}||_2 = O(\text{tol}_\exp).
\]

In order to compute the “real” residual, we first form the approximation \( y_m(t) = V_m u_m(t) \) explicitly, and then compute \( \mathbf{r}^{\text{real}} \) by (3.26). The convergence threshold \( \text{tol}_\text{sys} \) for the Toeplitz systems is determined by using (3.34).

There are two test problems in this example, both of which are from [15]. The first test matrix is the non-Hermitian Toeplitz matrix generated by the function \( f(\theta) = \theta^2 + i \cdot \theta^3, \theta = \sqrt{-1}, \theta \in [−π, π] \). Notice that \( \text{Re}(f) = \theta^2 \geq 0 \) is an even function, and \( \text{Im}(f) = \theta^3 \) is an odd function. Table 2 lists the numerical results of Algorithm 2 for \( \exp(-tA)v \) with \( t = 1, γ = 1/10, \) and \( n = 3000 \). For the first test problem, we have \( \kappa_1^\text{GSF}(I + γA) ≈ 1.275 \times 10^2 \), which is of medium sized. In the second test problem, we consider pricing options for a single underlying asset in Merton’s jump-diffusion model [15] [17]. As the real part
of the eigenvalues of the Toeplitz matrix are less equal to zero, we are interested in computing $\exp(tA)v$ with $t > 0$, for more details, see Example 3 of [15]. Table 3 gives the numerical results of Algorithm 2 with $t = 1, \gamma = 1, n = 3000$. For this test problem, we have $\kappa_1^{GSF}(I + \gamma A) \approx 6.296 \times 10^7$, which is relatively large.

Two remarks are in order. First, we see that $\|r^{\text{real}} - r^{\text{comp}}\|_2$ and $tol_{\text{exp}}$ are about in the same order in all the cases. This illustrates the effectiveness of Theorem 3.3 as well as the efficiency of the inexact strategy (3.34). Second, we observe from Table 2 and Table 3 that, if the GSF condition number $\kappa_1^{GSF}(I + \gamma A)$ is medium sized, one can solve the Toeplitz systems (2.3) with a relatively low accuracy. Otherwise, we have to solve them with a relatively high accuracy. For instance, if we choose $tol_{\text{exp}} = 10^{-6}$, one has to solve the Toeplitz systems in an accuracy of $O(10^{-9})$ for the first test problem, while an accuracy of $O(10^{-13})$ is required for the second test problem.

| tol_{\text{exp}} | tol_{\text{sys}} | \|r^{\text{real}} - r^{\text{comp}}\|_2 | Error |
|------------------|------------------|------------------|-------|
| $10^{-2}$        | $1.010 \times 10^{-5}$ | $1.519 \times 10^{-3}$ | $2.679 \times 10^{-4}$ |
| $10^{-4}$        | $1.010 \times 10^{-7}$ | $5.352 \times 10^{-5}$ | $6.480 \times 10^{-6}$ |
| $10^{-6}$        | $1.010 \times 10^{-9}$ | $4.839 \times 10^{-5}$ | $3.985 \times 10^{-6}$ |
| $10^{-8}$        | $1.010 \times 10^{-11}$ | $1.679 \times 10^{-8}$ | $1.701 \times 10^{-9}$ |
| $10^{-10}$       | $1.010 \times 10^{-13}$ | $2.667 \times 10^{-9}$ | $2.607 \times 10^{-10}$ |

Table 2, the 1st test problem of Example 2: Numerical results of Algorithm 2 with different $tol_{\text{exp}}$ for computing $e^{-tA}v$, $t = 1, \gamma = 1/10, n = 3000; \kappa_1^{GSF}(I + \gamma A) \approx 1.275 \times 10^2$.

| tol_{\text{exp}} | tol_{\text{sys}} | \|r^{\text{real}} - r^{\text{comp}}\|_2 | Error |
|------------------|------------------|------------------|-------|
| $10^{-2}$        | $4.236 \times 10^{-9}$ | $6.958 \times 10^{-2}$ | $9.375 \times 10^{-5}$ |
| $10^{-4}$        | $4.236 \times 10^{-11}$ | $7.347 \times 10^{-4}$ | $6.817 \times 10^{-7}$ |
| $10^{-6}$        | $4.236 \times 10^{-13}$ | $3.320 \times 10^{-5}$ | $3.056 \times 10^{-9}$ |
| $10^{-8}$        | $4.236 \times 10^{-15}$ | $1.417 \times 10^{-7}$ | $2.364 \times 10^{-11}$ |
| $10^{-10}$       | $4.236 \times 10^{-17}$ | $5.105 \times 10^{-11}$ | $2.021 \times 10^{-11}$ |

Table 3, the 2nd test problem of Example 2: Numerical results of Algorithm 2 with different $tol_{\text{exp}}$ for computing $e^{tA}v$, $t = 1, \gamma = 1, n = 3000; \kappa_1^{GSF}(I + \gamma A) \approx 6.296 \times 10^7$.

When $n = 1000, 2000, 3000$ and $4000$, we list in Table 4 the 1-norm GSF condition number $\kappa_1^{GSF}(I + \gamma A)$ (where we use $\max\|\text{fcol}\|_1, \|\text{frow}\|_1$ instead of $\|I + \gamma A\|_1$), the 1-norm classical condition number $\kappa_1(I + \gamma A)$ (evaluated by using the MATLAB command $\text{cond}(I + \gamma A, 1)$) and its estimation $\kappa_1^{est}(I + \gamma A)$ (evaluated by using the MATLAB command $\text{condest}(I + \gamma A)$); as well as the CPU time in seconds for solving them (in brackets). It is seen that the GSF condition number is about one to two times larger than the classical condition number, and the former is a good estimation to the latter. Furthermore, the CPU time for $\kappa_1^{GSF}(I + \gamma A)$ is much less than that for $\kappa_1(I + \gamma A)$ and $\kappa_1^{est}(I + \gamma A)$, especially when $n$ is large. Thus, the 1-norm GSF condition number is a competitive alternative to the classical condition number for Toeplitz matrices.

**Example 3.** In this example, we try to show that our new bounds (3.15) and (3.16) are sharper than (3.22) and (3.28). The test matrix is the “gallery” matrix generated by the MATLAB command $A =$ 

| tol_{\text{exp}} | tol_{\text{sys}} | \|r^{\text{real}} - r^{\text{comp}}\|_2 | Error |
|------------------|------------------|------------------|-------|
| $10^{-2}$        | $4.236 \times 10^{-9}$ | $6.958 \times 10^{-2}$ | $9.375 \times 10^{-5}$ |
| $10^{-4}$        | $4.236 \times 10^{-11}$ | $7.347 \times 10^{-4}$ | $6.817 \times 10^{-7}$ |
| $10^{-6}$        | $4.236 \times 10^{-13}$ | $3.320 \times 10^{-5}$ | $3.056 \times 10^{-9}$ |
| $10^{-8}$        | $4.236 \times 10^{-15}$ | $1.417 \times 10^{-7}$ | $2.364 \times 10^{-11}$ |
| $10^{-10}$       | $4.236 \times 10^{-17}$ | $5.105 \times 10^{-11}$ | $2.021 \times 10^{-11}$ |
where for (3.15) and (3.16), and 2-norm for (3.22) and (3.23). The vector running the preconditioned (unrestarted) GMRES algorithm with (3.15) is a vector of length $2000\times 1$.

Table 4, Example 2 : The values of $\kappa_{SSF}^{est}(I + \gamma A)$, $\kappa_{est}(I + \gamma A)$, $\kappa_{1}(I + \gamma A)$ and the CPU time in seconds for computing them (in brackets), $n = 1000, 2000, 3000, 4000$.

gallery('parter', n) 

It is a Toeplitz matrix whose singular values are close to $\pi$. Let $x$ and $y$ be the “exact” solutions of the systems $(I + \gamma A)x = e_1$ and $(I + \gamma A)y = e_n$, respectively, which are computed from running the preconditioned (unrestarted) GMRES algorithm with $tol_{sys} = 10^{-14}$. Then we form $\tilde{x}$ in the following way:

$$
\tilde{f} = \text{randn}(n, 1); \quad \tilde{f} = f/\|f\|; \quad \tilde{x} = x + \varepsilon \|x\| \cdot f;
$$

where $\text{randn}(n, 1)$ is a vector of length $n$ with normally distributed random entries, and $\| \cdot \|$ is 1-norm for (3.15) and (3.16), and 2-norm for (3.22) and (3.23). The vector $\tilde{y}$ is formed in a similar way. In this example, we choose $\varepsilon = 10^{-6}, 10^{-9}, 10^{-12}$ and $n = 1000, 2000, 3000, 4000$, respectively. In order to show the sharpness of our results, we also present the “exact” absolute and relative errors $\|T^{-1} - \tilde{T}^{-1}\|_2$ and $\|T^{-1} - \tilde{T}^{-1}\|_2/\|T^{-1}\|_2$. Tables 4 and 5 report the numerical results. It is seen that our upper bounds are sharper than those due to Gutknecht and Hochbruck, especially when $n$ is large.

| $\varepsilon$ | $n$ | $\tilde{f}$ | $\tilde{g}$ | $\|T^{-1} - \tilde{T}^{-1}\|_2$ |
|---------------|-----|-------------|-------------|---------------------|
| $10^{-6}$     | 1000| $1.114 \times 10^{-5}$ | $3.358 \times 10^{-3}$ | $3.238 \times 10^{-6}$ |
|               | 2000| $1.217 \times 10^{-5}$ | $6.717 \times 10^{-3}$ | $3.672 \times 10^{-6}$ |
|               | 3000| $1.281 \times 10^{-5}$ | $1.007 \times 10^{-2}$ | $3.948 \times 10^{-6}$ |
|               | 4000| $1.329 \times 10^{-5}$ | $1.343 \times 10^{-2}$ | $3.767 \times 10^{-6}$ |
| $10^{-9}$     | 1000| $1.113 \times 10^{-8}$ | $3.358 \times 10^{-6}$ | $3.182 \times 10^{-9}$ |
|               | 2000| $1.218 \times 10^{-8}$ | $6.717 \times 10^{-6}$ | $3.414 \times 10^{-9}$ |
|               | 3000| $1.282 \times 10^{-8}$ | $1.007 \times 10^{-5}$ | $3.947 \times 10^{-9}$ |
|               | 4000| $1.328 \times 10^{-8}$ | $1.343 \times 10^{-5}$ | $3.961 \times 10^{-9}$ |
| $10^{-12}$    | 1000| $1.113 \times 10^{-11}$ | $3.358 \times 10^{-9}$ | $3.385 \times 10^{-12}$ |
|               | 2000| $1.217 \times 10^{-11}$ | $6.717 \times 10^{-9}$ | $4.102 \times 10^{-12}$ |
|               | 3000| $1.282 \times 10^{-11}$ | $1.007 \times 10^{-8}$ | $3.930 \times 10^{-12}$ |
|               | 4000| $1.328 \times 10^{-11}$ | $1.343 \times 10^{-8}$ | $4.071 \times 10^{-12}$ |

Table 5, Example 3: A comparison of the absolute error bounds (3.15) and (3.22), $t = 1, \gamma = 1/10$, $\varepsilon = 10^{-6}, 10^{-9}, 10^{-12}$ and $n = 1000, 2000, 3000, 4000$. 

14
Table 6, Example 3: A comparison of the relative error bounds (3.16) and (3.23), $t = 1, \gamma = 1/10, 
\varepsilon = 10^{-6}, 10^{-9}, 10^{-12}$ and $n = 1000, 2000, 3000, 4000.$

| $\varepsilon$ | $n$ | (3.16) | (3.23) | $\|T^{-1} - T^{-1}\|$ |
|--------------|-----|--------|--------|----------------|
| $10^{-6}$    | 1000  | $3.524 \times 10^{-4}$ | $4.813 \times 10^{-3}$ | $2.932 \times 10^{-6}$ |
|              | 2000  | $5.447 \times 10^{-4}$ | $9.642 \times 10^{-3}$ | $3.739 \times 10^{-6}$ |
|              | 3000  | $7.018 \times 10^{-4}$ | $1.447 \times 10^{-2}$ | $3.829 \times 10^{-6}$ |
|              | 4000  | $8.403 \times 10^{-4}$ | $1.931 \times 10^{-2}$ | $3.652 \times 10^{-6}$ |
| $10^{-9}$    | 1000  | $3.519 \times 10^{-7}$ | $4.813 \times 10^{-6}$ | $3.626 \times 10^{-9}$ |
|              | 2000  | $5.443 \times 10^{-7}$ | $9.642 \times 10^{-6}$ | $3.328 \times 10^{-9}$ |
|              | 3000  | $7.018 \times 10^{-7}$ | $1.447 \times 10^{-5}$ | $3.618 \times 10^{-9}$ |
|              | 4000  | $8.403 \times 10^{-7}$ | $1.931 \times 10^{-5}$ | $3.718 \times 10^{-9}$ |
| $10^{-12}$   | 1000  | $3.521 \times 10^{-10}$ | $4.813 \times 10^{-9}$ | $3.427 \times 10^{-12}$ |
|              | 2000  | $5.443 \times 10^{-10}$ | $9.642 \times 10^{-9}$ | $3.964 \times 10^{-12}$ |
|              | 3000  | $7.017 \times 10^{-10}$ | $1.447 \times 10^{-8}$ | $4.893 \times 10^{-12}$ |
|              | 4000  | $8.402 \times 10^{-10}$ | $1.931 \times 10^{-8}$ | $3.991 \times 10^{-12}$ |

5 Conclusion

In this paper, we analyze and further develop an inexact shift-and-invert Arnoldi method for the problem of numerical approximation to the product of Toeplitz matrix exponential with a vector. First, we give an improved stability analysis on the Gohberg-Semencul formula (GSF) for the inverse of a Toeplitz matrix, and our result is independent of the size of the matrix in question. Moreover, we define the “GSF condition number” of a Toeplitz matrix. An advantage is that we can evaluate the “classical” condition number and the effective condition numbers of a Toeplitz matrix via solving Toeplitz systems, with no need to form the Toeplitz inverse explicitly. Second, we establish a relation between the error in approximating Toeplitz systems and the residual of its matrix exponential. Third, we provide a practical stopping criterion for the accuracy in approximating the Toeplitz systems in the inexact shift-and-invert Arnoldi algorithm for Toeplitz matrix exponential. It is shown that if the 1-norm “GSF condition number” $\kappa_1^{GSF}(I + \gamma A)$ is medium sized, then the Toeplitz systems can be solved in a relatively low accuracy.

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