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PRECONDITIONERS FOR SYMMETRIZED TOEPLITZ AND MULTILEVEL TOEPLITZ MATRICES*

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Abstract. When solving linear systems with nonsymmetric Toeplitz or multilevel Toeplitz matrices using Krylov subspace methods, the coefficient matrix may be symmetrized. The preconditioned MINRES method can then be applied to this symmetrized system, which allows rigorous upper bounds on the number of MINRES iterations to be obtained. However, effective preconditioners for symmetrized (multilevel) Toeplitz matrices are lacking. Here, we propose novel ideal preconditioners and investigate the spectra of the preconditioned matrices. We show how these preconditioners can be approximated and demonstrate their effectiveness via numerical experiments.

Key words. Toeplitz matrix, multilevel Toeplitz matrix, symmetrization, preconditioning, Krylov subspace method

AMS subject classifications. 65F08, 65F10, 15B05, 35R11

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1. Introduction.

Linear systems

$$A_n x = b, \tag{1.1}$$

where $A_n \in \mathbb{R}^{n\times n}$ is a Toeplitz or multilevel Toeplitz matrix, and $b \in \mathbb{R}^n$ arise in a range of applications. These include the discretization of partial differential and integral equations, time series analysis, and signal and image processing [7, 27]. Additionally, demand for fast numerical methods for fractional diffusion problems—which have recently received significant attention—has renewed interest in the solution of Toeplitz and Toeplitz-like systems [10, 26, 31, 32, 46].

Preconditioned iterative methods are often used to solve systems of the form (1.1). When A_n is Hermitian, the conjugate gradient method (CG) [18] and MINRES [29] can be applied, and their descriptive convergence rate bounds guide the construction of effective preconditioners [7, 27]. On the other hand, convergence rates of preconditioned iterative methods for nonsymmetric Toeplitz matrices are difficult to describe. Consequently, preconditioners for nonsymmetric problems are typically motivated by heuristics.

As described in [35] for Toeplitz matrices, and discussed in subsection 2.2 for the multilevel case, A_n is symmetrized by the exchange matrix

$$Y_n = \begin{bmatrix} & & 1 \\ & \iddots & \\ 1 & & \end{bmatrix}, \tag{1.2}$$

so that (1.1) can be replaced by

$$Y_n A_n x = Y_n b, \tag{1.3}$$

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with the symmetric coefficient matrix Y_nA_n. Although we can view Y_n as a preconditioner, its role is not to accelerate convergence, and there is no guarantee that (1.3) is easier to solve than (1.1) [12, 23]. Instead, the presence of Y_n allows us to use preconditioned MINRES, with its nice properties and convergence rate bounds, to solve (1.3). We can then apply a secondary preconditioner $P_n \in \mathbb{R}^{n\times n}$ to improve the spectral properties of Y_nA_n and therefore accelerate convergence. An additional benefit is that MINRES may be faster than GMRES [37] even when iteration numbers are comparable, since it requires only short-term recurrences.

Preconditioned MINRES requires a symmetric positive definite preconditioner P_n, but it is not immediately clear how to choose this matrix when A_n is nonsymmetric. In [35] it was shown that absolute value circulant preconditioners, which we describe in the next section, give fast convergence for many Toeplitz problems. However, for some problems there may be more effective alternatives based on Toeplitz matrices (see, e.g., [4, 17]). Moreover, multilevel circulant preconditioners generally are not effective for multilevel Toeplitz problems [40, 41, 42]. Thus, alternative preconditioners for (1.3) are needed.

In this paper, we describe ideal preconditioners for symmetrized (multilevel) Toeplitz matrices and show how these can be effectively approximated. To set the scene, we present background material in section 2. Sections 3 and 4 describe the ideal preconditioners for Toeplitz and multilevel Toeplitz problems, respectively. Numerical experiments in section 5 verify our results and show how the ideal preconditioners can be efficiently approximated by circulant matrices or multilevel methods. Our conclusions can be found in section 6.

2. Background. In this section we collect pertinent results on Toeplitz and multilevel Toeplitz matrices.

2.1. Toeplitz and Hankel matrices. Let $A_n \in \mathbb{R}^{n\times n}$ be the nonsingular Toeplitz matrix

$$A_n = \begin{bmatrix} a_0 & a_{-1} & \dots & a_{-n+2} & a_{-n+1} \\ a_1 & a_0 & a_{-1} & & a_{-n+2} \\ \vdots & a_1 & a_0 & \ddots & \vdots \\ a_{n-2} & & \ddots & \ddots & a_{-1} \\ a_{n-1} & a_{n-2} & \dots & a_1 & a_0 \end{bmatrix}. \quad (2.1)$$

In many applications, the matrix A_n is associated with a generating function $f \in L^1([-\pi,\pi])$ via its Fourier coefficients

$$a_k = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(\theta)\mathrm{e}^{-\mathrm{i}k\theta}\mathrm{d}\theta, \quad k \in \mathbb{Z}. \quad (2.2)$$

We use the notation $A_n(f)$ when we wish to stress that a Toeplitz matrix A_n is associated with the generating function f. An important class of generating functions is the Wiener class, which is the set of functions satisfying

$$f(\theta) = \sum_{k=-\infty}^{\infty} a_k\mathrm{e}^{-\mathrm{i}k\theta}, \quad \sum_{k=-\infty}^{\infty} |a_k| < \infty.$$

Many properties of $A_n(f)$ can be determined from f. For example, if f is real, then $A_n(f)$ is Hermitian and its eigenvalues are characterized by f [16, pp. 64–65].

On the other hand, if f is complex-valued, then $A_n(f)$ is non-Hermitian for at least some n, and its singular values are characterized by $|f|$ [2, 33, 47].

Circulant matrices are Toeplitz matrices of the form

$$C_n = \begin{bmatrix} c_0 & c_{n-1} & \cdots & c_2 & c_1 \\ c_1 & c_0 & c_{n-1} & & c_2 \\ \vdots & c_1 & c_0 & \ddots & \vdots \\ c_{n-2} & & \ddots & \ddots & c_{n-1} \\ c_{n-1} & c_{n-2} & \cdots & c_1 & c_0 \end{bmatrix}.$$

They are diagonalized by the Fourier matrix, i.e., $C_n = F_n^* \Lambda_n F_n$, where

$$(F_n)_{j,k} = \frac{1}{\sqrt{n}} \mathrm{e}^{\frac{2\pi \mathrm{i} jk}{n}}, \quad j,k = 0,\ldots,n-1,$$

and $\Lambda_n = \mathrm{diag}(\lambda_0, \ldots, \lambda_{n-1})$, with

$$\lambda_k = \sum_{j=0}^{n-1} c_j \mathrm{e}^{\frac{2\pi \mathrm{i} jk}{n}}. \tag{2.3}$$

We denote by $C_n(f)$ the circulant with eigenvalues $\lambda_j = f(2\pi j/n)$, $j = 0,\ldots,n-1$. The absolute value circulant [5, 28, 35] derived from a circulant C_n is the matrix

$$|C_n| = F_n^* |\Lambda_n| F_n. \tag{2.4}$$

Closely related to Toeplitz matrices are Hankel matrices $H_n \in \mathbb{R}^{n\times n}$,

$$H_n = \begin{bmatrix} a_1 & a_2 & a_3 & \cdots & a_n \\ a_2 & a_3 & & \iddots & a_{n+1} \\ a_3 & & \iddots & \iddots & \vdots \\ \vdots & \iddots & \iddots & & a_{2n-2} \\ a_n & a_{n+1} & \cdots & a_{2n-2} & a_{2n-1} \end{bmatrix},$$

which have constant antidiagonals. It is well known that a Toeplitz matrix can be converted into a Hankel matrix, or vice versa, by flipping the rows (or columns), i.e., via Y_n in (1.2). Since Hankel matrices are necessarily symmetric, this means that any nonsymmetric Toeplitz matrix A_n can be symmetrized by applying Y_n, so that

$$Y_n A_n = A_n^T Y_n. \tag{2.5}$$

Alternatively, we may think of A_n as being self-adjoint with respect to the bilinear form induced by Y_n [14, 34].

A matrix $G_n \in \mathbb{R}^{n\times n}$ is centrosymmetric if

$$G_n Y_n = Y_n G_n \tag{2.6}$$

and is skew-centrosymmetric if $G_n Y_n = -Y_n G_n$. Thus, (2.5) shows that symmetric Toeplitz matrices are centrosymmetric. It is clear from (2.6) that the inverse of a nonsingular centrosymmetric matrix is again centrosymmetric. Furthermore, nonsingular centrosymmetric matrices have a centrosymmetric square root [22, Corollary 1].[1]

[1] In [22] the proof is given only for a centrosymmetric matrix of even dimension. However, the extension to matrices of odd dimension is straightforward.

2.2. Multilevel Toeplitz and Hankel matrices. Multilevel Toeplitz matrices are generalizations of Toeplitz matrices. To define a generating function for a multilevel Toeplitz matrix, let $j = (j_1, \ldots, j_p) \in \mathbb{Z}^p$ be a multi-index, and consider a p-variate function $f \in L^1([-\pi, \pi]^p)$, $f : [-\pi, \pi]^p \to \mathbb{C}$. The Fourier coefficients of f are defined as

$$a_j = a_{(j_1,\ldots,j_p)} = \frac{1}{(2\pi)^p} \int_{[-\pi,\pi]^p} f(\theta) \mathrm{e}^{-\mathrm{i}\langle \theta, j\rangle} \, \mathrm{d}\theta, \qquad j \in \mathbb{Z}^p,$$

where $\langle \theta, j\rangle = \sum_{k=1}^p \theta_k j_k$, and $\mathrm{d}\theta = \mathrm{d}\theta_1 \cdots \mathrm{d}\theta_p$ is the volume element with respect to the p-dimensional Lebesgue measure.

If $n = (n_1, \ldots, n_p) \in \mathbb{N}^p$, with $n_i > 1$, $i = 1, \ldots, p$, and $\pi(n) = n_1 \cdots n_p$, then f is the generating function of the multilevel Toeplitz matrix $A_n(f) \in \mathbb{R}^{\pi(n)\times\pi(n)}$, where

$$A_n(f) = \sum_{j_1=-n_1+1}^{n_1-1} \cdots \sum_{j_p=-n_p+1}^{n_p-1} J_{n_1}^{(j_1)} \otimes \cdots \otimes J_{n_p}^{(j_p)} a_{(j_1,\ldots,j_p)}.$$

Here, $J_r^{(k)} \in \mathbb{R}^{r\times r}$ is the matrix whose (i, j)th entry is one if $i - j = k$ and zero otherwise.

Similarly, we can define a multilevel Hankel matrix as

$$H_n(f) = \sum_{j_1=1}^{2n_1-1} \cdots \sum_{j_p=1}^{2n_p-1} K_{n_1}^{(j_1)} \otimes \cdots \otimes K_{n_p}^{(j_p)} a_{(j_1,\ldots,j_p)},$$

where $K_r^{(k)} \in \mathbb{R}^{r\times r}$ is the matrix whose (i, j)th entry is one if $i + j = k + 1$ and zero otherwise. Although a multilevel Hankel matrix does not necessarily have constant antidiagonals, it is symmetric.

Multilevel Toeplitz matrices can also be symmetrized by the exchange matrix $Y_n \in \mathbb{R}^{\pi(n)\times\pi(n)}$, $Y_n = Y_{n_1} \otimes \cdots \otimes Y_{n_p}$. To see this, we use an approach analogous to that in the proof of [11, Lemma 5]. The key point is that $Y_r J_r^{(k)} = K_r^{(r-k)}$, so that

$$\begin{aligned} Y_n A_n(f) &= \sum_{j_1=-n_1+1}^{n_1-1} \cdots \sum_{j_p=-n_p+1}^{n_p-1} \left((Y_{n_1} J_{n_1}^{(j_1)}) \otimes \cdots \otimes (Y_{n_p} J_{n_p}^{(j_p)}) \right) a_{(j_1,\ldots,j_p)} \\ &= \sum_{j_1=-n_1+1}^{n_1-1} \cdots \sum_{j_p=-n_p+1}^{n_p-1} \left(K_{n_1}^{(n_1-j_1)} \otimes \cdots \otimes K_{n_p}^{(n_p-j_p)} \right) a_{(j_1,\ldots,j_p)} \\ &= \sum_{j_1=1}^{2n_1-1} \cdots \sum_{j_p=1}^{2n_p-1} K_{n_1}^{(j_1)} \otimes \cdots \otimes K_{n_p}^{(j_p)} b_{(j_1,\ldots,j_p)}, \end{aligned}$$

where $b_{(j_1,\ldots,j_p)} = a_{(n_1-j_1,\ldots,n_p-j_p)}$. Thus, $Y_n A_n(f)$ is a multilevel Hankel matrix and hence is symmetric.

2.3. Assumptions and notation. Throughout, we assume that all Toeplitz or multilevel Toeplitz matrices A_n are real and are associated with generating functions in $L^1([-\pi, \pi]^p)$. We denote the real and imaginary parts of f by f_R and f_I, respectively, so that $f = f_R + \mathrm{i} f_I$. We assume that the symmetric part of A_n, given by $A_R = (A_n + A_n^T)/2$, is positive definite, which is equivalent to requiring that f_R is essentially positive. Similarly, we assume that $|f| \geq \delta > 0$ for some constant δ, so that $A_n(|f|)$ is positive definite with $\lambda_{\min}(A_n(|f|) \geq \delta$. Moreover, $\lambda_{\min}(A_n(|f|) > \delta$ if $\operatorname{esssup} |f| > \delta = \operatorname{essinf} |f|$ (see Lemma 3.1).

3. Preconditioning Toeplitz matrices. In this section we introduce our ideal preconditioners for (1.3) when A_n is a Toeplitz matrix, and we analyze the spectrum of the preconditioned matrices. Although these preconditioners may be too expensive to apply exactly, they can be approximated by, e.g., a circulant matrix or multigrid solver.

3.1. The preconditioner A_R. The first preconditioner we consider is the symmetric part of A_n, namely $A_R = (A_n + A_n^T)/2$, which was previously used to precondition the nonsymmetric problem (1.1) (see [21]). When the preconditioner A_R is applied to the symmetrized system (1.3), spectral information can be used to bound the convergence rate of preconditioned MINRES. Accordingly, in this section we characterize the eigenvalues of $A_R^{-\frac{1}{2}} Y_n A_n A_R^{-\frac{1}{2}}$.

We begin by stating a powerful result that characterizes the spectra of preconditioned Hermitian Toeplitz matrices in terms of generating functions.

LEMMA 3.1 (see [39, Theorem 3.1]). *Let $f, g \in L^1([-\pi,\pi])$ be real-valued functions with g essentially positive. Let $A_n(f)$ and $A_n(g)$ be the Hermitian Toeplitz matrices with generating functions f and g, respectively. Then, $A_n(g)$ is positive definite, and the eigenvalues of $A_n^{-1}(g)A_n(f)$ lie in (r,R), where $r < R$ and*

$$r = \operatorname*{essinf}_{x\in[-\pi,\pi]} \frac{f(\theta)}{g(\theta)}, \qquad R = \operatorname*{esssup}_{\theta\in[-\pi,\pi]} \frac{f(\theta)}{g(\theta)}.$$

If $r = R$, then $A_n^{-1}(g)A_n(f) = I_n$, the identity matrix of dimension n.

Lemma 3.1 shows that in the Hermitian case, we can bound the extreme eigenvalues of preconditioned Toeplitz matrices using scalar quantities. If bounds on the eigenvalues nearest the origin are also available, it is possible to estimate the convergence rate of preconditioned MINRES applied to the Toeplitz system. Unfortunately, this result neither carries over to nonsymmetric matrices nor is an eigenvalue inclusion region alone sufficient to bound the convergence rate of a Krylov subspace method for nonsymmetric problems [1, 15]. However, in the following we show that by symmetrizing the Toeplitz matrix A_n, we can obtain results analogous to Lemma 3.1—even for nonsymmetric A_n. As a first step, we quantify the perturbation of the (nonsymmetric) preconditioned matrix $A_R^{-\frac{1}{2}} A_n A_R^{-\frac{1}{2}}$ from the identity.

LEMMA 3.2. *Let $f \in L^1([-\pi,\pi])$, and let $f = f_R + \mathrm{i} f_I$, where f_R and f_I are real-valued functions with f_R essentially positive. Additionally, let $A_n := A_n(f) \in \mathbb{R}^{n\times n}$ be the Toeplitz matrix associated with f. Then $A_R = A_n(f_R) = (A_n + A_n^T)/2$ is symmetric positive definite and*

$$A_R^{-\frac{1}{2}} A_n A_R^{-\frac{1}{2}} = I_n + E_n,$$

where

$$\|E_n\|_2 = \epsilon < \operatorname*{esssup}_{\theta\in[-\pi,\pi]} \left| \frac{f_I(\theta)}{f_R(\theta)} \right|.$$

Proof. It is easily seen from (2.2) that $A_n(f) = A_n(f_R) + \mathrm{i}A_n(f_I)$. Moreover, from Lemma 3.1 we also know that $A_R = A_n(f_R)$ is symmetric positive definite and $A_n(f_I)$ is Hermitian. It follows that

$$A_R^{-\frac{1}{2}} A_n A_R^{-\frac{1}{2}} = A_R^{-\frac{1}{2}} (A_R + \mathrm{i}A_n(f_I)) A_R^{-\frac{1}{2}} = I_n + E_n,$$

where $E_n = \mathrm{i}\widehat{E}_n = \mathrm{i}A_R^{-\frac{1}{2}} A_n(f_I) A_R^{-\frac{1}{2}}$.

To bound $\epsilon := \|E_n\|_2 = \|\widehat{E}_n\|_2$, note that since $\widehat{E}_n$ is Hermitian, $\|\widehat{E}_n\|_2$ is equal to the spectral radius of $\widehat{E}_n$. Applying Lemma 3.1 thus gives that

$$\epsilon < \operatorname*{esssup}_{\theta\in[-\pi,\pi]} \left|\frac{f_I(\theta)}{f_R(\theta)}\right|,$$

which completes the proof. ∎

The above result tells us that the nonsymmetric preconditioned matrix will be close to the identity when the skew-Hermitian part of A_n is small, as expected. Although this enables us to bound the singular values of $A_R^{-\frac{1}{2}} A_n A_R^{-\frac{1}{2}}$, these cannot be directly related to the convergence of, e.g., GMRES. In contrast, the following result will enable us to characterize the convergence rate of MINRES applied to (1.3).

LEMMA 3.3. *Let $f \in L^1([-\pi,\pi])$, and let $f = f_R + \mathrm{i} f_I$, where f_R and f_I are real-valued functions with f_R essentially positive. Additionally, let $A_n := A_n(f) \in \mathbb{R}^{n\times n}$ be the Toeplitz matrix associated with f. Then the symmetric positive definite matrix $A_R = A_n(f_R) = (A_n + A_n^T)/2$ is such that*

$$A_R^{-\frac{1}{2}}(Y_n A_n)A_R^{-\frac{1}{2}} = Y_n + Y_n E_n, \tag{3.1}$$

where Y_n is the exchange matrix in (1.2) *and*

$$\|Y_n E_n\|_2 = \epsilon < \operatorname*{esssup}_{\theta\in[-\pi,\pi]} \left|\frac{f_I(\theta)}{f_R(\theta)}\right|.$$

Proof. Since A_R is a symmetric Toeplitz matrix, it is centrosymmetric. Hence, $A_R^{-\frac{1}{2}}$ is centrosymmetric (see (2.6) and [22]), so that $Y_n A_R^{-\frac{1}{2}} = A_R^{-\frac{1}{2}} Y_n$. Combining this with Lemma 3.2 shows that

$$A_R^{-\frac{1}{2}}(Y_n A_n)A_R^{-\frac{1}{2}} = Y_n(A_R^{-\frac{1}{2}} A_n A_R^{-\frac{1}{2}}) = Y_n(I_n + E_n) = Y_n + Y_n E_n.$$

Since Y_n is orthogonal, $\|Y_n E_n\|_2 = \|E_n\|_2$, and the result follows from Lemma 3.2. ∎

Applying Weyl's theorem [20, Theorem 4.3.1] to (3.1) shows that the eigenvalues of $A_R^{-\frac{1}{2}}(Y_n A_n)A_R^{-\frac{1}{2}}$ lie in $[-1-\epsilon, -1+\epsilon] \cup [1-\epsilon, 1+\epsilon]$. However, as ϵ grows, eigenvalues could move close to the origin and hamper MINRES convergence. In the following result, we show that this cannot happen.

THEOREM 3.4. *Let $f \in L^1([-\pi,\pi])$, and let $f = f_R + \mathrm{i} f_I$, where f_R and f_I are real-valued functions with f_R essentially positive. Additionally, let $A_n := A_n(f) \in \mathbb{R}^{n\times n}$ be the Toeplitz matrix associated with f, and let $A_R = A_n(f_R) = (A_n + A_n^T)/2$. Then, the eigenvalues of $A_R^{-\frac{1}{2}}(Y_n A_n)A_R^{-\frac{1}{2}}$ lie in $[-1-\epsilon, -1] \cup [1, 1+\epsilon]$, where*

$$\epsilon < \operatorname*{esssup}_{\theta\in[-\pi,\pi]} \left|\frac{f_I(\theta)}{f_R(\theta)}\right|. \tag{3.2}$$

Proof. We know from Lemma 3.3 that

$$A_R^{-\frac{1}{2}}(Y_n A_n)A_R^{-\frac{1}{2}} = Y_n + Y_n E_n,$$

where $\|Y_n E_n\|_2 < \epsilon$ and Y_n has eigenvalues ± 1. Thus, as discussed above, the eigenvalues of $A_R^{-\frac{1}{2}}(Y_n A_n)A_R^{-\frac{1}{2}}$ lie in $[-1-\epsilon, -1+\epsilon] \cup [1-\epsilon, 1+\epsilon]$. Hence, all that remains is to improve the bounds on the eigenvalues nearest the origin. Our strategy for doing so will be to apply successive similarity transformations to $Y_n + Y_nE_n$; as a by-product, we will characterize the eigenvalues of $A_R^{-\frac{1}{2}}(Y_nA_n)A_R^{-\frac{1}{2}}$ in terms of the eigenvalues of Y_nE_n.

Before applying our first similarity transform, we recall from the proofs of Lemmas 3.2 and 3.3 that $\mathrm{i}A_n(f_I)$ is skew-symmetric and Toeplitz, while $A_R^{-\frac{1}{2}}$ is symmetric and centrosymmetric. It follows that Y_nE_n is symmetric but skew-centrosymmetric. Skew-centrosymmetry implies that whenever (λ, x), $\lambda \neq 0$ is an eigenpair of Y_nE_n, then so is $(-\lambda, Y_nx)$ [19, 36, 44]. Additionally, any eigenvectors of Y_nE_n corresponding to a zero eigenvalue can be expressed as a linear combination of vectors of the form $x \pm Y_nx$, $x \in \mathbb{R}^n$ [44, Theorem 17]. Therefore, Y_nE_n has eigendecomposition $Y_nE_n = U_n\Lambda_nU_n^T$, where

$$\Lambda_n = \begin{array}{c} \\ m_1 \\ m_1 \\ m_2 \end{array}\begin{array}{c} \begin{array}{ccc} m_1 & m_1 & m_2 \end{array} \\ \begin{bmatrix} \Lambda_{\text{pos}} & & \\ & -\Lambda_{\text{pos}} & \\ & & 0 \end{bmatrix} \end{array} \tag{3.3}$$

and

$$U_n = \begin{array}{c} \begin{array}{cccc} m_1 & m_1 & m_3 & m_4 \end{array} \\ [U_{\text{pos}} \quad Y_nU_{\text{pos}} \quad U_{\text{sym}} + Y_nU_{\text{sym}} \quad U_{\text{skew}} - Y_nU_{\text{skew}}] \end{array}, \tag{3.4}$$

where $n = 2m_1 + m_2$ and $m_2 = m_3 + m_4$. Since Y_nE_n is symmetric, we may assume that U_n is orthogonal. We can now apply the first similarity transform, namely,

$$U_n^T(Y_n + Y_nE)U_n = U_n^TY_nU_n + \Lambda_n. \tag{3.5}$$

Using the orthogonality of the columns of U_n, it is straightforward to show that

$$U_n^TY_nU_n = \begin{bmatrix} & I_{m_1} & & \\ I_{m_1} & & & \\ & & I_{m_3} & \\ & & & -I_{m_4} \end{bmatrix}.$$

Thus, $U_n^TY_nU_n = Q_n\Gamma_nQ_n^T$, where

$$\Gamma_n = \begin{bmatrix} \widehat{\Gamma}_{2m_1} & & \\ & I_{m_3} & \\ & & -I_{m_4} \end{bmatrix} \quad \text{and} \quad Q_n = \left[\begin{array}{c|cc} \widehat{Q} & I_{m_3} & \\ & & -I_{m_4} \end{array}\right].$$

Here, $\widehat{\Gamma}_{2m_1} = \mathrm{diag}(1, -1, \ldots, 1, -1)$, and the kth column of $\widehat{Q} \in \mathbb{R}^{n \times 2m_1}$ is given by

$$\widehat{q}_k = \begin{cases} \frac{1}{\sqrt{2}}(e_k + e_{m_1+k}), & k \text{ odd}, \\ \frac{1}{\sqrt{2}}(e_k - e_{m_1+k}), & k \text{ even}, \end{cases}$$

with $e_j \in \mathbb{R}^n$ the jth unit vector. Consequently, our second similarity transform gives

$$Q_n^TU_n^T(Y_n + Y_nE_n)U_nQ_n = \Gamma_n + Q_n^T\Lambda_nQ_n, \tag{3.6}$$

with

$$Q_n^T \Lambda_n Q_n = \left[\begin{array}{cccc|cc} \Sigma_1 & & & & & \\ & \Sigma_2 & & & & \\ & & \ddots & & & \\ & & & \Sigma_{m_1} & & \\ \hline & & & & 0 & \\ & & & & & 0 \end{array}\right],$$

where if $\Lambda_{\text{pos}} = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_{m_1})$, then

$$\Sigma_k = \begin{bmatrix} 0 & \lambda_k \\ \lambda_k & 0 \end{bmatrix}.$$

Hence, letting

$$Z = \begin{bmatrix} 1 & \\ & -1 \end{bmatrix},$$

we find that

$$\Gamma + Q_n^T \Lambda_n Q_n = \begin{bmatrix} Z + \Sigma_1 & & & & & \\ & Z + \Sigma_2 & & & & \\ & & \ddots & & & \\ & & & Z + \Sigma_{m_1} & & \\ & & & & I_{m_3} & \\ & & & & & -I_{m_4} \end{bmatrix}.$$

Since the eigenvalues of $Z + \Sigma_k$ are $\pm\sqrt{1 + \lambda_k^2}$, we see from (3.6) that the eigenvalues of $A_R^{-\frac{1}{2}}(Y_n A_n)A_R^{-\frac{1}{2}}$ are $\pm\sqrt{1 + \lambda_k^2}$, $k = 1, \dots, m_1$, and possibly 1 or both 1 and -1. Hence, the eigenvalues are at least 1 in magnitude. This completes the proof. ∎

Theorem 3.4 characterizes the eigenvalues of $A_R^{-\frac{1}{2}}(Y_n A_n)A_R^{-\frac{1}{2}}$, and hence the convergence rate of preconditioned MINRES, in terms of the scalar quantity in (3.2). Thus, we expect that the preconditioner A_R will perform best when A_n is nearly symmetric, and we investigate this in section 5. However, irrespective of the degree of nonsymmetry of A_n, Theorem 3.4 shows that the eigenvalues of the preconditioned matrix are at least bounded away from the origin.

3.2. The preconditioner A_M. We saw in subsection 3.1 that A_R is an effective preconditioner when the degree of nonsymmetry of A_n is not too large. For problems that are highly nonsymmetric, however, a different preconditioner may be more effective. Here, motivated by the success of absolute value preconditioning, we consider the preconditioner $A_M = A_n(|f|)$ instead. The following result describes the asymptotic eigenvalue distribution of $A_M^{-1} Y_n A_n$.

THEOREM 3.5. *Assume that* $f \in L^\infty([-\pi, \pi])$ *with* $0 < \delta \le |f(\theta)|$ *for all* $\theta \in [-\pi, \pi]$. *Then, if* $A_M = A_n(|f|)$,

$$(A_M)^{-1} Y_n A_n(f) = Y_n A_n(\widetilde{f}) + E_n,$$

where $\widetilde{f} = f/|f|$ *and* $\|E_n\|_2 = o(n)$ *as* $n \to \infty$. *Moreover, the eigenvalues of* $Y_n A_n(\widetilde{f})$ *lie in* $[-1, 1]$.

Proof. The conditions on $|f|$ guarantee that $A_n(|f|)$ is invertible and that its eigenvalues (singular values) are bounded away from 0. Thus, by Proposition 5 in [9],

$$A_n(|f|)^{-1}A_n(f) - A_n(\widetilde{f}) = \widetilde{E}_n,$$

where $\|\widetilde{E}_n\|_2 = o(n)$ as $n \to \infty$. Since A_M is Hermitian and Toeplitz, both A_M and its inverse are centrosymmetric. It follows that

$$(A_M)^{-1}(Y_nA_n(f)) = Y_n\left((A_M)^{-1}A_n(f)\right) = Y_nA_n(\widetilde{f}) + E_n,$$

where $E_n = Y_n\widetilde{E}_n$ and $\|E_n\|_2 = \|Y\widetilde{E}_n\|_2 = \|\widetilde{E}_n\|_2$. Hence, $\|E_n\|_2 = o(n)$ as $n \to \infty$. Since Y_n is unitary and $Y_nA_n(\widetilde{f})$ is symmetric, the absolute values of the eigenvalues of $Y_nA_n(\widetilde{f})$ coincide with the singular values of $A_n(\widetilde{f})$, which in turn are bounded above by one [47]. This proves the result. ∎

A consequence of Theorem 3.5 is that the eigenvalues of $A_n(|f|)^{-1}Y_nA_n$ lie in $[-1-\epsilon, 1+\epsilon]$, where for large enough n the parameter ϵ is small. Although eigenvalues may be close to the origin, most cluster at -1 and 1, in line with Theorem 3.4 in [23].

To conclude this section, we show how A_M can be approximated by circulant preconditioners. First, recall from subsection 2.1 that $C_n(f)$ is the preconditioner with eigenvalues $\lambda_j = f(2\pi j/n)$, $j = 0, \ldots, n-1$. For large enough dimension n, we have that $A_M = C_n(|f|) + E_n + R_n$, where E_n has small norm and R_n has small rank [13, pp. 108–110], so that $C_n(|f|)$ is a good approximation to A_M for large n.

The matrix $C_n(|f|)$ can in turn be approximated by the Strang absolute value circulant preconditioner $|C_n^{(S)}|$ [5, 28, 35], where if $C_n^{(S)}$ is the Strang circulant preconditioner [43] for A_n, with eigenvalues λ_j, $j = 1, \ldots, n$, then the corresponding absolute value circulant preconditioner $|C_n^{(S)}|$ has eigenvalues $|\lambda_j|$, $j = 1, \ldots, n$. For this preconditioner, we obtain the following result.

THEOREM 3.6. *Let $f : [-\pi, \pi] \to \mathbb{C}$ be in the Wiener class, and let $A_n = A_n(f) \in \mathbb{R}^{n\times n}$. Then the Strang preconditioner $C_n^{(S)}$ is such that $|C_n^{(S)}| \to C_n(|f|)$ as $n \to \infty$.*

Proof. Assume that n, the dimension of A_n, is $n = 2m + 1$. (This idea can be extended to the case of even n, as in [6, p. 37].) Then, $C_n^{(S)} = C_n(\mathcal{D}_m \star f)$, where

$$(\mathcal{D}_m \star f)(\theta) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathcal{D}_m(\phi)f(\theta - y)\,\mathrm{d}\phi = \sum_{-m}^{m} a_k \mathrm{e}^{\frac{2\pi \mathrm{i} jk}{n}}$$

is the convolution of f with the Dirichlet kernel $\mathcal{D}$ [6], and a_k is as in (2.2).

Since both $|C_n^{(S)}| = |C_n(\mathcal{D}_m \star f)|$ and $C_n(|f|)$ are diagonalized by the Fourier matrix, they will be identical if all their eigenvalues, defined by (2.3), match. The eigenvalues of $C_n(\mathcal{D}_m \star f)$ are $(\mathcal{D}_m * f)(2\pi j/n)$, $j = 0, \ldots, n-1$. Hence, the jth eigenvalue of $|C_n(\mathcal{D}_m \star f)|$ is

$$\lambda_j(|C_n(\mathcal{D}_m \star f)|) = \left((\mathcal{D}_m \star f)\left(\frac{2\pi j}{n}\right)\overline{(\mathcal{D}_m \star f)\left(\frac{2\pi j}{n}\right)}\right)^{\frac{1}{2}}.$$

Since f is in the Wiener class, $(\mathcal{D}_m \star f)(\theta)$ converges absolutely and hence uniformly to $f(\theta)$. Thus,

$$\lim_{n\to\infty}\lambda_j(|C_n(\mathcal{D}_m\star f)|)=\lim_{n\to\infty}\left((\mathcal{D}_m\star f)\left(\frac{2\pi j}{n}\right)\overline{(\mathcal{D}_m\star f)\left(\frac{2\pi j}{n}\right)}\right)^{\frac{1}{2}}$$
$$=\left(f\left(\frac{2\pi j}{n}\right)\overline{f\left(\frac{2\pi j}{n}\right)}\right)^{\frac{1}{2}}=\left|f\left(\frac{2\pi j}{n}\right)\right|=\lambda_j(C_n(|f|)).$$

Since the eigenvalues of $|C_n(\mathcal{D}_m\star f)|$ approach those of $C_n(|f|)$ as $n\to\infty$, we obtain the result. ◻

4. Multilevel Toeplitz problems.

We now extend the results of section 3 to multilevel Toeplitz matrices.

4.1. The preconditioner A_R.

The results of subsection 3.1 carry over straightforwardly to the multilevel case. They depend on the following generalization of Lemma 3.1. This result essentially appeared in Theorem 2.4[2] in [38].

LEMMA 4.1 (see [38]). *Let $f,g\in L^1([-\pi,\pi]^p)$ with g essentially positive. Let*

$$r:=\operatorname*{essinf}_{\theta\in[-\pi,\pi]^p}\frac{f(\theta)}{g(\theta)},\quad R:=\operatorname*{esssup}_{\theta\in[-\pi,\pi]^p}\frac{f(\theta)}{g(\theta)}.$$

Then the eigenvalues of $A_n^{-1}(g)A_n(f)$ lie in (r,R) if $r<R$. If $r=R$, then $A_n^{-1}(g)A_n(f)=I_n$, where I_n is the identity matrix of dimension $\pi(n)=n_1\cdots n_p$.

With this result, Lemmas 3.2 and 3.3 and Theorem 3.4 carry over directly to the multilevel case. In particular, we have the following characterization of the eigenvalues of $A_R^{-\frac{1}{2}}(Y_nA_n)A_R^{-\frac{1}{2}}$.

THEOREM 4.2. *Let $f\in L^1([-\pi,\pi]^p)$, and let $f=f_R+\mathrm{i}f_I$, where f_R and f_I are real-valued functions with f_R essentially positive. Additionally, let $A_n:=A_n(f)\in\mathbb{R}^{\pi(n)\times\pi(n)}$ be the multilevel Toeplitz matrix associated with f, and let $A_R=A_n(f_R)=(A_n+A_n^T)/2$. Then, the eigenvalues of $A_R^{-\frac{1}{2}}(Y_nA_n)A_R^{-\frac{1}{2}}$ lie in $[-1-\epsilon,-1]\cup[1,1+\epsilon]$, where*

$$\epsilon<\operatorname*{esssup}_{\theta\in[-\pi,\pi]^p}\left(\left|\frac{f_I(\theta)}{f_R(\theta)}\right|\right). \tag{4.1}$$

Theorem 4.2 characterizes the eigenvalues of $A_R^{-\frac{1}{2}}(Y_nA_n)A_R^{-\frac{1}{2}}$, which are bounded away from the origin. In turn, this allows us to bound the convergence rate of preconditioned MINRES in terms of the easily computed quantity in (4.1).

4.2. The preconditioner A_M.

We can also extend the results in subsection 3.2 to the multilevel case. However, for multilevel problems this preconditioner is more challenging to approximate. Matrix algebra, e.g., block circulant, preconditioners will generally result in iteration counts that increase as the dimension increases, as previously discussed. On the other hand, constructing effective banded Toeplitz, or efficient multilevel, algorithms is challenging since it is generally necessary to compute elements of A_M. Nonetheless, we present the following result for completeness. It directly generalizes the result for Toeplitz matrices, so it is presented without proof.

[2]Although the result is stated for f,g nonnegative, the proof also holds for indefinite f.

THEOREM 4.3. *Let $f : L^\infty([-\pi,\pi]^p)$, with $0 < \delta < |f(\theta)|$ for all $\theta \in [-\pi,\pi]^p$. Then, if $A_M = A_n(|f|)$ is the multilevel Toeplitz matrix generated by $|f|$,*

$$(A_M)^{-1} Y_n A_n(f) = Y_n A_n(\tilde{f}) + E_n,$$

where $\tilde{f} = f/|f|$ and $\|E_n\|_2 = o(n)$ as $n \to \infty$. Moreover, the eigenvalues of $Y_n A_n(\tilde{f})$ lie in $[-1,1]$.

5. Numerical experiments. In this section we investigate the effectiveness of the preconditioners described above, and approximations to them, for the symmetrized system (1.3). We also compare the proposed approach to using nonsymmetric preconditioners for (1.1) within preconditioned GMRES and LSQR [30]. All code is written in MATLAB (version 9.4.0) and run on a quad-core, 62 GB RAM, Intel i7-6700 CPU with 3.20 GHz.[3] We apply MATLAB versions of LSQR and MINRES, and a version of GMRES that performs right preconditioning. (Note that LSQR requires two matrix-vector products with the coefficient matrix and two preconditioner solves per iteration.) We take as our initial guess $x_0 = (1, 1, \ldots, 1)^T/\sqrt{n}$, and we stop all methods when $\|r_k\|_2/\|r_0\|_2 < 10^{-8}$. When more than 200 iterations are required, we denote this by "—" in the tables.

When A_R or A_M are too expensive to apply directly, we use either a circulant or multigrid approximation. The multigrid preconditioner consists of a single V-cycle with damped Jacobi smoothing and Galerkin projections, namely linear or bilinear interpolation and restriction by full-weighting. The coarse matrices are also built by projection. The number of smoothing steps and the damping factor ω are stated below for each problem. The damping parameter is chosen by trial and error to minimize the number of iterations needed for small problems. When applying circulant preconditioners to (1.3), we use the absolute value preconditioner in (2.4) based on the Strang [43], optimal [8], or superoptimal [45] circulant preconditioner.

Example 5.1. Our first example is from [21, Example 2], where numerical experiments indicated that A_R is an effective preconditioner for the nonsymmetric system (1.1) when GMRES is applied. The Toeplitz coefficient matrix $A_n = A_n(f)$ is formed from the generating function $f(\theta) = (2 - 2\cos(\theta))(1 + \mathrm{i}\theta)$. Since computing the Fourier coefficients for larger problems is time-consuming, smaller problems are examined here. The right-hand side is a random vector (computed using the MATLAB function `randn`).

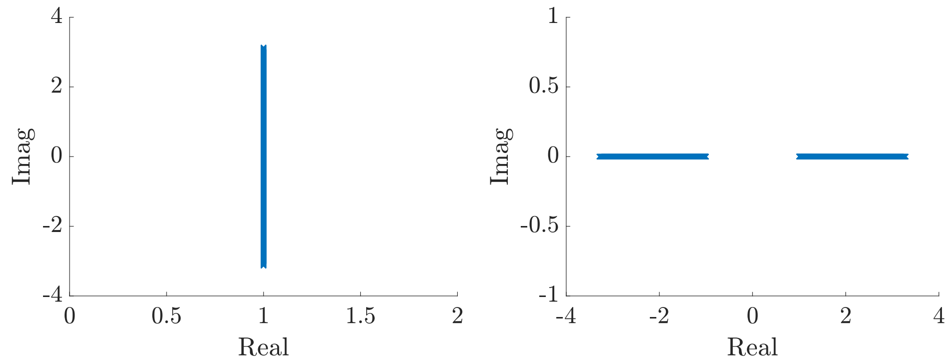
The preconditioner $A_R := A_n(f_R)$ is positive definite since $f_R(\theta) = 2 - 2\cos(\theta)$ is essentially positive. Indeed, A_R is the second-order finite difference matrix, namely the tridiagonal matrix with 2 on the diagonal and -1 on the sub- and superdiagonals. Accordingly, A_R can be applied directly with $O(n)$ cost. For comparison we also apply the optimal circulant preconditioner C_n and its absolute value counterpart $|C_n|$. (The optimal circulant outperformed the Strang and superoptimal circulant preconditioners for this problem.) The absolute value circulant approximates A_M.

Table 5.1 shows that A_R requires fewer iterations than C_n for MINRES and LSQR, and that MINRES with A_R is the fastest method overall. The good performance of A_R with MINRES can be explained by the clustered eigenvalues of $A_R^{-1} Y_n A_n$. Theorem 3.4 tells us that these eigenvalues lie in $[-1-\pi, -1] \cup [1, 1+\pi]$, and Figure 5.1 (b) shows that these bounds are tight. As discussed in [21], the eigenvalues of $A_R^{-1} A_n$ are also nicely clustered (see Figure 5.1 (a)), with real part equal to 1, and imaginary part in $[-\pi, \pi]$. Although we cannot rigorously link this eigenvalue characterization

[3]Code is available from https://github.com/jpestana/fracdiff.

Table 5.1
Iteration numbers and CPU times (in parentheses) for the optimal circulant preconditioner C_n and tridiagonal preconditioner A_R for Example 5.1.

n	GMRES				LSQR				MINRES			
	C_n		A_R		C_n		A_R		$\|C_n\|$		A_R	
1023	37	(0.058)	67	(0.067)	105	(0.15)	62	(0.05)	82	(0.057)	68	(0.029)
2047	48	(0.13)	68	(0.12)	186	(0.4)	67	(0.081)	111	(0.12)	70	(0.046)
4095	62	(0.25)	69	(0.22)	—	—	73	(0.13)	170	(0.21)	71	(0.065)
8191	—	—	72	(0.51)	—	—	78	(0.2)	—	—	72	(0.13)



(a) A_n (b) Y_nA_n

Fig. 5.1. *Eigenvalues of $A_R^{-1}A_n$ and $A_R^{-1}Y_nA_n$ for Example* 5.1 *with* $n = 2047$.

to the rate of GMRES convergence, Table 5.1 indicates that in this case, A_R is also a reasonable preconditioner for GMRES.

We now consider A_M, which is dense since $|f(\theta)| = (2-2\cos(\theta))\sqrt{1+\theta^2}$. Accordingly, as well as applying A_M exactly—to confirm our theoretical results—we approximate A_M via our V-cycle multigrid method with two pre- and two postsmoothing steps, the coarsest grid of dimension 15, $\omega = 0.1$ for GMRES, $\omega = 0.4$ for LSQR, and $\omega = 0.5$ for MINRES. For LSQR, multigrid with A_M gave lower timings and iteration counts than multigrid with A_n, and so was used instead.

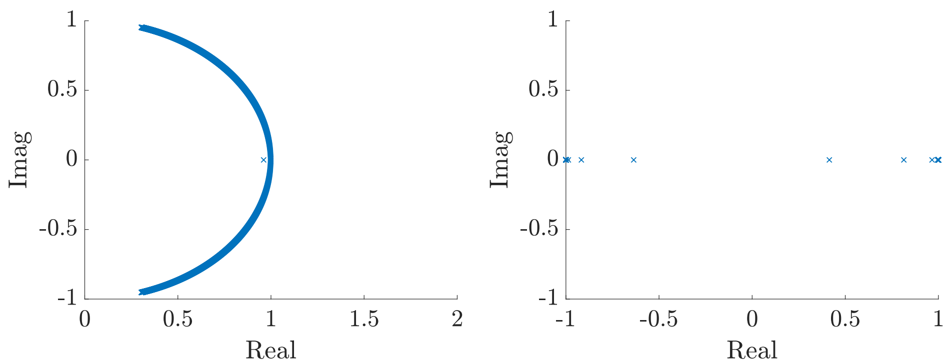
Iteration counts and CPU times (excluding the time to construct A_M but including the time to set up the multigrid preconditioner) are given in Table 5.2. Both A_M and its multigrid approximation give lower iteration counts than A_R, with the multigrid method especially effective for MINRES applied to the symmetrized system. However, timings are higher than for A_R since the $O(n\log(n))$ multigrid method is more expensive than the $O(n)$ solve with A_R. The eigenvalues of $A_M^{-1}Y_nA_n$, when $n = 2047$, are as expected from Theorem 3.5 (see Figure 5.2), since all eigenvalues lie in $[-1, 1]$. Indeed, most cluster at the endpoints of this interval. The eigenvalues of $A_M^{-1}A_n$ are also localized, but not as clustered, indicating that the spectrum of $A_M^{-1}A_n$ may differ significantly from that of $A_M^{-1}Y_nA_n$.

Example 5.2. We now examine the linear system obtained by discretizing a fractional diffusion problem from [3], which we alter so as to make it nonsymmetric. The problem is to find $u(x,t)$ that satisfies

$$\frac{\partial u(x,t)}{\partial t} = d_+\frac{\partial_+^\alpha u(x,t)}{\partial x^\alpha} + d_-\frac{\partial_-^\alpha u(x,t)}{\partial x^\alpha} + f(x,t), \quad (x,t) \in (0,1)\times(0,1], \tag{5.1}$$

TABLE 5.2
Iteration numbers and CPU times (in parentheses) for the exact preconditioner A_M and its multigrid approximation $MG(A_M)$ for Example 5.1. The second column shows the time needed to compute the elements of A_M.

n	A_M time	GMRES		LSQR		MINRES	
		A_n	$MG(A_n)$	A_n	$MG(A_M)$	A_M	$MG(A_M)$
1023	6.4	1 (0.06)	39 (0.15)	1 (0.068)	33 (0.11)	11 (0.11)	24 (0.044)
2047	21	1 (0.28)	41 (0.28)	1 (0.33)	37 (0.24)	11 (0.6)	24 (0.082)
4095	73	1 (1.9)	39 (0.36)	1 (1.9)	39 (0.27)	12 (3.6)	25 (0.096)
8191	2.5×10^2	1 (8.7)	42 (0.88)	1 (11)	43 (0.67)	12 (22)	25 (0.21)



(a) A_n (b) $Y_n A_n$

FIG. 5.2. *Eigenvalues of $A_M^{-1}A_n$ and $A_M^{-1}Y_nA_n$ for Example 5.1 with $n = 2047$.*

where $\alpha \in (1, 2)$, and d_+ and d_- are nonnegative constants. We impose the absorbing boundary conditions $u(x \le 0, t) = u(x \ge 1, t) = 0$, $t \in [0, 1]$, while $u(x, 0) = 80\sin(20x)\cos(10x)$, $x \in [0, 1]$. The Riemann–Liouville derivatives in (5.1) are

$$\frac{\partial_+^\alpha u(x,t)}{\partial x^\alpha} = \frac{1}{\Gamma(n-\alpha)}\frac{\partial^n}{\partial x^n}\int_L^x \frac{u(\xi,t)}{(x-\xi)^{\alpha+1-n}}\mathrm{d}\xi,$$
$$\frac{\partial_-^\alpha u(x,t)}{\partial x^\alpha} = \frac{(-1)^n}{\Gamma(n-\alpha)}\frac{\partial^n}{\partial x^n}\int_x^R \frac{u(\xi,t)}{(\xi-x)^{\alpha+1-n}}\mathrm{d}\xi,$$

where n is the integer for which $n - 1 < \alpha \le n$.

Discretizing by the shifted Grünwald–Letnikov method in space, and the backward Euler method in time [24, 25], gives the linear system

$$\underbrace{(\nu I + d_+ L_\alpha + d_- L_\alpha^T)}_{A} u^m = \nu u^{m-1} + h^\alpha f^m, \tag{5.2}$$

$$L_\alpha = -\begin{bmatrix} g_{\alpha,1} & g_{\alpha,0} & & & \\ g_{\alpha,2} & g_{\alpha,1} & g_{\alpha,0} & & \\ \vdots & \ddots & \ddots & \ddots & \\ g_{\alpha,n-1} & & \ddots & \ddots & g_{\alpha,0} \\ g_{\alpha,n} & g_{\alpha,n-1} & \cdots & g_{\alpha,2} & g_{\alpha,1} \end{bmatrix}, \tag{5.3}$$

where $g_{\alpha,k} = (-1)^k\binom{\alpha}{k}$, $\nu = \frac{\tau}{h^\alpha}$, and $h = \frac{1}{n+1}$. We set $\tau = 1/\lceil n^\alpha \rceil$, which makes ν constant, so that all of the theory in section 3 can be directly applied, but comparable results are obtained for $\tau = 1/n$. Stated CPU times and iteration counts in this example are for the first time step. (Iteration counts and timings decrease at later time steps.) CPU times include the preconditioner setup time and solve time.

Entries of A in (5.2) are generated by [10]

$$\varphi(\theta) = \nu + d_+ f_\alpha(\theta) + d_- f_\alpha(-\theta), \qquad f_\alpha(\theta) = -\mathrm{e}^{-\mathrm{i}\theta}\left(1 - \mathrm{e}^{\mathrm{i}\theta}\right)^\alpha.$$

The real part of φ is essentially positive, so $A_R = (A_n + A_n^T)/2$ is positive definite. However, since A_R is dense, we approximate it by our V-cycle multigrid method (analyzed in [32]) with the coarsest grid of dimension 127, two pre- and two postsmoothing steps, and $\omega = 0.7$ for all Krylov solvers. The matrix A_M is also dense and positive definite, and we approximate it using two different approaches. The first is the absolute value Strang preconditioner discussed at the end of subsection 3.2. The second is multigrid (with the same parameters as for A_R, except that we use one pre- and one postsmoothing step) applied to a banded Toeplitz approximation of A_M. Specifically, if r and c are the first row and column of A_M, respectively, when $\alpha = 1.25$ we compute the first 50 elements in r and c, and when $\alpha > 1.25$ we take the first $\lceil \beta(1.1)^{\log_2(n+1)} \rceil$ elements in r and c, where $\beta = 40$ when $\alpha = 1.5$ and $\beta = 100$ when $\alpha = 1.75$. This balances the time to compute these coefficients and the resulting MINRES iteration count.

We see from Table 5.3 that our approximations to A_R and A_M are robust with respect to n, but both require slightly more iterations for larger α. The multigrid preconditioner for A_R requires fewer iterations than the circulant, but the latter results in a lower CPU time because the preconditioner application is cheap, and indeed the absolute value preconditioner with MINRES is the fastest method overall. Of the multigrid methods, the approximation to A_R with MINRES is fastest for $\alpha \le 1.5$, while the multigrid approximation of A_n with GMRES is slightly faster for large α.

TABLE 5.3
Iteration numbers and CPU times (in parentheses) for the Strang circulant C_n, absolute value Strang circulant $|C_n|$, and multigrid preconditioners when $d_+ = 0.5$ and $d_- = 1$ for Example 5.2.

α	n	GMRES C_n		GMRES $MG(A_n)$		LSQR C_n		LSQR $MG(A_n)$		MINRES $\|C_n\|$		MINRES $MG(A_M)$		MINRES $MG(A_R)$	
1.25	1023	5	(0.01)	4	(0.016)	6	(0.011)	6	(0.02)	10	(0.0084)	12	(0.18)	8	(0.014)
	4095	6	(0.017)	4	(0.045)	6	(0.016)	6	(0.053)	10	(0.013)	12	(0.18)	8	(0.043)
	16383	6	(0.065)	4	(0.17)	6	(0.066)	7	(0.22)	10	(0.054)	13	(0.32)	8	(0.17)
	65535	6	(0.25)	4	(0.66)	6	(0.25)	7	(0.76)	9	(0.19)	13	(0.82)	8	(0.6)
	262143	6	(0.99)	4	(4.4)	6	(1)	7	(5)	9	(0.72)	13	(4.5)	8	(4.3)
1.5	1023	6	(0.0062)	4	(0.021)	6	(0.0062)	7	(0.025)	10	(0.0048)	13	(0.37)	8	(0.013)
	4095	6	(0.018)	4	(0.046)	6	(0.018)	7	(0.061)	10	(0.015)	13	(0.5)	8	(0.044)
	16383	6	(0.062)	4	(0.17)	6	(0.067)	7	(0.21)	9	(0.05)	13	(0.76)	9	(0.19)
	65535	6	(0.24)	5	(0.7)	7	(0.28)	8	(0.8)	9	(0.19)	13	(1.4)	9	(0.66)
	262143	6	(0.93)	5	(5.2)	7	(1.1)	8	(5.7)	9	(0.72)	15	(6.1)	9	(4.7)
1.75	1023	6	(0.0085)	5	(0.043)	7	(0.0088)	7	(0.021)	9	(0.0062)	13	(1.6)	9	(0.014)
	4095	6	(0.015)	5	(0.046)	7	(0.015)	8	(0.058)	9	(0.01)	15	(2.2)	9	(0.036)
	16383	6	(0.062)	5	(0.2)	7	(0.075)	8	(0.24)	9	(0.049)	15	(3.2)	10	(0.21)
	65535	6	(0.24)	5	(0.71)	7	(0.28)	8	(0.81)	9	(0.19)	15	(4.8)	11	(0.75)
	262143	6	(0.9)	5	(5.2)	7	(1.1)	9	(6.3)	9	(0.72)	16	(11)	11	(5.7)

In Table 5.4 we investigate the effect of d_+ and d_-, i.e., of nonsymmetry, on the preconditioners. The results are unchanged when d_+ and d_- are swapped, so we tabulate results for $d_+ \le d_-$ only. As expected, our approximation to A_R is best suited to problems for which d_+ and d_- do not differ too much. The hardest problem for A_R is when $d_+ = 0$, since in this case A_n is a Hessenberg matrix and hence highly

TABLE 5.4
Iteration numbers and CPU times (in parentheses) for the Strang circulant C_n, absolute value, Strang circulant $|C_n|$, and multigrid preconditioners when $\alpha = 1.5$ for Example 5.2.

(d_+, d_-)	n	GMRES C_n	GMRES $MG(A_n)$	LSQR C_n	LSQR $MG(A_n)$	MINRES $\lvert C_n \rvert$	MINRES $MG(A_M)$	MINRES $MG(A_R)$
(0,3)	4095	5 (0.031)	5 (0.053)	7 (0.02)	5 (0.059)	10 (0.016)	10 (0.47)	13 (0.049)
	16383	4 (0.044)	5 (0.21)	7 (0.078)	5 (0.23)	10 (0.058)	10 (0.83)	13 (0.27)
	65535	4 (0.18)	6 (0.84)	7 (0.29)	6 (0.93)	10 (0.22)	10 (1.6)	14 (0.97)
	262143	4 (0.75)	6 (6.2)	7 (1.2)	6 (6.7)	11 (0.92)	11 (6.8)	14 (7.1)
(1,3)	4095	7 (0.015)	5 (0.042)	7 (0.014)	5 (0.045)	10 (0.013)	10 (0.4)	9 (0.037)
	16383	7 (0.072)	5 (0.21)	7 (0.078)	5 (0.23)	11 (0.06)	10 (0.81)	10 (0.21)
	65535	7 (0.29)	5 (0.71)	8 (0.33)	5 (0.77)	11 (0.24)	11 (1.6)	10 (0.7)
	262143	7 (1.1)	6 (6.2)	8 (1.3)	6 (6.6)	11 (0.93)	11 (6.6)	10 (5.3)
(1,1)	4095	6 (0.013)	4 (0.031)	6 (0.013)	5 (0.041)	10 (0.01)	9 (0.39)	9 (0.034)
	16383	6 (0.064)	4 (0.17)	6 (0.068)	5 (0.23)	10 (0.058)	9 (0.79)	9 (0.19)
	65535	6 (0.25)	4 (0.57)	6 (0.26)	5 (0.77)	9 (0.19)	9 (1.4)	9 (0.64)
	262143	6 (0.93)	5 (5.2)	7 (1.2)	5 (5.8)	9 (0.79)	9 (5.9)	9 (4.9)

nonsymmetric. However, even here the iteration numbers are fairly low, since the eigenvalues are bounded away from the origin independently of n. The circulant and multigrid preconditioners based on A_M are not greatly affected by altering d_+ and d_-.

The low iteration numbers and mesh-size–independent results for A_R in Table 5.4 are explained by Theorem 3.4 and the relatively small upper bound (3.2), which describes how far eigenvalues of $A_R^{-1} Y_n A_n$ can deviate from 1 in magnitude. This bound is 0 when $d_+ = d_-$ or when $\alpha = 2$, since in both cases A_n is symmetric. However, Table 5.5 shows that even when A_n is nonsymmetric, the bound is quite small. Additionally, it does not change when the values of d_+ and d_- are swapped.

TABLE 5.5
Upper bound in (3.2) *for Example* 5.2.

α	(d_+, d_-) (0,3)	(1,3)	(0.5,1)	(1,1)
1	1.13	0.67	0.25	0.00
1.25	0.70	0.39	0.17	0.00
1.5	0.42	0.23	0.11	0.00
1.75	0.20	0.11	0.05	0.00

Example 5.3. We now solve a two-level Toeplitz problem that also arises from fractional diffusion and is based on the symmetric problem in [3]. We seek $u(x, y, t)$ in the domain $\Omega = (0, 1)^2 \times (0, 1]$ that satisfies

$$\begin{aligned}\frac{\partial u(x,y,t)}{\partial t} =& d_+ \frac{\partial_+^\alpha u(x,y,t)}{\partial x^\alpha} + d_- \frac{\partial_-^\alpha u(x,y,t)}{\partial x^\alpha} \\ &+ e_+ \frac{\partial_+^\beta u(x,y,t)}{\partial y^\beta} + e_- \frac{\partial_-^\beta u(x,y,t)}{\partial y^\beta} + f(x,y,t),\end{aligned}$$

where $\alpha, \beta \in (1, 2)$, and d_+, d_-, e_+, and e_- are nonnegative constants. We impose absorbing boundary conditions, and the initial condition is $u(x, 0) = 100 \sin(10x) \cos(y) + \sin(10t)xy$.

We again discretize by the shifted Grünwald–Letnikov method in space, and the backward Euler method in time [24, 25], which leads to the following linear system:

$$\underbrace{\left(I_{n_x n_y} - I_{n_y} \otimes L_x - L_y \otimes I_{n_x}\right)}_{A_n} u^m = u^{m-1} + \tau f^m. \tag{5.4}$$

Here n_x and n_y are the number of spatial degrees of freedom in the x and y directions, respectively; we choose $n_x = n_y = n$. Also,

$$L_x = \frac{\tau}{h_x^\alpha}(d_+ L_\alpha + d_- L_\alpha^T), \qquad L_y = \frac{\tau}{h_y^\beta}(e_+ L_\beta + e_- L_\beta^T),$$

where L_α is given by (5.3), and $h_x = 1/(n_x+1)$ and $h_y = 1/(n_y+1)$ are the mesh widths in the x and y directions. Unless $\alpha = \beta$, both τ/h_x^α and τ/h_y^β cannot be independent of n; we choose $\tau = 1/\lceil n_x^\alpha \rceil$. Note that the theory for A_R still applies in this case. Stated CPU times and iteration counts are again for the first time step.

It is too costly to approximate A_M by a banded Toeplitz matrix or a multigrid method, simply because it is expensive to obtain the Fourier coefficients of $|f|$, and so we present results for a multigrid approximation to A_R only. We also apply the nonsymmetric block circulant $C_n = I_{n_x n_y} - I_{n_y} \otimes C_x - C_y \otimes I_{n_x}$ preconditioner and the symmetric positive definite block circulant $|C_n| = I_{n_x n_y} + I_{n_y} \otimes |C_x| + |C_y| \otimes I_{n_x}$ preconditioner, where C_x and C_y are Strang circulant approximations to L_x and L_y, respectively. Our multigrid method comprises four pre- and four postsmoothing steps and a damping parameter of 0.9. The coarsest grid has $n_x = n_y = 7$.

The results in Table 5.6 show that the multigrid approximation of A_R gives mesh-size-independent iteration counts, and that MINRES with this preconditioner is the fastest method for larger problems. For the block circulant preconditioners, we see different behaviors depending on whether $\alpha > \beta$. Specifically, when $\alpha > \beta$, $\tau/h_y^\beta \to 0$ as $n \to \infty$, which makes this problem easier to solve in some sense. On the other hand, when $\alpha < \beta$, the problems become harder to solve as n increases, and the block circulants with LSQR and MINRES suffer from growing iteration counts.

TABLE 5.6

Iteration numbers and CPU times (in parentheses) for the circulant preconditioners C_n and $|C_n|$ and for the multigrid preconditioners when $d_+ = 2$, $d_- = 0.5$, $e_+ = 0.3$, and $e_- = 1$ for Example 5.3.

(α,β)	n^2	GMRES				LSQR				MINRES			
		C_n		$MG(A_n)$		C_n		$MG(A_n)$		$\lvert C_n\rvert$		$MG(A_R)$	
	961	16	(0.032)	5	(0.011)	23	(0.033)	5	(0.014)	42	(0.028)	12	(0.013)
(1.5,1.25)	16129	15	(0.12)	5	(0.058)	21	(0.11)	6	(0.07)	39	(0.12)	12	(0.07)
	261121	14	(1.5)	5	(1.1)	18	(1.4)	6	(1.3)	34	(1.5)	12	(1.0)
	961	21	(0.029)	4	(0.0086)	28	(0.038)	4	(0.0099)	43	(0.027)	10	(0.01)
(1.5,1.75)	16129	21	(0.16)	4	(0.051)	35	(0.2)	5	(0.065)	57	(0.19)	10	(0.049)
	261121	20	(2.1)	5	(1.2)	40	(3.1)	5	(1.0)	67	(2.8)	12	(0.97)

6. Conclusions. In this paper we presented two novel ideal preconditioners for (multilevel) Toeplitz matrices by considering the generating function f. The first, A_R, is formed using the real part of f. While it works best when the (multilevel) Toeplitz matrix is close to symmetric, it is reasonably robust with respect to the degree of nonsymmetry. This performance is likely attributable to the eigenvalue distribution, which remains bounded away from the origin. Our second preconditioner, A_M, is based on $|f|$, and its performance is less affected by nonsymmetry. The bigger challenge is to construct efficient approximations to A_M in the multilevel case.

Our numerical results not only illustrate the effectiveness of the preconditioners but also highlight the value of symmetrization, which enables us to compute bounds on convergence rates that depend only on the scalar function f. Additionally, the combination of symmetrization and preconditioned MINRES can be more computationally efficient than applying GMRES or LSQR to these problems.

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