# Fast computation of the matrix exponential for a Toeplitz matrix 

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#### Abstract

The computation of the matrix exponential is a ubiquitous operation in numerical mathematics, and for a general, unstructured $n \times n$ matrix it can be computed in $\mathcal{O}\left(n^{3}\right)$ operations. An interesting problem arises if the input matrix is a Toeplitz matrix, for example as the result of discretizing integral equations with a time invariant kernel. In this case it is not obvious how to take advantage of the Toeplitz structure, as the exponential of a Toeplitz matrix is, in general, not a Toeplitz matrix itself. The main contribution of this work are fast algorithms for the computation of the Toeplitz matrix exponential. The algorithms have provable quadratic complexity if the spectrum is real, or sectorial, or more generally, if the imaginary parts of the rightmost eigenvalues do not vary too much. They may be efficient even outside these spectral constraints. They are based on the scaling and squaring framework, and their analysis connects classical results from rational approximation theory to matrices of low displacement rank. As an example, the developed methods are applied to Merton's jump-diffusion model for option pricing.


## 1 Introduction

Let us consider an $n \times n$ Toeplitz matrix

$$
T=\left[\begin{array}{cccc}
t_{0} & t_{-1} & \cdots & t_{-n+1}  \tag{1}\\
t_{1} & t_{0} & \ddots & \vdots \\
\vdots & \ddots & \ddots & t_{-1} \\
t_{n-1} & \cdots & t_{1} & t_{0}
\end{array}\right]
$$

In this work, we propose a new class of fast algorithms for computing a highly accurate approximation of the matrix exponential $\exp (T)$. An important source of applications for $\exp (T)$ arises from the discretization of integro-differential equations with a shift-invariant kernel. Such equations play a central role in, e.g., the pricing of single-asset options modelled by jump-diffusion processes [5, 28]. The related problem of computing the exponential of a block Toeplitz matrix appears in the Erlangian approximation of Markovian fluid queues [3].

It is well known that the multiplication of a Toeplitz matrix with a vector can be implemented in $\mathcal{O}(n \log n)$ operations, using the FFT. This suggests the use of a Krylov subspace method, such as the Lanczos method, for computing the product of $\exp (T)$ with a vector $b$; see, e.g., [23]. For a matrix $T$ of large norm, the Krylov subspace method can be expected to converge slowly [15]. In this case, the use of rational Krylov subspace methods is advisable. For example, Lee, Pang, and Sun 20 have suggested a shift-and-invert Arnoldi method for approximating $\exp (T) b$. Every step of this method requires the solution of a linear system

[^0]with a Toeplitz matrix. The fast and superfast solution of such linear systems has received broad attention in the literature; we refer to [12, [19, 24, [25] for overviews. Recent work in this direction includes an algorithm based on a combination of rank structured matrices and randomized sampling 31.

If, additionally, $T$ is upper triangular then $T^{2}$ and, more generally, any matrix function of $T$ is again an upper triangular Toeplitz matrix. This very desirable property allows for the design of efficient algorithms that directly aim at the computation of generators for $\exp (T)$; see [3] and the references therein. It is important to note that this property does not extend to general Toeplitz matrices.

The approach proposed in this work is different from existing approaches, because it aims at approximating the full matrix exponential $\exp (T)$, instead of $\exp (T) b$, and it does not impose additional structure on $T$. Our approach is based on a combination of the scaling and squaring method for the matrix exponential of unstructured matrices [10, 13, 14] with approximations of low displacement rank [19. Specifically, we show that the displacement rank of a rational function of $T$ is bounded by the degree of the rational function. In turn, we obtain an approximate representation of $\exp (T)$, which requires $\mathcal{O}(n)$ storage under suitable assumptions and allows to conveniently multiply $\exp (T)$ with a vector in $\mathcal{O}(n \log n)$ operations. The latter property is particularly interesting in option pricing; it allows for quickly evaluating prices for times to maturity that are integer multiplies of a fixed time period. The availability of an approximation to the full matrix exponential also allows us to quickly access parts of that matrix. For example, the diagonal entries can be computed in $\mathcal{O}(n)$ operations, which would be significantly more expensive using Krylov subspace methods.

## 2 Toeplitz matrices

In this section, we recall and establish basic properties of Toeplitz matrices needed for our developments. Following [18], we define the displacement $\nabla_{F}(A)$ of $A \in \mathbb{C}^{n \times n}$ with respect to $F \in \mathbb{C}^{n \times n}$ as

$$
\nabla_{F}(A):=A-F A F^{*}
$$

We will mostly use the downward shift matrix for $F$, in which case we omit the subscript:

$$
\nabla(A)=A-Z A Z^{*}, \quad Z=\left[\begin{array}{cccc}
0 & & & \\
1 & 0 & & \\
& \ddots & \ddots & \\
& & 1 & 0
\end{array}\right]
$$

The rank of $\nabla(A)$ is called the displacement rank of $A$. Toeplitz matrices have displacement rank at most two. Matrices of "small" displacement rank are often called Toeplitz-like matrices. Given an invertible matrix $A$ with $\operatorname{rank}(\nabla(A)) \leq r$, it follows that $\operatorname{rank}\left(\nabla\left(A^{-1}\right)\right) \leq$ $r+2$. More generally, any Schur complement of $A$ has bounded displacement rank, see 18 , Thm. 2.2]. These displacement rank properties are discussed with great detail in Section 3.1.

It follows that the inverse of a Toeplitz matrix $T$ has displacement rank at most 2. This property does not extend to general matrix functions of $T$. In particular, $\exp (T)$ usually has full displacement rank. However, as we will see below in Section 3.2, it turns out that matrix functions of $T$ can often be well approximated by a matrix of low displacement rank.

### 2.1 Generators, reconstruction, and fast matrix-vector products

For $r \geq \operatorname{rank}(\nabla(A))$, there are matrices $G, B \in \mathbb{C}^{n \times r}$ such that

$$
\begin{equation*}
\nabla(A)=A-Z A Z^{*}=G B^{*} \tag{2}
\end{equation*}
$$

We call such a pair $(G, B)$ a generator for $A$. Note that $A$ admits many generators and $(G, B)$ is called a minimal generator for $A$ if $r=\operatorname{rank}(\nabla(A))$. A generator for the Toeplitz matrix (1) is given by

$$
G=\left[\begin{array}{cc}
t_{0} & 1  \tag{3}\\
t_{1} & 0 \\
\vdots & \vdots \\
t_{n-1} & 0
\end{array}\right], \quad B=\left[\begin{array}{cc}
1 & 0 \\
0 & \bar{t}_{-1} \\
\vdots & \vdots \\
0 & \bar{t}_{-n+1}
\end{array}\right]
$$

Fast algorithms for Toeplitz-like matrices operate directly on the generator of $A$ instead of $A$ itself. When needed, the full matrix can be reconstructed from the generators by noting that (2) is a matrix Stein equation admitting the unique solution

$$
\begin{equation*}
A=\mathcal{T}(G, B):=\sum_{k=0}^{n-1} Z^{k} G B^{*}\left(Z^{*}\right)^{k} \tag{4}
\end{equation*}
$$

Letting $g_{j}, b_{j} \in \mathbb{C}^{n}$ for $j=1, \ldots, r$ denote the columns of $G, B$, we can rewrite (4) as

$$
\begin{equation*}
A=\mathcal{T}(G, B)=L\left(g_{1}\right) U\left(b_{1}^{*}\right)+L\left(g_{2}\right) U\left(b_{2}^{*}\right)+\cdots+L\left(g_{r}\right) U\left(b_{r}^{*}\right), \tag{5}
\end{equation*}
$$

with the triangular Toeplitz matrices

$$
L(x):=\left[\begin{array}{cccc}
x_{1} & 0 & \cdots & 0 \\
x_{2} & x_{1} & \ddots & \vdots \\
\vdots & \ddots & \ddots & 0 \\
x_{n} & \cdots & x_{2} & x_{1}
\end{array}\right], \quad U(x):=\left[\begin{array}{cccc}
x_{1} & x_{2} & \cdots & x_{n} \\
0 & x_{1} & \ddots & \vdots \\
\vdots & \ddots & \ddots & x_{2} \\
0 & \cdots & 0 & x_{1}
\end{array}\right]
$$

Using the Fast Fourier Transform (FFT), the matrix-vector product with a Toeplitz matrix can be done in $O(n \log n)$ operations; see, e.g., [2, Sec. 10.2.3]. In turn, (5) shows that the multiplication of $A$ with a vector can be computed in $O(r n \log n)$ operations; see 19, Chap. 1] for more details.

### 2.2 Generator Truncation

Operations like matrix addition or multiplication typically increase the displacement rank of Toeplitz-like matrices. Even worse, the result of such operations may lead to non-minimal, that is, rank deficient generators with many more columns than necessary. To limit this increase in generator size, we will truncate the singular values of the generators. The following results justify our procedure.
Lemma 2.1. The displacement $\nabla(A)$ for $A \in \mathbb{C}^{n \times n}$ satisfies

$$
\frac{1}{2}\|\nabla(A)\|_{*} \leq\|A\|_{*} \leq n\|\nabla(A)\|_{*}
$$

where $\|\cdot\|_{*}$ denotes any unitarily invariant norm.
Proof. Note that $\left\|Z^{k}\right\|_{2}=1$ for $0 \leq k<n$. The first inequality follows directly from the definition of the displacement operator, viz.

$$
\|\nabla(A)\|_{*}=\left\|A-Z A Z^{*}\right\|_{*} \leq\|A\|_{*}+\|Z\|_{2}\|A\|_{*}\|Z\|_{2} \leq 2\|A\|_{*}
$$

For the second inequality we compute from (4) that

$$
\|A\|_{*} \leq \sum_{k=0}^{n-1}\left\|Z^{k} \nabla(A)\left(Z^{*}\right)^{k}\right\|_{2} \leq \sum_{k=0}^{n-1}\left\|Z^{k}\right\|_{2}\|\nabla(A)\|_{*}\left\|\left(Z^{*}\right)^{k}\right\|_{2}=n\|\nabla(A)\|_{*}
$$

The bounds of Lemma 2.1 may not be sharp. In particular, one may question whether the factor $n$ of the upper bound is necessary. The following example shows that this linear dependence on $n$ can, in general, not be removed.

Example 2.2. Let $g=[1,1, \ldots, 1]^{*} \in \mathbb{R}^{n}$ and $A=\mathcal{T}\left(g g^{*}\right)$. Then the kth entry of $f=A g$ is given by $f(k)=k n-k(k-1) / 2$. Since $f$ is monotonically increasing, this allows us to estimate

$$
\|f\|_{2}^{2}=\sum_{k=1}^{n} f(k)^{2} \geq \int_{0}^{n} f(k)^{2} \mathrm{~d} k \geq \frac{2}{15} n^{5} .
$$

In turn,

$$
\|A\|_{2} \geq \frac{\|A g\|_{2}}{\|g\|_{2}} \geq \sqrt{\frac{2}{15}} n^{2}=\sqrt{\frac{2}{15}} n\|\nabla(A)\|_{2}
$$

which shows that $\|A\|_{2} /\|\nabla(A)\|_{2}$ grows linearly with $n$.
Lemma 2.1 allows us to analyze the effect of generator truncation in terms of the approximation error.
Theorem 2.3. Let $A \in \mathbb{C}^{n \times n}$ be a Toeplitz-like matrix of displacement rank $r$ and consider the singular value decomposition (SVD)

$$
\nabla(A)=U \Sigma V^{*}=\left[\begin{array}{ll}
U_{1} & U_{2}
\end{array}\right]\left[\begin{array}{cc}
\Sigma_{1} & 0 \\
0 & \Sigma_{2}
\end{array}\right]\left[\begin{array}{l}
V_{1}^{*} \\
V_{2}^{*}
\end{array}\right]
$$

where $\Sigma_{1} \in \operatorname{diag}\left(\sigma_{1}, \ldots, \sigma_{\tilde{r}}\right)$ and $\Sigma_{2}=\operatorname{diag}\left(\sigma_{\tilde{r}+1}, \ldots, \sigma_{r}\right)$. Letting $\tilde{A}=\mathcal{T}\left(U_{1} \Sigma_{1}, V_{1}\right)$, it holds that

$$
\begin{equation*}
\|A-\tilde{A}\|_{2} \leq n \sigma_{\tilde{r}+1} \quad \text { and } \quad\|A-\tilde{A}\|_{F} \leq n \sqrt{\sigma_{\tilde{r}+1}^{2}+\cdots+\sigma_{r}^{2}} \tag{6}
\end{equation*}
$$

Proof. By linearity of the displacement operator $\nabla$ we find

$$
\nabla(A-\tilde{A})=\nabla(A)-\nabla(\tilde{A})=U \Sigma V^{*}-U_{1} \Sigma_{1} V_{1}^{*}=U_{2} \Sigma_{2} V_{2}^{*}
$$

Hence, the claimed bounds follow from applying Lemma 2.1 to $A-\tilde{A}$.
Note that (6) improves upon a result by Pan [26, Eq. (3.5)].
We will use the construction of Theorem 2.3 to compress a generator $(G, B)$ with $G, B \in$ $\mathbb{C}^{n \times r}$ to a generator $(\tilde{G}, \tilde{B})$ with $\tilde{G}, \tilde{B} \in \mathbb{C}^{n \times \tilde{r}}$ and $\tilde{r}<r$. By (6), the singular values of $G B^{*}$ allow us to quantify the compression error and choose $\tilde{r}$ adaptively. In the particular case of a non-minimal (rank deficient) generator $(G, B)$ with $r>\tilde{r}=\operatorname{rank}\left(G B^{*}\right)$, the construction returns an exact minimal generator. Typically we have $r \ll n$, in which case the cost greatly reduces from $\mathcal{O}\left(n^{3}\right)$ FLOPs for computing the SVD of $G B^{*}$ to $\mathcal{O}\left(r^{2} n+r^{3}\right)$ FLOPs by first computing thin QR decompositions of $G$ and $B$. This well-known procedure is summarized in Algorithm

```
Algorithm 1 Generator Compression
Input: Generator matrices \(G, B \in \mathbb{C}^{n \times r}\), integer \(\tilde{r}<r\).
Output: Generator matrices \(\tilde{G}, \tilde{B} \in \mathbb{C}^{n \times \tilde{r}}\) such that \(\mathcal{T}(G, B) \approx \mathcal{T}(\tilde{G}, \tilde{B})\).
    1: Compute thin QR factorizations \(Q_{G} R_{G}=G\) and \(Q_{B} R_{B}=B\)
    Compute \(S=R_{G} R_{B}^{*} \in \mathbb{C}^{r \times r}\)
    Compute truncated SVD \(U_{1} \Sigma_{1} Y_{1}^{*} \approx S\) with \(\Sigma_{1} \in \mathbb{R}^{\tilde{r} \times \tilde{r}}\)
    Set \(\tilde{G}=Q_{G} X_{1} \Sigma_{1}^{\frac{1}{2}}\) and \(\tilde{B}=Q_{B} Y_{1} \Sigma_{1}^{\frac{1}{2}}\)
```

Generators are not uniquely determined. For every $Z \in \mathrm{GL}_{r}(\mathbb{C})$, the generators $(G, B)$ and $\left(G Z, B Z^{-*}\right)$ correspond to the same Toeplitz-like matrix. The following lemma shows that this relation in fact characterizes the set of all minimal generators.

Lemma 2.4. Let $A \in \mathbb{C}^{n \times n}$ be a Toeplitz-like matrix of displacement rank $r$, and let $\left(G_{1}, B_{1}\right),\left(G_{2}, B_{2}\right)$ be two minimal generators for $A$. Then there exists a matrix $Z \in \mathrm{GL}_{r}(\mathbb{C})$ such that $G_{1}=G_{2} Z$ and $B_{1}=B_{2} Z^{-*}$.
Proof. By minimality of the generators all of $G_{i}$ and $B_{i}, i=1,2$, have full rank. Hence $G_{1}$ is right-equivalent to $G_{2}$, and $B_{1}$ is right-equivalent to $B_{2}$, i.e., there exist $Z, W \in \mathrm{GL}_{r}(\mathbb{C})$ such that $G_{1}=G_{2} Z$ and $B_{1}=B_{2} W$. But then

$$
G_{2} B_{2}^{*}=G_{1} B_{1}^{*}=G_{2} Z W^{*} B_{2}^{*}
$$

so $G_{2}\left(I-Z W^{*}\right) B_{2}^{*}=0$. Since $G_{2}$ and $B_{2}$ have full rank it follows that $W=Z^{-*}$.

## 3 Bounds on the displacement rank of functions of Toeplitz matrices

The scaling and squaring method [13, chap. 10] for the evaluation of $\exp (T)$ takes three phases: First, the matrix $T$ is scaled by a power of two, then a Pade approximant of the scaled matrix is computed, and in a third step, the approximant is repeatedly squared in order to undo the initial scaling. In the context of Toeplitz matrices, the main challenge is to control the growth of the displacement rank in the second and third phase.

### 3.1 Polynomial and rational functions of Toeplitz matrices

In the following, we analyze the impact of various operations on the displacement rank of Toeplitz-like matrices and provide explicit expressions for the resulting generators. The following result is a variation of the well-known result that Schur complements do not increase the displacement rank.
Lemma 3.1 (Generator block update). Consider $M=\left[\begin{array}{cc}D & U \\ L & M_{1}\end{array}\right] \in \mathbb{C}^{n \times n}$ with $D \in \mathbb{C}^{k \times k}$ invertible and

$$
\nabla_{F}(M)=G B^{*}, \quad G, B \in \mathbb{C}^{n \times r}
$$

for a strictly lower triangular matrix $F$. Let us partition $F=\left[\begin{array}{cc}\hat{F} & 0 \\ \star & F_{1}\end{array}\right]$ with $\hat{F} \in \mathbb{C}^{k \times k}$, $F_{1} \in \mathbb{C}^{(n-k) \times(n-k)}$, and $G=\left[\begin{array}{c}\hat{G} \\ \star\end{array}\right], B=\left[\begin{array}{c}\hat{B} \\ \star\end{array}\right]$ with $\hat{G}, \hat{B} \in \mathbb{C}^{k \times r}$ ( $\star$ is used as a placeholder referring to an arbitrary block). Then the Schur complement of $D$ in $M$ satisfies

$$
\nabla_{F_{1}}\left(M_{1}-L D^{-1} U\right)=G_{1} B_{1}^{*}
$$

where the generator matrices $G_{1}, B_{1} \in \mathbb{R}^{(n-k) \times r}$ are defined by the relations

$$
\begin{align*}
& {\left[\begin{array}{c}
0 \\
G_{1}
\end{array}\right]=G+\left(F-I_{n}\right)\left[\begin{array}{l}
D \\
L
\end{array}\right] D^{-1}\left(I_{k}-\hat{F}\right)^{-1} \hat{G}}  \tag{7}\\
& {\left[\begin{array}{c}
0 \\
B_{1}
\end{array}\right]=B+\left(F-I_{n}\right)\left[\begin{array}{l}
D^{*} \\
U^{*}
\end{array}\right] D^{-*}\left(I_{k}-\hat{F}\right)^{-1} \hat{B}} \tag{8}
\end{align*}
$$

Proof. The result is a direct extension of [29, Alg. 3.3] from the Hermitian to the nonHermitian case.

It is well known that the displacement rank of the product $T_{1} T_{2}$ of two Toeplitz matrices $T_{1}, T_{2}$ is at most 4 [17, Example 2]. The following theorem extends this result to Toeplitz-like matrices.

Theorem 3.2. Let $A_{1}, A_{2} \in \mathbb{C}^{n, n}$ be two Toeplitz-like matrices of displacement ranks $r_{1}, r_{2}$ with generators $\left(G_{1}, B_{1}\right)$ and $\left(G_{2}, B_{2}\right)$, respectively. Then $A_{1} A_{2}$ is a Toeplitz-like matrix of displacement rank at most $r_{1}+r_{2}+1$, and a generator $(G, B)$ for $A_{1} A_{2}$ is given by

$$
\begin{aligned}
& G=\left[\begin{array}{lll}
(Z-I) A_{1}(Z-I)^{-1} G_{2} & G_{1} & -(Z-I) A_{1}(Z-I)^{-1} e_{1}
\end{array}\right] \\
& B=\left[\begin{array}{lll}
B_{2} & (Z-I) A_{2}^{*}(Z-I)^{-1} B_{1} & (Z-I) A_{2}^{*}(Z-I)^{-1} e_{1}
\end{array}\right]
\end{aligned}
$$

where $e_{1} \in \mathbb{R}^{n}$ denotes the first unit vector. If, additonally, $e_{1} \in \operatorname{ran}\left(G_{2}\right) \cup \operatorname{ran}\left(B_{1}\right)$ then $A_{1} A_{2}$ has displacement rank at most $r_{1}+r_{2}$.

Proof. Consider the matrix

$$
M=\left[\begin{array}{cc}
-I & A_{2} \\
A_{1} & 0
\end{array}\right]
$$

and set $F=Z \oplus Z$. One computes that

$$
\nabla_{F}(M)=M-F M F^{*}=\left[\begin{array}{cc}
-e_{1} e_{1}^{*} & G_{2} B_{2}^{*} \\
G_{1} B_{1}^{*} & 0
\end{array}\right]=\left[\begin{array}{ccc}
G_{2} & 0 & -e_{1} \\
0 & G_{1} & 0
\end{array}\right]\left[\begin{array}{cc}
0 & B_{2}^{*} \\
B_{1}^{*} & 0 \\
e_{1}^{*} & 0
\end{array}\right]
$$

Since $A_{1} A_{2}$ is the Schur complement of $-I$ in $M$, Lemma 3.1 implies that $A_{1} A_{2}$ has displacement rank at most $r_{1}+r_{2}+1$. Moreover, by (7)-(8), a generator $(G, B)$ for $A_{1} A_{2}$ is given by

$$
\begin{aligned}
G & =\left[\begin{array}{lll}
0 & G_{1} & 0
\end{array}\right]+(Z-I) A_{1}(Z-I)^{1}\left[\begin{array}{lll}
G_{2} & 0 & -e_{1}
\end{array}\right] \\
& =\left[\begin{array}{lll}
(Z-I) A_{1}(Z-I)^{-1} G_{2} & G_{1} & -(Z-I) A_{1}(Z-I)^{-1} e_{1}
\end{array}\right] \\
B & =\left[\begin{array}{lll}
B_{2} & 0 & 0
\end{array}\right]+(Z-I) A_{2}^{*}(Z-I)^{-1}\left[\begin{array}{lll}
0 & B_{1} & e_{1}
\end{array}\right] \\
& =\left[\begin{array}{lll}
B_{2} & (Z-I) A_{2}^{*}(Z-I)^{-1} B_{1} & (Z-I) A_{2}^{*}(Z-I)^{-1} e_{1}
\end{array}\right] .
\end{aligned}
$$

Note that at least one of these matrices becomes rank deficient if $e_{1} \in \operatorname{ran}\left(G_{2}\right) \cup \operatorname{ran}\left(B_{1}\right)$, which shows the second part of the theorem.

Because of (3), the additional condition of Theorem 3.2 is satisfied for Toeplitz matrices. An analogous condition plays a role in controlling the displacement rank for the inverse of a Toeplitz-like matrix.

Theorem 3.3. Let $A$ be an invertible Toeplitz-like matrix of displacement rank $r$ with generator $(G, B)$. Then $A^{-1}$ is a Toeplitz-like matrix of displacement rank at most $r+2$, and a generator $(\tilde{G}, \tilde{B})$ is given through

$$
\begin{aligned}
\tilde{G} & =\left[\begin{array}{lll}
-(Z-I) A^{-1}(Z-I)^{-1} G & (Z-I) A^{-1}(Z-I)^{-1} e_{1} & e_{1}
\end{array}\right], \\
\tilde{B} & =\left[\begin{array}{lll}
(Z-I) A^{-*}(Z-I) B & e_{1} & (Z-I) A^{-*}(Z-I) e_{1}
\end{array}\right] .
\end{aligned}
$$

If, additionally, $e_{1} \in \operatorname{ran}(G) \cup \operatorname{ran}(B)$ then $A^{-1}$ has displacement rank at most $r+1$.
Proof. The result follows from applying the technique from the proof of Theorem 3.2 to the embedding $M=\left[\begin{array}{cc}-A & I \\ I & 0\end{array}\right]$, which has the generator $\hat{G}=\left[\begin{array}{ccc}G & 0 & e_{1} \\ 0 & e_{1} & 0\end{array}\right], \hat{B}=\left[\begin{array}{ccc}B & e_{1} & 0 \\ 0 & 0 & e_{1}\end{array}\right]$. The second part follows from the observation that at least one of $\hat{G}, \hat{B}$ has at most rank $r+1$ if $e_{1} \in \operatorname{ran}(G) \cup \operatorname{ran}(B)$.

Remark 3.4. We remark that the special shape (3) of $B, G$ for a Toeplitz matrix $T$ imply that the matrix $\hat{G} \hat{B}^{*}$ in the proof of Theorem 3.3 has rank $\leq 2$ and, in turn, the displacement rank of $T^{-1}$ is $\leq 2$. In fact, letting $(G, B)=\left(\left[g e_{1}\right],\left[e_{1} b\right]\right)$ denote the generator (33) for $T$, the matrices

$$
\begin{aligned}
& \hat{G}=\left[\begin{array}{ll}
e_{1} & 0
\end{array}\right]+(Z-I) T^{-1}(Z-I)^{-1}\left[\begin{array}{ll}
-g & e_{1}
\end{array}\right], \\
& \hat{B}=\left[\begin{array}{ll}
0 & e_{1}
\end{array}\right]+(Z-I) T^{-*}(Z-I)^{-1}\left[\begin{array}{ll}
e_{1} & -b
\end{array}\right]
\end{aligned}
$$

constitute a generator for $T^{-1}$. This result is well known and a corollary of Lemma 3.1.
While Theorems 3.2 and 3.3 are variations of well-known results, we are not aware of existing results on the displacement ranks of powers and polynomials of Toeplitz matrices analyzed in the following.

Lemma 3.5. Let $T$ be a Toeplitz matrix. Then $T^{s}$ is a Toeplitz-like matrix of displacement rank at most $2 s$ for any integer $s \geq 1$. Letting $(G, B)$ denote a generator for $T$, a sequence of (non-minimal) generators $\left(G_{1}, B_{1}\right), \ldots,\left(G_{s}, B_{s}\right)$ for $T, T^{2}, \ldots, T^{s}$ is given by

$$
\begin{align*}
G_{1}=G, & G_{i+1}=\left[\begin{array}{lllllll}
P_{G}^{i} G & P_{G}^{i-1} G & \ldots & G & -P_{G} e_{1} & \ldots & -P_{G}^{i} e_{1}
\end{array}\right]  \tag{9}\\
B_{1}=B, & B_{i+1}
\end{align*}=\left[\begin{array}{lllllll}
B & P_{B} B & \ldots & P_{B}^{i} B & P_{B}^{i} e_{1} & \ldots & P_{B} e_{1} \tag{10}
\end{array}\right], ~ l
$$

for $i=1, \ldots, s-1$, where $P_{G}:=(Z-I) T(Z-I)^{-1}$ and $P_{B}:=(Z-I) T^{*}(Z-I)^{-1}$. Moreover,

$$
\begin{equation*}
e_{1} \in \operatorname{ran}\left(G_{1}\right) \subset \cdots \subset \operatorname{ran}\left(G_{s}\right) \quad \text { and } \quad e_{1} \in \operatorname{ran}\left(B_{1}\right) \subset \cdots \subset \operatorname{ran}\left(B_{s}\right) . \tag{11}
\end{equation*}
$$

Proof. The proof is by induction on $i$. For $G_{1}, B_{1}$, the claim (11) follows directly from the expression (3) for the generator of $T$.

Now assume that (9)-(11) hold for all $G_{i}, B_{i}$ with $i<s$. Invoking Theorem 3.2 with $T_{1}=T^{i}$ and $T_{2}=T$ yields the formulas (9)-(10). Further, since all columns of $G_{i}$ and $B_{i}$ are also columns of $G_{i+1}$ and $B_{i+1}$, respectively, we directly obtain $\operatorname{ran}\left(G_{i}\right) \subset \operatorname{ran}\left(G_{i+1}\right)$ and $\operatorname{ran}\left(B_{i}\right) \subset \operatorname{ran}\left(B_{i+1}\right)$.

Finally, since $e_{1} \in \operatorname{ran}(G)$, each of the last $i$ columns of $G_{i+1}$ and $B_{i+1}$ is a linear combination of one of the first $i+1$ block columns. In turn,

$$
\begin{aligned}
& \operatorname{ran}\left(G_{i+1}\right)=\operatorname{ran}\left(\left[\begin{array}{llll}
P_{G}^{i} G & P_{G}^{i-1} G & \ldots & G
\end{array}\right]\right), \\
& \operatorname{ran}\left(B_{i+1}\right)=\operatorname{ran}\left(\left[\begin{array}{llll}
B & P_{B} B & \ldots & P_{B}^{i} B
\end{array}\right]\right),
\end{aligned}
$$

which implies $\operatorname{rank}\left(G_{i+1}\right) \leq 2(i+1)$ and $\operatorname{rank}\left(B_{i+1}\right) \leq 2(i+1)$. In particular, the displacement rank of $T^{i+1}$ is at most $2(i+1)$.

Theorem 3.6. Let $T$ be a Toeplitz matrix and $p \in \mathcal{P}_{s}$, where $\mathcal{P}_{s}$ denotes the set of polynomials of degree at most s. Then $p(T)$ is a Toeplitz-like matrix of displacement rank at most $2 s$.

Proof. Let $p=\sum_{i=0}^{s} a_{k} z^{k}$ and consider the generators $\left(G_{i}, B_{i}\right), 1 \leq i \leq s$, for the monomials $T^{i}$ constructed in (19)-(10). Setting $G_{0}:=B_{0}:=e_{1}$ and using the linearity of the displacement operator $\nabla$ we obtain

$$
\nabla(p(T))=\sum_{i=0}^{s} a_{i} \nabla\left(T^{i}\right)=\sum_{i=0}^{s} a_{i} G_{i} B_{i}^{*}=\left[\begin{array}{llll}
a_{0} e_{1} & a_{1} G_{1} & \ldots & a_{s} G_{s}
\end{array}\right]\left[\begin{array}{c}
e_{1}^{*} \\
B_{1}^{*} \\
\vdots \\
B_{s}^{*}
\end{array}\right]=: G_{p} B_{p}^{*}
$$

It follows from (11) that $\operatorname{rank}\left(G_{p}\right)=\operatorname{rank}\left(G_{s}\right) \leq 2 s, \operatorname{rank}\left(B_{p}\right)=\operatorname{rank}\left(B_{s}\right) \leq 2 s$, and hence $\operatorname{rank}(\nabla(p(T))) \leq 2 s$ 。

The following theorem is the main result of this section and quantifies the effect of a rational function on the displacement rank. It shows that the displacement rank grows at most linearly with the degree of the rational function, defined as the maximal degree of the numerator and denominator.

Theorem 3.7. Let $T$ be a Toeplitz matrix, and let $p \in \mathcal{P}_{s_{p}}, q \in \mathcal{P}_{s_{q}}$ be such that $q(T)$ is invertible. Let $\left(G_{p}, B_{p}\right)$ and $\left(G_{q}, B_{q}\right)$ denote generators of $p(T)$ and $q(T)$, respectively. Then $r(T)=\frac{p(T)}{q(T)}$ is a Toeplitz-like matrix of displacement rank at most $2 \max \left\{s_{p}, s_{q}\right\}+1$, and a generator is given by

$$
\begin{align*}
G & =\left[\begin{array}{llll}
-(Z-I) q(T)^{-1}(Z-I)^{-1} G_{q} & (Z-I) q(T)^{-1}(Z-I)^{-1} G_{p} & e_{1},
\end{array}\right]  \tag{12}\\
B & =\left[\begin{array}{llll}
(Z-I) p(T)^{*} q(T)^{-*}(Z-I)^{-1} B_{q} & B_{p} & (Z-I) p(T)^{*} q(T)^{-*}(Z-I)^{-1} e_{1}
\end{array}\right] . \tag{13}
\end{align*}
$$

Proof. The Schur complement of the leading diagonal block in the embedding $M=\left[\begin{array}{cc}-q(T) & p(T) \\ I\end{array}\right]$, is $q(T)^{-1} p(T)$, and setting $F=Z \oplus Z$ one computes

$$
M-F M F^{*}=\left[\begin{array}{cc}
-G_{q} B_{q}^{*} & G_{p} B_{p}^{*}  \tag{14}\\
e_{1} e_{1}^{*} & 0
\end{array}\right]=\left[\begin{array}{ccc}
-G_{q} & G_{p} & 0 \\
0 & 0 & e_{1}
\end{array}\right]\left[\begin{array}{cc}
B_{q}^{*} & 0 \\
0 & B_{p}^{*} \\
e_{1}^{*} & 0
\end{array}\right] .
$$

The formulas (12) and (13) are obtained by applying Lemma 3.1.
To see that the matrix (14) has rank at most $2 \max \left\{s_{p}, s_{q}\right\}+1$, we recall from (11) that the ranges of the generator matrices for monomials are nested and thus Theorem 3.6 implies $\operatorname{rank}\left[-G_{q} G_{p}\right] \leq 2 \max \left\{s_{p}, s_{q}\right\}$.

### 3.2 Low displacement rank approximation of matrix exponential

If the singular values of a matrix are rapidly decaying, the limits of finite precision arithmetic effect that the numerical rank of the matrix is smaller than its rank. In order to formulate quantitative statements involving the numerical rank, we use the following notion of $\varepsilon$-rank.

Definition 3.8. Let $A \in \mathbb{C}^{n, n}$ and $\varepsilon>0$. We say that $A$ has $\varepsilon$-rank $k$, if

$$
\min _{B \in \mathbb{C}^{n}, n}\left\{\|A-B\|_{2}: \operatorname{rank}(B) \leq k\right\} \leq \varepsilon
$$

or, equivalently, if the $k+1$ st singular value of $A$ does not exceed $\varepsilon$. The matrix $A$ is said to have $\varepsilon$-displacement rank $k$, if $\nabla(A)$ has $\varepsilon$-rank $k$.

Theorem 3.6 allows us to derive a priori bounds on the numerical displacement rank of $\exp (T)$, using rational approximations of the exponential function. To see this, let us first recall a seminal result by Gonchar and Rakhmanov [7].

Theorem 3.9. There is a constant $C$ such that

$$
\inf _{p_{1}, p_{2} \in \mathcal{P}_{s}} \max _{\lambda \in(-\infty, 0]}\left|e^{\lambda}-p_{1}(\lambda) / p_{2}(\lambda)\right| \leq C V^{-s}
$$

holds for all $s \geq 1$ with $V \approx 9.28903 \ldots$
Corollary 3.10. Let $T \in \mathbb{C}^{n, n}$ be a diagonalizable Toeplitz matrix with all eigenvalues real and contained in $(-\infty, \mu]$ for some $\mu \in \mathbb{R}$. Then

$$
\min \left\{\|\exp (T)-A\|_{2}: \operatorname{rank}(\nabla(A)) \leq 2 s+1\right\} \leq \tilde{C} V^{-s},
$$

for $\tilde{C}=\kappa(X) e^{\mu} C$, where $C, V$ are as in Theorem 3.9 and $\kappa(X)$ is the condition number of a matrix $X$ such that $X^{-1} T X$ is diagonal.

Proof. According to Theorem 3.7 the matrix $A=e^{\mu} p_{2}(T)^{-1} p_{1}(T)$ with $p_{1}, p_{2} \in \mathcal{P}_{s}$ has displacement rank at most $2 s+1$. From

$$
\begin{aligned}
\|\exp (T)-A\|_{2} & =\|\exp (\mu I) \exp (T-\mu I)-A\|_{2} \\
& \leq \kappa(X) e^{\mu} \max _{\lambda \in(-\infty, 0]}\left|e^{\lambda}-p_{1}(\lambda) / p_{2}(\lambda)\right|
\end{aligned}
$$

the result follows using Theorem 3.9.
Corollary 3.10 implies that the singular values of $\nabla(\exp (T))$ decay at least exponentially to zero, with a decay rate that does not deteriorate even if $T$ has very small eigenvalues. This property is retained by approximations to the matrix exponential.

Corollary 3.11. Under the assumptions of Corollary 3.10 , let $B \in \mathbb{C}^{n \times n}$ satisfy $\|B-\exp (T)\|_{2} \leq$ $\tau$ for $\tau \geq 0$. If $s$ is an integer such that

$$
\tilde{C} V^{-s} \leq \tau
$$

then $B$ has $2 \tau$-displacement rank $2 s+1$.
Proof. The result follows from the triangular inequality

$$
\|B-A\|_{2} \leq\|B-\exp (T)\|_{2}+\|\exp (T)-A\|_{2} \leq 2 \tau
$$

and Corollary 3.10.
The case of complex spectra is more difficult. A common approach to obtain rational approximations is to consider the contour integral representation

$$
\begin{equation*}
\exp (T)=\frac{1}{2 \pi \mathrm{i}} \int_{\Gamma} e^{z}(z I-T)^{-1} \mathrm{~d} z \tag{15}
\end{equation*}
$$

where $\Gamma$ is a contour enclosing the spectrum of $T$. Applying numerical quadrature with $s$ points to (15) yields an approximation $r(T) \approx \exp (T)$, where $r$ is a rational function of degree $s$ and hence $r(T)$ has displacement rank at most $2 s+1$ by Theorem 3.7. In the absence of information on the spectrum of $T$, one might choose $\Gamma$ to be a circle of radius larger than $\|T\|_{2}$. Applying the composite trapezoidal rule yields exponential convergence but the convergence rate deteriorates as $\|T\|_{2}$ grows; see, e.g., [30]. Sometimes, much better results can be obtained if more information on the spectrum is available. For example, if $A$ is sectorial (that is, its eigenvalues are contained in a sector strictly contained in the left half plane), López-Fernández et al. [21, Thm. 1] establish a bound of the form

$$
\|\exp (T)-r(T)\|_{2} \leq C \gamma^{s}
$$

where the rate $0<\gamma<1$ depends on the opening angle of the sector but not on the norm of $A$. The rational function $r$ has degree $s$ and is obtained by applying quadrature to (15) with $\Gamma$ chosen to be the left branch of a hyperbola. Analogous results hold for the case that the numerical range of $A$ is contained in the open left half complex plane; see [9, Sec. 4.2] for an overview.

If $T$ has large norm and eigenvalues on or close to the imaginary axis then it cannot be expected that $\exp (T)$ admits a good approximation of low displacement rank. In turn, the methods developed in this paper are not efficient, i.e., of quadratic complexity in $n$, for this type of matrices. The following example illustrates such a situation.
Example 3.12. Let $T \in \mathbb{R}^{2000 \times 2000}$ be a skew-symmetric Toeplitz matrix (11) with $t_{1}=1$, $t_{-1}=-1$ and all other entries zero. The following table shows the numerical displacement rank of $\exp (\alpha T)$, which we compute as the number of singular values of $\nabla(\exp (\alpha T))$ larger than $10^{-10}$ times the first singular value (see also Figure [1):

| $\alpha$ | 1 | 10 | 100 | 1000 |
| :---: | :---: | :---: | :---: | :---: |
| num. displacement rank | 11 | 29 | 153 | 1309 |

Clearly, as $\alpha$ grows it becomes increasingly difficult to approximate $\exp (\alpha T)$ by a Toeplitz-like matrix.

## 4 Algorithmic tools

In Section 5 we will adapt two variants of the scaling and squaring method for Toeplitz matrices. The algorithmic tools needed for an efficient implementation are the same for both, and we will describe them in this section without making reference to either algorithm.


Figure 1: Decay of the singular values of $\nabla(\exp (\alpha T))$ for $\alpha \in\{1,10,100,1000\}$ and the Toeplitz matrix $T$ from Example 3.12. The plots show the singular value ratios $\sigma_{j} / \sigma_{1}$ vs. $1 \leq j \leq 2000$ for each choice of $\alpha$.

### 4.1 Norm estimation and scaling

The first step of the scaling and squaring method consists of determining a scaling parameter $\rho \in \mathbb{N}$ such that $\left\|2^{-\rho} T\right\| \approx 1$, which necessitates computing $\|T\|$ or an estimate thereof.

Since matrix-vector products with a Toeplitz matrices can be carried out in $\mathcal{O}(n \log n)$ operations, the power method for estimating $\|T\|_{2}$ can be implemented with the same complexity per iteration. Alternatively, $\|T\|_{1}$ can be computed at little cost.

Lemma 4.1. Let $T \in \mathbb{C}^{n \times n}$ be a Toeplitz matrix. Then $\|T\|_{1}$ can be computed in $\mathcal{O}(n)$ operations.

Proof. Let us denote the first column and row of $T$ by $c$ and $r$, respectively, and set $\mu_{j}:=$ $\left\|T e_{j}\right\|_{1}, 1 \leq j \leq n$. From the structure of $T$ we find that

$$
\mu_{1}=\sum_{i=1}^{n}\left|c_{i}\right|, \quad \mu_{j+1}=\mu_{j}-\left|c_{n-j+1}\right|+\left|r_{j}\right| \text { for } 1 \leq j<n
$$

and hence $\|T\|_{1}=\max _{1 \leq j \leq n}\left\{\mu_{j}\right\}$ can be computed in $\mathcal{O}(n)$.
Once the scaling parameter $\rho$ is determined, the generator of $T$ is scaled accordingly, which obviously requires only $\mathcal{O}(n)$ operations.

### 4.2 Fast solution of Toeplitz and Toeplitz-like systems

In order to compute generators for rational functions of Toeplitz matrices, we need to solve linear systems of equations with Toeplitz and Toeplitz-like matrices; see Theorem 3.7. We will now briefly summarize a well established technique for the solution of such systems in quadratic time (the "GKO algorithm" [6).

Let $A \in \mathbb{C}^{n \times n}$ be a Toeplitz-like matrix of displacement rank $r \ll n$, so that $A$ satisfies the matrix Stein equation (2) with a low-rank right hand side. It is well known (see, e.g., [6, sec. 0.2] and the references therein) that $T$ also satisfies numerous other matrix equations, including the Sylvester equation

$$
\begin{equation*}
\Delta_{Z_{1}, Z_{-1}}(T):=Z_{1} T-T Z_{-1}=\tilde{G} \tilde{B}^{*} \tag{16}
\end{equation*}
$$

with low-rank right-hand side and $Z_{\delta}:=Z+\delta e_{1} e_{n}^{*}$.

One could directly apply the generalized Schur algorithm [18 to either representation (2) or (16) in order to solve linear systems with $A$ in $\mathcal{O}\left(r n^{2}\right)$ operations, but without further assumptions on $A$, such as well-conditioned leading principal submatrices, or more involved algorithmic techniques [4] a numerically stable solution is not guaranteed.

Instead, we propose to use a transformation [6, prop. 3.1] (see also [11) of (16) to a Cauchy-like Sylvester displacement equation

$$
\begin{equation*}
D_{1} C-C D_{2}=\hat{G} \hat{B}^{*} \tag{17}
\end{equation*}
$$

with the same displacement rank and where $D_{1}, D_{2}$ are diagonal matrices. The transformation between (16) and (17) involves only FFTs and diagonal scalings. The fact that the Sylvester operator matrices $D_{1}$ and $D_{2}$ are now diagonal allows for pivoting within the generalized Schur algorithm, requiring in total $\mathcal{O}\left(r n^{2}\right)$ operations. Combined with further safeguarding techniques one obtains an efficient algorithm for the solution of linear systems with $A$ that enjoys similar stability properties as traditional Gaussian elimination with pivoting [8].

For our purpose of evaluating rational matrix functions of Toeplitz matrices only one minor technicality needs to be resolved: The generator matrices $G, B$ with respect to the matrix Stein equation (21) need to be transformed to generator matrices with respect to the Sylvester equation (16). The following lemma shows that the corresponding displacement rank increases at most by two.

Lemma 4.2. Let $A \in \mathbb{C}^{n \times n}$ be a Toeplitz-like matrix, and let $\left[\begin{array}{c}c \\ \alpha\end{array}\right]$ and $\left[\begin{array}{rl}r \alpha\end{array}\right]$ denote its last column and row, respectively. If $T$ denotes the Toeplitz matrix with first column $\left[\begin{array}{c}\alpha \\ c\end{array}\right]$ and first row $[\alpha r]$ then

$$
\Delta_{Z_{1}, Z_{-1}}(A)=(\nabla(T)-\nabla(A)) Z_{-1}
$$

Proof. One directly calculates that

$$
\begin{aligned}
\Delta_{Z_{1}, Z_{-1}}(A) Z_{-1}^{*} & =Z_{1} A Z_{-1}^{*}-A=\left(Z+e_{1} e_{n}^{*}\right) A\left(Z^{*}-e_{n} e_{1}^{*}\right)-A \\
& =Z A Z^{*}-A+e_{1} e_{n}^{*} A Z^{*}-Z A e_{n} e_{1}^{*}-e_{1} e_{n}^{*} A e_{n} e_{1}^{*} \\
& =-\nabla(A)+\left[\begin{array}{cc}
\alpha & r \\
c & 0_{n-1, n-1}
\end{array}\right]=-\nabla(A)+\nabla(T) .
\end{aligned}
$$

To compute a $\Delta_{Z_{1}, Z_{-1}}$ generator for $A$ using Lemma 4.2, one needs to reconstruct the last column and row of $A$ from a generator with respect to $\nabla$. According to (5) this requires $2 r$ matrix-vector multiplications with triangular Toeplitz matrices and can hence be computed in $\mathcal{O}(r n \log n)$ operations. We can summarize the preceding discussion as follows.

Corollary 4.3. Let $A \in \mathbb{C}^{n \times n}$ be a Toeplitz-like matrix of displacement rank $r$. Then linear systems with $A$ can be solved in $\mathcal{O}\left(r n^{2}\right)$ operations.

### 4.3 Computing generators of Toeplitz matrix polynomials

In Lemma 3.5 we computed explicit expressions for generators of monomials $T, T^{2}, T^{3}, \ldots$. Within these expressions, one needs to (repeatedly) apply the matrices

$$
(Z-I) T(Z-I)^{-1} \quad \text { and } \quad(Z-I) T^{*}(Z-I)^{-1}
$$

to a given canonical Toeplitz generator $(G, B)$. Note that applying $(Z-I)^{-1}$ to a vector amounts simply to computing the vector of its cumulative sums, and that the application of $Z-I$ to a vector can be evaluated with $n-1$ subtractions. Hence, both operations require $\mathcal{O}(n)$ operations. Finally, as mentioned in Section 2 matrix-vector products with $T$ and $T^{*}$ can be evaluated in $\mathcal{O}(n \log n)$ operations, so that we have the following result.

Corollary 4.4. Let $T \in \mathbb{R}^{n, n}$ be a Toeplitz matrix, then a set of generators for the monomials $T, T^{2}, \ldots, T^{s}$ can be computed with $\mathcal{O}(s n \log n)$ operations.

Because of the nested structure of the monomial generators (cf. (9)-(10)), only the generator $\left(G_{s}, B_{s}\right)$ for the leading monomial $T^{s}$ is actually needed for the evaluation of $p(T):=\sum_{k=0}^{s} a_{k} T^{k}$. A generator for $p(T)$ can be computed by appropriate linear combination of the block columns of $G_{s}$, i.e., there exists a matrix $X \in \mathbb{R}^{3 s-1,3 s-1}$ defined through the coefficients $a_{0}, \ldots, a_{s}$, such that $\left(G_{s} X, B_{s}\right)$ is a generator for $p(T)$. For example, if we set

$$
X=\left[\begin{array}{ccc}
a_{2} I_{2} & 0 & 0 \\
0 & a_{2} I_{2} & 0 \\
0 & 0 & a_{2}
\end{array}\right]+\left[\begin{array}{ccc}
0 & a_{1} I_{2} & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{array}\right]
$$

then $\left(G_{2} X, B_{2}\right)$ is a generator for $a_{2} T^{2}+a_{1} T$.
Alternatively, a Horner-like scheme can be used to compute a generator for $p(T)$. Let $T_{k}, 0 \leq k \leq s$ be the $k$ th Horner polynomial, defined via the recursion

$$
T_{0}:=a_{s} I, \quad T_{k}:=T T_{k-1}+a_{s-k} I \text { for } 1 \leq k \leq s
$$

then $T_{k}$ is the Schur complement of $-I$ in the embedding

$$
M=\left[\begin{array}{cc}
-I & T_{k-1}  \tag{18}\\
T & a_{k} I
\end{array}\right]
$$

Using similar arguments and techniques as for the evaluation of monomials in $T$, it follows that the evaluation of $p(T)$ based on (18) can be carried out in $\mathcal{O}(s n \log n)$ operations. In contrast to the evaluation based on monomials of $T$, the resulting generator has length $2 s$.

### 4.4 Evaluating rational approximants by solving Toeplitz-like systems

We now turn to the computation of generators for rational functions of $T$. Let $r(z)=\frac{p(z)}{q(z)}$ be a rational function, and let $\left(G_{p}, B_{p}\right)$ and $\left(G_{q}, B_{q}\right)$ be generators for $p(T)$ and $q(T)$, respectively; see Section 4.3. From equations (12)-(13), we see that a generator for $r(T)=$ $q(T)^{-1} p(T)$ is found by solving the linear Toeplitz-like systems

$$
q(T)^{-1}(Z-I)^{-1}\left[\begin{array}{ll}
G_{q} & G_{p}
\end{array}\right] \quad \text { and } \quad q(T)^{-*}(Z-I)^{-1}\left[\begin{array}{ll}
B_{q} & e_{1} \tag{19}
\end{array}\right] .
$$

In total there are $2 \operatorname{deg}(q)+\operatorname{deg}(p)+1$ right hand sides to solve for, and since the displacement rank of $q(T)$ is at most $2 \operatorname{deg}(q)$, the techniques outlined in Section 4.2 yield the following result.

Corollary 4.5. Let $T \in \mathbb{C}^{n \times n}$ be a Toeplitz matrix, and $r(z)=\frac{p(z)}{q(z)}$ a rational function of degree $s=\max \{\operatorname{deg}(p), \operatorname{deg}(q)\}$. Then a generator for $r(T)=q(T)^{-1} p(T)$ can be computed with $\mathcal{O}\left(s^{2} n^{2}\right)$ operations.

The dependence on $s^{2}$ in the above statement is nearly negligible in our context, since the degrees of the Padé approximants we will be using are typically small, and never larger than thirteen. Note also that (12)-(13) involve matrix-vector multiplications with $p(T)$ and $p\left(T^{*}\right)$, but the cost for these are dominated by solving the linear systems (19).

### 4.5 Evaluating rational approximants by partial fraction expansion

Any rational function with simple poles can be expressed as a partial fraction expansion

$$
r(z)=\sum_{i=1}^{m} \frac{\beta_{i}}{z-\alpha_{i}}+p(z)
$$

where $m$ is the number of poles $\alpha_{i}$ with residues $\beta_{i}$, and $p$ is a polynomial. Let $T \in \mathbb{C}^{n \times n}$ be a Toeplitz matrix, and assume that none of the poles of $r$ is an eigenvalue of $T$. Generators for $p(T)$ can be computed using the techniques described in Section4.3 and we now discuss the computation of generators for the Toeplitz-like matrix

$$
\begin{equation*}
\sum_{i=1}^{m} \beta_{i}\left(T-\alpha_{i} I\right)^{-1} \tag{20}
\end{equation*}
$$

First note that for any $\alpha \in \mathbb{C}$ the matrix $T_{\alpha}=T+\alpha I$ is a Toepliz matrix as well, with the generator

$$
G_{\alpha}=\left[\begin{array}{cc}
t_{0}+\alpha & 1 \\
t_{1} & 0 \\
\vdots & \vdots \\
t_{n-1} & 0
\end{array}\right], \quad B_{\alpha}=\left[\begin{array}{cc}
1 & 0 \\
0 & t_{-1} \\
\vdots & \vdots \\
0 & t_{-n+1}
\end{array}\right]
$$

Hence, the evaluation of (20) is simply the sum of $m$ inverse Toeplitz matrices and we can therefore apply the result from Remark 3.4 and the related Gohberg-Semuncul formulas (see, e.g., [16] for an overview) to compute a generator for (20) by solving $\mathcal{O}(m)$ linear Toeplitz systems using the technique described in Section 4.2.

In the common case where $T$ is real, and the expansion (20) involves pairs of complex conjugates shifts $\alpha, \bar{\alpha}$ and residues $\beta, \bar{\beta}$, then

$$
\bar{\beta}(T-\bar{\alpha})^{-1}=\overline{\beta(T-\alpha)^{-1}},
$$

so that a real generator for $\beta(T-\alpha)^{-1}+\bar{\beta}(T-\bar{\alpha})^{-1}$ can be computed by means of solving two linear Toeplitz systems (instead of four). So let $(G, B)$ be a generator for $\beta(T-\alpha)^{-1}$, then

$$
\begin{aligned}
& \nabla\left(\beta(T-\alpha)^{-1}+\bar{\beta}(T-\bar{\alpha})^{-1}\right)=\nabla\left(\beta(T-\alpha)^{-1}\right)+\overline{\nabla\left(\beta(T-\alpha)^{-1}\right)} \\
& =G B^{*}+\overline{G B^{*}}=2 \operatorname{Re}\left(G B^{*}\right)=2\left(\operatorname{Re}(G) \operatorname{Re}(B)^{*}+\operatorname{Im}(G) \operatorname{Im}(B)^{*}\right)
\end{aligned}
$$

In the case of a Padé approximant, this implies that the number of Toeplitz matrix inversions is roughly halved. Of course, the asymptotic cost is unchanged, and we summarize our findings as follows.
Corollary 4.6. Let $T \in \mathbb{C}^{n \times n}$ be a Toeplitz matrix, and $r(z)=\sum_{i=1}^{m} \beta_{i}\left(z-\alpha_{i}\right)^{-1} a$ rational function. Then $r(T)$ can be evaluated in $\mathcal{O}\left(m n^{2}\right)$ operations involving at most $2 m+2$ solutions of linear Toeplitz systems.

### 4.6 Iterative squaring

At the final stage of scaling and squaring algorithms we have at hand a rational approximation $r\left(2^{-\rho} T\right) \approx \exp \left(2^{-\rho} T\right)$, and in order to obtain an approximation for $\exp (T)$, the initial scaling is undone by squaring the matrix $r\left(2^{-\rho} T\right) \rho$ times.

Let $(G, B)$ be a generator of length $s$ for the Toeplitz-like matrix $A$. Then a generator of length $2 s+1$ for $A^{2}$ can be computed using Theorem 3.2. The cost for computing the new generator is dominated by the evaluation of the products $A G$ and $A^{*} B$. Each of these products can be computed based on the expansion (5), involving $2 s^{2}$ multiplications with triangular Toeplitz matrices, resulting in an operation of complexity $\mathcal{O}\left(s^{2} n \log n\right)$.

Each squaring operation effectively doubles the length of the generator matrices, and hence after $\rho$ squaring operations we would obtain generator matrices of length $\mathcal{O}\left(2^{\rho} s\right)$, which is computationally feasible only for tiny values of $\rho$. However, if the spectrum of $T$ allows for low degree rational approximation of $\exp (T)$ (see Sec. (3) , the same is true for each scaled matrix $2^{-k} T, 1 \leq k \leq \rho$. Consequently, if the rational approximation to $\exp \left(2^{-\rho} T\right)$ is such that

$$
\begin{equation*}
r\left(2^{-\rho} T\right)^{2^{k}} \approx \exp \left(2^{\rho-k} T\right), \quad 0 \leq k \leq \rho, \tag{21}
\end{equation*}
$$

then Corollary 3.11 shows that each displacement $\nabla\left(r\left(2^{-\rho} T\right)^{2^{k}}\right)$ is close to a low rank matrix, and a generator compression (Alg. (1) applied after every squaring operation will reduce the intermediate generator length back to $\mathcal{O}(s)$, without compromising the approximation quality of the final approximation to $\exp (T)$. The computational cost for each of this compressions is dominated by the matrix multiplications $A G$ and $A^{*} B$. The following Corollary summarizes the discussion.

Corollary 4.7. Generators for the sequence $r\left(2^{-\rho} T\right)^{2}, \ldots, r\left(2^{-\rho} T\right)^{2^{\rho}}$ can be computed in $\mathcal{O}\left(\rho s^{2} n \log n\right)$, provided that each intermediate displacement $\nabla\left(r\left(2^{-\rho} T\right)^{2}\right), \ldots, \nabla\left(r\left(2^{-\rho} T\right)^{2^{\rho}}\right)$ has numerical rank $\mathcal{O}(s)$.

### 4.7 Reconstruction of Toeplitz-like matrices

As mentioned in Section 2 a Toeplitz-like matrix can be reconstructed from a generator based on (44). We note next that this operation can be implemented efficiently.

Lemma 4.8. Let $A \in \mathbb{C}^{n \times n}$ be a Toeplitz-like matrix, and $(G, B)$ a generator for $T$ of length $r$. Then $A$ can be computed from $(G, B)$ in $\mathcal{O}\left(r n^{2}\right)$ operations.

Proof. The number of operations for computing $D=G B^{*}$ is $\mathcal{O}\left(r n^{2}\right)$. Then the expression

$$
A=\sum_{k=0}^{n-1} Z^{k} D\left(Z^{*}\right)^{k}
$$

can be evaluated in $\mathcal{O}\left(n^{2}\right)$ operations by noting that the $k$ th subdiagonal (superdiagonal) of $A$ is just the vector of cumulative sums of the $k$ th subdiagonal (superdiagonal) of $D$.

Remark 4.9. If only the diagonal of $A$ is of interest then the proof of Lemma 4.8 shows that this diagonal can be reconstructed by forming the cumulative sum of the vector $d=$ $\operatorname{diag}\left(G B^{*}\right)$. The arithmetic cost for forming $d$ and thus the entire cost of extracting the diagonal of $A$ is $\mathcal{O}(n r)$. In fact any banded section of $A$ can be reconstructed by only computing the corresponding banded section of $G B^{*}$.

### 4.8 A remark on the use of the FFT

Many of the operations discussed in this section involve or even reduce to matrix-vector multiplication with Toeplitz and Toeplitz-like matrices, cf. Secs. 4.1, 4.3, 4.4, 4.6 The complexity of computing a matrix-vector product $A x$ for a Toeplitz-like matrix $A \in \mathbb{C}^{n, n}$ of displacement rank $r$ is $r n \log n$. Although carrying out these multiplications using the FFT is asymptotically faster than standard matrix-vector multiplication, an actual computational advantage is gained only for sufficiently large matrix dimension $n$.

If that is not the case, it is preferable to resort to standard matrix-vector multiplication. Since $A$ is of displacement rank $r$, the reconstruction of $A$ from a generator can be done in $\mathcal{O}\left(r n^{2}\right)$ operations, as described in Sec. 4.7. Consequently, a single matrix-vector product can be computed using standard multiplication in $\mathcal{O}\left(r n^{2}+n^{2}\right)$ operations, and $\ell$ matrixvector products with $A$ can be evaluated in $\mathcal{O}\left((r+\ell) n^{2}\right)$ operations. Note that in this latter case, the cost for FFT based multiplication is $\mathcal{O}(\ell r n \log n)$.

## 5 Scaling and squaring algorithms for Toeplitz matrices

In Section 3 we have shown that rational approximations to the matrix exponential of a Toeplitz matrix $T$ enjoy low displacement rank, provided that $T$ is negative real or sectorial. We will now use scaling and squaring algorithms that take advantage of this property. Based on the techniques presented in Section 4 the resulting algorithms will require $\mathcal{O}\left(n^{2}\right)$ operations for computing $\exp (T)$, which is optimal since the output is also of size $n^{2}$.

Denote by $r_{k, m}(z)=\frac{p_{k, m}(z)}{q_{k, m}(z)}$ the $(k, m)$-Padé approximant to the exponential function, meaning that the numerator polynomial is of degree $k$, and the denominator polynomial of degree $m$. Scaling and squaring algorithms take advantage of the fact that Pade approximations are very accurate close to origin. An input matrix $A$ is thus scaled by a power of two, so that $\left\|2^{-\rho} A\right\| \lesssim 1$, and then the Padé approximant $r_{k, m}\left(2^{-\rho} A\right)$ is computed. Finally, an approximation to $\exp (A)$ is obtained by squaring the result repeatedly, viz.

$$
\exp (A) \approx r_{k, m}\left(2^{-\rho} A\right)^{2^{\rho}}
$$

using the identity $\exp (A)=\exp \left(\sigma^{-1} A\right)^{\sigma}, \sigma \in \mathbb{C} \backslash\{0\}$.
Different strategies for choosing the scaling parameter $\rho$ and the Pade degree ( $k, m$ ) yield different methods. We will discuss two recently proposed scaling and squaring methods. The first one, described by Higham [14, is based on a diagonal Padé approximation of degree at most 13 and makes no assumption on the spectrum of the input matrix. The second one by Güttel and Nakatsukasa [10] employs a subdiagonal Padé approximation of much smaller degree, and is particularly useful if the imaginary parts of the rightmost eigenvalues do not vary too much. Both scaling and squaring methods have been shown to behave in a forward stable manner for normal matrices.

### 5.1 A diagonal scaling and squaring method

The scaling and squaring method designed by Higham [14 was until recently the default method to compute the matrix exponential in Matlab, available via the command expm. It scales the input matrix $A$ so that $\left\|2^{-\rho} A\right\|_{1} \lesssim 5.4$, and approximates $\exp (A)$ using a diagonal Padé approximation, i.e., $k=m$ in the notation from above. The approximation degree is at most 13, or less for matrices that need not be scaled. This parameter choice is designed such that the approximation error can be interpreted as a backward error $E$ (in any consistent matrix norm)

$$
\begin{equation*}
r_{m, m}\left(2^{-\rho} A\right)^{2^{\rho}}=\exp (A+E),\|E\| \leq u\|A\|, \tag{22}
\end{equation*}
$$

where $u$ denotes the unit roundoff in double precision; see [14, Thm. 2.1]. Note that no assumption on the spectral properties of $A$ have been made. The matrix $E$ can be shown to commute with $A$, and hence one obtains immediately

$$
\begin{align*}
\left\|r_{m, m}\left(2^{-\rho} A\right)^{2^{\rho}}-\exp (A)\right\| & \leq\|\exp (A)(\exp (E)-I)\| \\
& \leq\|\exp (A)\|\|E\|\|\exp (E)\| \leq\|\exp (A)\| u\|A\| e^{u\|A\|}, \tag{23}
\end{align*}
$$

which bounds the forward error of the approximation. At the same time, Higham shows that the matrix $q_{m, m}(A)$ is well conditioned under this parameter regime.

We now show for the case of real spectra that the numerical rank is bounded throughout the squaring phase (cf. (21)). By effecting a shift $T \leftarrow T-\mu I$ we may assume that the spectrum is actually negative real, which simplifies the notation in what follows.

Lemma 5.1. Let $T$ be a diagonalizable Toeplitz matrix with spectrum in $(-\infty, 0]$. Set $\tau=u\|T\| \exp (u\|T\|)$, and

$$
s=\left\lceil\frac{\log (\tilde{C})-\log (\tau)}{\log (V)}\right\rceil \text {, }
$$

with $\tilde{C}$ and $V$ as in Corollary 3.10 (we may safely assume that $s \geq 0$ ). Then $r_{m, m}\left(2^{-\rho} A\right)^{2^{\sigma}}$ and all the intermediate matrices in the squaring phase have $2 \tau$-displacement rank $2 s+1$.

Proof. We abbreviate $r:=r_{m, m}$. The squaring phase involves the quantities

$$
r\left(2^{-\sigma} T\right), r\left(2^{-\sigma} T\right)^{2^{1}}, r\left(2^{-\sigma} T\right)^{2^{2}}, \ldots, r\left(2^{-\sigma} T\right)^{2^{\sigma}}
$$

and we proceed by showing that each of these powers is close to the matrix exponential of the matrix $T_{k}:=2^{-k} T$. Regarding $T_{k}$ as the input matrix to expmt, the scaling power

```
Algorithm 2 expmt - Diagonal scaling \& squaring from 14 for Toeplitz matrices
Input: Toeplitz matrix \(T \in \mathbb{C}^{n \times n}\), given by its first column \(c\) and row \(r\).
Output: Generator \((G, B)\) such that \(\mathcal{T}(G, B) \approx \exp (T)\)
    Compute \(\|T\|_{1} \quad\{\mathcal{O}(n)\), Sec. 4.1] \(\}\)
    Chose scaling parameter \(\rho\) and Padé approximant \(r_{m}(z)=\frac{p_{m}(z)}{q_{m}(z)} \quad\{[14\}\)
    Scale \(c \leftarrow 2^{-\rho} c, r \leftarrow 2^{-\rho} r\)
    \(\left(G_{p}, B_{p}\right) \leftarrow\) generator for \(p_{m}(T)\)
    \(\left(G_{q}, B_{q}\right) \leftarrow\) generator for \(q_{m}(T)\)
    \((G, B) \leftarrow\) generator for \(r_{m}(T)=q_{m}(T)^{-1} p_{m}(T)\)
    for \(k=1\) to \(\rho\) do
        \((\tilde{G}, \tilde{B}) \leftarrow\) generator for \(\mathcal{T}(G, B)^{2} \quad\left\{\mathcal{O}\left(m^{2} n \log n\right)\right.\), Sec. 4.6 \(\}\)
        \((G, B) \leftarrow\) compress \((\tilde{G}, \tilde{B})\)
    end for
    \{optionally\} reconstruct \(\mathcal{T}(G, B) \quad\left\{\mathcal{O}\left(m n^{2}\right)\right.\), Sec. 4.7\}
```

selected by the algorithm design is $\sigma-k$, and the approximant $r$ is the same for all $k$. So we obtain from (22) for $0 \leq k \leq \sigma$

$$
r\left(2^{-\sigma+k} 2^{-k} T\right)^{2^{k}}=r\left(2^{-\sigma} T\right)^{2^{k}}=\exp \left(T_{k}+E_{k}\right), \quad\left\|E_{k}\right\| \leq 2^{-k} u\|T\|
$$

A forward error bound for the approximation of the intermediate exponentials, that is, for each squaring iteration $k$, follows from (23),

$$
\begin{aligned}
\left\|r\left(2^{-\sigma} T\right)^{2^{k}}-\exp \left(T_{k}\right)\right\| & =\left\|\exp \left(T_{k}+E_{k}\right)-\exp \left(T_{k}\right)\right\| \\
& \leq u 2^{-k}\|T\| \exp \left(u 2^{-k}\|T\|\right) \leq \tau
\end{aligned}
$$

Since all the matrices $T_{k}$ (trivially) have negative real spectra, the result now follows from Corollary 3.11

Note that the non-normality of $T$ is reflected in the constant $\tilde{C}$, via the condition number of an eigenbasis for $T$. If $T$ arises from a discretization process, the lemma shows that the $2 \tau$ numerical displacement rank remains bounded as long as this condition number is bounded. For highly non-normal matrices, the usefulness of our result is limited. We remark, however, that the behaviour of scaling and squaring, in particular its stability, is not well understood in this case.

We now leave the regime of negative real spectra, but continue to assume that $T$ is not highly non-normal, that is, $T$ can be diagonalized by a reasonably well-conditioned matrix. The preceding discussion in fact applies to any Toeplitz matrix $T$ whose spectrum is contained in a subset of the complex plane, where the error of the rational best approximation to $e^{z}$ decays exponentially in the approximation degree (the involved constants change, however). Another well known example for this situation are sectorial matrices (see Section 3.2).

In the absence of such a rational best approximation result, which are in general quite difficult to obtain, the displacement rank of $\exp (T)$, as well as the intermediates in the squaring phase, are not bounded a priori and independently of the scaling power $\rho$. However the displacemnt ranks may still remain small, see Section 6.2 for an example.

Assuming that the numerical displacement ranks during the squaring phase are bounded, a practical algorithm of quadratic complexity is obtained by replacing the unstructured matrix computations used in [14] by their structured counterparts explained in Sec. 4. The resulting method is shown in Algorithm 2.

We close the discussion by noting that Algorithm 2 almost achieves our goal of designing a method of quadratic complexity for the Toeplitz matrix exponential. While the approximation degree $m$ is bounded by 13 , the scaling power $\rho$ still grows logarithmically with
$\|A\|_{1}$, and consequently the number of squaring iterations is not bounded independently of the numerical values of $A$. From a practical point of view Algorithm 2 still behaves like an algorithm of quadratic complexity.

### 5.2 A subdiagonal scaling and squaring method

The second scaling and squaring method we adapted for the Toeplitz case is described and analyzed in [10]. In contrast to Higham's design, it (typically) employs a subdiagonal Padé approximation (hence "sexpm"), which is appropriate if the spectrum is located on the negative real line, or close to it. If the input matrix $T$ does not have this property, say, the eigenvalues are only real, this subdiagonal approximation may be applied to the shifted matrix

$$
T-\lambda_{\max } I
$$

where $\lambda_{\max }$ denotes the largest eigenvalue of $T$. (The approximation to $\exp (T)$ is then recovered by multiplication with $\left.e^{\lambda_{\text {max }}}\right)$.

Put more generally, it suffices that the rightmost eigenvalues of $T$ do not have widely varying imaginary parts for this subdiagonal approximation to be very accurate. We refer to [10] for a complete discussion of this shifting technique, and the quality of the obtained approximation.

Compared to expm, sexpm has several attractive features:

1. For the Padé degree $(k, m)$ we have $k, m \leq 5$, resulting in computational cost savings over the diagonal approximation from the previous section.
2. The Padé approximant can be stably evaluated as a partial fraction expansion. Hence the rational approximation $q_{k, m}(T)^{-1} p_{k, m}$ involves only solves with Toeplitz matrices instead of Toeplitz-like matrices.
3. The number of scaling iterations $\rho$ is bounded by four, independently of $A$, implying that the generator length can increase at most by a factor of $2^{4}=16$ during the squaring phase. (In light of the results from Section 3.2, this factor likely still is a gross overestimate, however). Hence, the displacement rank of the approximation to the exponential is bounded independently of $A$ as well. In other words, the potential displacement rank growth as discussed in Section 4.6 is not an issue for this method.

If $A \in \mathbb{C}^{n, n}$ is normal, the approximation $B$ of $\exp (A)$ obtained through sexpm satisfies

$$
\|B-\exp (A)\|_{2} \leq u\|A\|_{2}
$$

and the authors in fact show that their method is a forward stable method [10, Thm. 4.1]. The adaption to the Toeplitz case, coined sexpmt, is shown in Algorithm 3. Since the number of squaring iterations is bounded independently of $n$ and $\|A\|_{2}$, it follows that the complexity of Algorithm 3 is $\mathcal{O}\left(n^{2}\right)$.

## 6 Numerical experiments

We have implemented Algorithms 2 and 3 in Matlab. For solving the Toeplitz-like systems as described in Section 4.2, we are using the drsolve1] package [1]. All experiments were conducted on a standard Linux box using a single computational thread. The expm function of Matlab that we used for various comparisons is described in [13].

```
Algorithm 3 sexpmt - Subdiagonal scaling \& squaring from 10 for Toeplitz matrices
Input: Toeplitz matrix \(T \in \mathbb{C}^{n \times n}\) with the spectral properties described in Section 5.2,
    given by its first column \(c\) and row \(r\).
Output: Generator \((G, B)\) such that \(\mathcal{T}(G, B) \approx \exp (T)\)
    Estimate \(\|T\|_{2} \quad\{\mathcal{O}(n \log n)\), Sec. 4.1] \(\}\)
    Chose scaling \(2^{\rho}\) and Padé approximant \(\left.r_{k, m}(z)=\sum_{i=1}^{m} \frac{\beta_{i}}{z-\alpha_{j}}+p(z) \quad\{10]\right\}\)
    Scale \(c \leftarrow 2^{-\rho} c, r \leftarrow 2^{-\rho} r \quad\{\mathcal{O}(n)\}\)
    Initialize \(G=[], B=[]\)
    for \(i=1\) to \(m\) do
        Compute generator \(\left(G_{i}, B_{i}\right)\) for \(\beta_{i}\left(T-\alpha_{i} I\right)^{-1} \quad\left\{\mathcal{O}\left(n^{2}\right)\right.\), Sec. 4.5 \}
        \(G \leftarrow\left[G, G_{i}\right], B \leftarrow\left[B, B_{i}\right]\)
    end for
    Compute generator for \(p(T)\), append to \((G, B) \quad\{\mathcal{O}(\operatorname{deg}(p) n \log n)\), Sec. 4.3\}
    for \(k=1\) to \(\rho\) do
        \((\tilde{G}, \tilde{B}) \leftarrow\) generator for \(\mathcal{T}(G, B)^{2} \quad\left\{\mathcal{O}\left(m^{2} n \log n\right)\right.\), Sec. 4.6 \(\}\)
        \((G, B) \leftarrow\) compress \((\tilde{G}, \tilde{B})\)
                            \(\left\{\mathcal{O}\left(m^{2} n\right)\right.\), Alg. [1]
    end for
    \{optionally\} reconstruct \(\mathcal{T}(G, B)\)
    \(\left\{\mathcal{O}\left(m n^{2}\right)\right.\), Sec. 4.7\}
```


### 6.1 Exact error on small matrices

As a first test we compute the exact normwise error of the approximation of $\exp (T)$ via Algorithm 2 on a diverse set of small Toeplitz matrices, from the following sources:

- The 16 Toeplitz matrices available via the smtgallery command of the structured matrix toolbox $\sqrt[2]{2}$ [27.
- Seven matrices from [20, sec. 5]. Specifically, we generated matrices according to Examples 1 and 2 from [20] for time steps 1,10 and 100 as well as one instance of Example 3 from [20] with time step 1. The last example refers to the Merton model, which is considered further in Section 6.3.

Figure 2 shows the normwise relative errors

$$
\frac{\|\exp (T)-\operatorname{expmt}(T)\|_{F}}{\|\exp (T)\|_{F}}
$$

where $\operatorname{expmt}(T)$ denotes the computed approximation to $\exp (T)$ obtained from Algorithm 2, The "exact" $\exp (T)$ was computed using Matlab's variable precision arithmetic with 150 digits. Further, we show for each matrix in the set an approximation to the relative condition number of the exponential condition number [13, chap. 10] (black line). The errors of a backward stable method would realize errors close to this line, and we see that the errors of expmt are roughly bounded by ten times this quantity.

### 6.2 Efficiency of expmt outside the sectorial regime

Let $T$ be a Toeplitz matrix. In Section 5.1 we concluded that that the displacement rank of $\exp (T)$, and ranks of the intermediate approximations (21), are bounded a priori only under certain conditions on the spectrum of $T$, e.g., real or sectorial. Further, in Example 3.12 we showed that one cannot expect an accurate, low displacement rank approximation of $\exp (T)$ if all the eigenvalues of $T$ are located on, or close to, the imaginary axis.

[^1]

Figure 2: Left: Normwise relative error for the approximation of $\exp (T)$ via Algorithm 2 for the matrices listed in Section 6.1 The solid black line indicates the condition numbers (times machine precision). Right: Displacement rank of $\exp (T)$ and the displacement rank of the approximation. All matrices have size $32 \times 32$.


Figure 3: Algorithm 2 applied to $\alpha T$, where $T$ is a random matrix and $\alpha \in\{1,10,100\}$. Left: Spectrum of $T$ in the complex plane. Right: Displacement rank of the intermediate approximations during the squaring phase. See Section 6.2 for a discussion.

This does not imply that Algorithm 2 is necessarily inefficient if applied to a matrix that is not sectorial. We illustrate this setting in Figure 3. There we consider a Toeplitz matrix $T$ as in (11) where the real and imaginary parts of each $t_{k},-n+1 \leq k \leq n-1(n=2000)$, have been drawn from $\mathcal{N}(0,1)$, followed by a scaling so that $\|T\|_{2}=1$. The spectrum of $T$ is shown on the left, and it is evident that $T$ is not sectorial.

We applied Algorithm 2 to $\alpha T$ for $\alpha \in\{1,10,100\}$, in order to provoke an increasing number of squaring iterations. The displacement ranks of the intermediate approximations over the course of the squaring iterations, lines 10, are shown on the right (iteration 0 corresponds to the initial rational approximation). We observe that the displacement rank grows very slowly in all of the three cases under consideration. In particular, the displacement rank does not double at each squaring iteration, which corresponds to the worst case bound discussed in Section 4.6. We remark that for $\alpha=100$ the run time of expmt was no more than 5 s , while expm took more than 40 s.

Finally we revisit Example 3.12. While Algorithm 2 will exhibit $\mathcal{O}\left(n^{3}\right)$ run time scaling when applied to matrices of this type, it is still faster than the corresponding standard expm algorithm, because the only costly operations are the very last squaring steps. In contrast,
all the squaring iterations, as well as the computations involved in evaluating the rational function, are operations of cubic complexity in expm.

A comparison of the run times for computing the exponentials in Example 3.12 is given in the following table.

| $\alpha$ | expm | expmt | expmt-GEMM |
| :--- | ---: | ---: | ---: |
| 1 | 4.55 s | 1.96 s | 2.01 s |
| 10 | 8.04 s | 2.92 s | 2.98 s |
| 100 | 13.15 s | 3.28 s | 3.41 s |
| 1000 | 19.47 s | 12.30 s | 5.77 s |

Comparing the timings of expm and exmpt, we find that Algorithm 2 is always faster than Matlab's built-in matrix exponential function. The last column ("expmt-GEMM") shows the run times for the following variation of expmt: As soon as the displacement rank exceeds a certain threshold during the squaring phase (here we chose $n / 6$ ), we use standard matrix-matrix multiplication instead of the generator based multiplication (see Section4.6). With this trivial twist enabled, the run time gains over expm remain quite pronounced even if the exponential is far from having low numerical displacement rank.

### 6.3 Option pricing using the Merton model

We now turn to the evaluation of option prices in the Merton model, for one single underlying asset [22]. There, in contrast to the Black-Scholes model, the expected return of the asset evolves as a mixture of continuous and jump processes. The option value $\omega(\xi, t)$ on $(-\infty, \infty) \times[0, T]$ satisfies the partial integro-differential equation (PIDE)

$$
\begin{equation*}
\omega_{t}=\frac{\nu^{2}}{2} \omega_{\xi \xi}+\left(r-\lambda \kappa-\frac{\nu^{2}}{2}\right) \omega_{\xi}-(r+\lambda) \omega+\lambda \int_{-\infty}^{\infty} \omega(\xi+\eta, t) \phi(\eta) d \eta \tag{24}
\end{equation*}
$$

where $T$ denotes time to maturity, $\nu \geq 0$ is the volatility, $r$ is the risk-free interest rate, $\lambda \geq 0$ is the arrival intensity of a Poisson process, $\phi$ is the normal distribution with mean $\mu$ and standard deviation $\sigma$, and $\kappa=e^{\mu+\sigma^{2} / 2}-1$.

The discretization of (24) first truncates the infinite domain $(-\infty, \infty) \times[0, T]$ to $\left(-\xi_{\min }, \xi_{\max }\right) \times$ $[0, T]$. Then central differences and the rectangle method are used to discretize the differential and integral terms in (24), respectively. Because the coefficients do not depend on $\xi$ and the integral kernel is shift invariant, the discretization yields a nonsymmetric, sectorial Toeplitz matrix $T$. We refrain from giving details and refer to the excellent summary given in [20, Example 3].

In all experiments, we used parameters identical to the ones used in [20: $\xi_{\text {min }}=-2$, $\xi_{\text {max }}=2, K=100, \nu=0.25, r=0.05, \lambda=0.1, \mu=\hat{a} L{ }_{L}{ }_{S} 0.9, \sigma=0.45$, as well as a full time step 1.

Figure 4 (left) shows the run time for the four matrix exponential approximations expm, expmt, sexpm, and sexpmt. From the complexity analysis in Section 4 we know that the run times of expmt and sexpmt scale quadratically in $n$ (expm and sexpm scale cubically), and the plot shows this qualitative different behaviour. The run time scaling exponents inferred from the measured times $t_{1}, t_{2}$ at dimensions $n_{1}=2048$ and $n_{2}=4096$ through $\log \left(t_{2} / t_{1}\right) / \log \left(n_{2} / n_{1}\right)$, is about 2.20 for expmt and 2.00 for sexpmt. From the shown data we also see that a saving in run time by using our fast algorithm over the standard ones is realized already for matrix sizes between $n=1000$ and $n=1500$, indicating that the constants hidden in the big- $\mathcal{O}$ complexity bounds for our algorithms are not too large.

We now discuss the accuracy of the obtained approximations. Since the computation of the matrix exponential using variable precision arithmetic is too expensive for the matrix sizes we are considering here, we assess the accuracy of expmt, sexpm, and sexpmt with


Figure 4: Experimental comparison of approximations to $\exp \left(A_{n}\right)$ for the Merton model (see Section 6.31). Left: Run time comparison for the computation of the full exponential approximation. Right: Relative error with respect to expm. The dashed gray line shows $u\left\|A_{n}\right\|_{F}$, a lower bound for the exponential condition number (times machine precision).


Figure 5: Displacement ranks of the exponentials computed for the Merton model.
reference to expm. Figure 4 (right), shows the relative distance

$$
\frac{\|B-\operatorname{expm}(T)\|_{F}}{\|\operatorname{expm}(T)\|_{F}}
$$

where $B$ is the approximation we want to compare. In addition, we show $u\|T\|_{F}$ (dashed line), which is a lower bound for the exponential condition number (times machine precision). Since the relative error w.r.t. expm is roughly bounded by this quantity, we conclude that our adapted scaling and squaring methods behave in a forward stable manner in this example.

In Figure 5 we show the displacement ranks of the approximations to the matrix exponentials. For expmt and sexpmt, this rank corresponds to the length of the generator obtained by the corresponding method after the squaring phase. For expm and sexpm, the shown rank is the numerical rank of the displacements, as determined by Matlab's rank function. As suggested by the discussion in Section 3, all these ranks are close to each other, and in particular quite small. Finally, Figure 6 shows how the displacement rank evolves during the squaring phase of expmt $(n=4096)$.


Figure 6: Evolution of the displacement ranks in the squaring phase of Alg. 2 for the Merton model discretized with $n=4096$ points.

## 7 Conclusions and future work

We have shown that the full matrix exponential of a Toeplitz matrix can be computed efficiently using scaling and squaring algorithms. A key result that enables this efficient computation is the low displacement rank of rational functions for Toeplitz matrices. Combined with classical results for rational best approximations of the exponential function, it asserts that the Toeplitz matrix exponential itself enjoys provable low displacement rank if its spectrum is real or sectorial, for example. By carefully adapting all the matrix computations in the general scaling and squaring framework, we obtain algorithms of quadratic complexity of the input size for computing $\exp (T)$ for a Toeplitz matrix $T$. Since the output size of the matrix exponential is quadratic as well, our algorithms hence achieve optimal complexity.

We also demonstrated by means of an example that a spectrum clustered along a long stretch of the imaginary axis does not allow for a low displacement rank approximation of the matrix exponential. The apparent reason is the periodicity of the exponential function on this set, which does not allow for a low degree rational approximation. It would be of interest to investigate this setting more rigorously.

In this work we have focused on analyzing the displacement rank of polynomials, rational functions and the matrix exponential itself. Two important aspects have received less attention than they probably deserve. One is the design of the scaling and squaring logic itself, for which we relied on the works of Higham [14, as well as Güttel and Nakatsukasa [10]. An important design goal for these methods is a small number of (unstructured) matrix operations of cubic complexity such as inversion or matrix-matrix multiplication. However, as our careful description in Section 4 shows, minimizing these operations is of much less importance in the Toeplitz case, as long as the overall quadratic complexity is maintained. It would thus be of interest to design a scaling and squaring method specifically for the case of Toeplitz matrices. We also did not attempt to analyze the forward stability in floating point arithmetic for our adapted methods in detail, although such an analysis is certainly of interest.

Finally, our results show that for Toeplitz matrices it is even possible to implement scaling and squaring algorithms of subquadratic complexity, provided that only the generators of $\exp (T)$ are requested, and not the full matrix exponential. Recall that the generators are already sufficient for applying the exponential to a vector. If, for example, the Toepliz inversions in Alg. 3 are carried out by superfast solvers (e.g., [19, 24, 31), then these generators can be computed in $\mathcal{O}(n \log n)$.

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[^1]:    ${ }^{1}$ http://bugs.unica.it/~gppe/soft/\#drsolve
    2http://bugs.unica.it/~gppe/soft/smt/

