A Note on Superoptimal Generalized Circulant Preconditioners

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Abstract

Circulant matrices can be effective preconditioners for linear systems of equations with a Toeplitz matrix. Several approaches to construct such preconditioners have been described in the literature. This paper focuses on the superoptimal circulant preconditioners proposed by Tyrtyshnikov, and investigates a generalization obtained by allowing generalized circulant matrices. Numerical examples illustrate that the new preconditioners so obtained can give faster convergence than available preconditioners based on circulant and generalized circulant matrices.

Key words: Toeplitz matrix, circulant matrix, generalized circulant, Krylov subspace methods, preconditioning

1 Introduction

Linear systems of equations with a nonsingular Toeplitz matrix,

$$A_n = \begin{bmatrix} a_0 & a_{-1} & a_{-2} & \dots & a_{-n+1} \\ a_1 & a_0 & a_{-1} & \dots & a_{-n+2} \\ \vdots & & \ddots & \ddots & \vdots \\ a_{n-2} & \dots & a_1 & a_0 & a_{-1} \\ a_{n-1} & \dots & a_2 & a_1 & a_0 \end{bmatrix} \in \mathbf{C}^{n\times n}, \tag{1}$$

arise, for instance, from the discretization of certain integral and differential equations, as well as in signal processing. A Toeplitz matrix (1) is said to be an $\{e^{i\theta}\}$-*circulant* matrix, or briefly a *generalized circulant*, if

$$a_\ell = e^{i\theta} a_{-n+\ell}, \qquad 0 \leq \ell < n, \tag{2}$$

for $i = \sqrt{-1}$ and some angle $\theta \in (-\pi, \pi]$. The angles $\theta = 0$ and $\theta = \pi$ give circulants and skew-circulants, respectively. Let $\mathbb{C}_{n,\theta}$ denote the set of $\{e^{i\theta}\}$-*circulant* matrices in $\mathbf{C}^{n\times n}$. Thus, $\mathbb{C}_{n,0}$ is the set of circulant matrices of order n. It is convenient to also define the set $\mathbb{C}_n$ of all generalized circulants of order n, i.e., $\mathbb{C}_n = \cup_{-\pi<\theta\leq\pi} \mathbb{C}_{n,\theta}$.

We associate with the infinite matrix A_∞ the function

$$f(x) = \sum_{k=-\infty}^{\infty} a_k e^{ikx}, \qquad x \in [-\pi, \pi],$$

which is referred to as the *symbol* for the sequence of Toeplitz matrices A_n, $n = 1, 2, 3, \ldots$. The entries of A_n are the Fourier coefficients of f:

$$a_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) e^{-ikx} dx, \qquad k = 0, \pm 1, \pm 2, \ldots \ .$$

When f is a real-valued function, the matrices A_n are Hermitian. If, in addition, f is positive, then the matrices A_n are positive definite. Generating functions provide information about the distribution of the eigenvalues of the matrices A_n, $n = 1, 2, 3, \ldots$; see, e.g., Böttcher [1] for an insightful discussion on Toeplitz matrices.

This paper is concerned with the iterative solution of Toeplitz systems of equations

$$A_n x = b, \qquad A_n \in \mathbf{C}^{n\times n}, \qquad x, b \in \mathbf{C}^n, \tag{3}$$

by Krylov subspace methods. A preconditioner $C \in \mathbf{C}^{n\times n}$, that approximates A_n in some sense, often is used in order to increase the rate of convergence of the iterative method. When both A_n and C are Hermitian positive definite, we apply the conjugate gradient (CG) method to the solution of the preconditioned system

$$C^{-1} A_n x = C^{-1} b. \tag{4}$$

If A_n or C are not Hermitian positive definite, then one can solve (4) by an iterative method designed for the solution of linear systems of equations with a non-Hermitian nonsingular matrix, such as GMRES, or apply the CG method to the normal equations associated with (4); see [16] for discussions on many Krylov subspace iterative methods.

Circulant matrices can be effective preconditioners for (3). Many different approaches to construct such preconditioners are described in [2,11]. Strang [17] proposed to determine a circulant preconditioner S_n for a Hermitian positive definite Toeplitz matrix A_n by requiring S_n to have as many central diagonals equal to those of A_n as possible. The preconditioners S_n are commonly referred to as Strang preconditioners. Subsequently, T. Chan [4] suggested to use the solution C_n of

$$\|C_n - A_n\|_F = \min_{C \in \mathbb{C}_{n,0}} \|C - A_n\|_F, \quad C_n \in \mathbb{C}_{n,0}, \tag{5}$$

as preconditioner, where $\|\cdot\|_F$ denotes the Frobenius norm. This preconditioner often is referred to as *optimal* preconditioner. Tyrtyshnikov [19] proposed to use the solution of

$$\min_{C \in \mathbb{C}'_{n,0}} \|I - C^{-1} A_n\|_F \tag{6}$$

as preconditioner, where $\mathbb{C}'_{n,0}$ denotes the subset of nonsingular matrices in $\mathbb{C}_{n,0}$. Tyrtyshnikov [19] referred to the preconditioners so determined as *superoptimal* preconditioners. Comparisons of these preconditioners with other circulant preconditioners are reported in [18], as well as in [2,11]. Further circulant preconditioners that are solutions of certain minimization problems relative to the Frobenius norm are considered in [10]. We denote the solution of (6) by T_n.

Preconditioning requires repeated evaluation of the product of the inverse of the preconditioner and a vector. A reason for the popularity of circulant preconditioners is that the spectral factorization of a circulant of order n can be computed in only $\mathcal{O}(n \log n)$ arithmetic floating-point operations (flops) with the aid of the fast Fourier transform, and this factorization makes it possible to evaluate the product of the inverse of the preconditioner and a vector in $\mathcal{O}(n \log n)$ flops.

The spectral factorization of a generalized circulant of order n also can be evaluated in $\mathcal{O}(n \log n)$ flops; see Section 2 or [6,11] for details. It therefore can be attractive to apply nonsingular generalized circulants as preconditioners. Potts and Steidl [15] applied these preconditioners to Toeplitz systems with ill-conditioned matrices. Generalized circulant preconditioners are determined by an angle θ, cf. (2), which can be chosen to obtain a preconditioner with better properties than a standard circulant preconditioner, which corresponds to the angle $\theta = 0$. Fischer and Huckle [7] generalized the optimal preconditioner proposed by T. Chan by minimizing (5) over generalized circulants. This generalization also is investigated in [12]. An extension of the Strang preconditioner to generalized circulants has recently been proposed in [13]. Certain skew-circulant preconditioners, which are obtained when $\theta = \pi$, are discussed in [2,9,11].

It is natural to generalize the superoptimal preconditioner introduced by Tyrtyshnikov by minimizing (6) over generalized circulants and investigate whether the angle θ can be chosen to yield superoptimal generalized circulant preconditioners with desirable properties. It is the purpose of this paper to address this question. We remark that other extensions of the superoptimal preconditioners have recently been discussed by Pang and Jin [14], who consider Hermitian preconditioners with an arbitrary but fixed unitary eigenvector matrix, and by Chen and Jin [5], who allow the matrix A_n to be singular.

This paper is organized as follows. Section 2 discusses properties of our generalization of the superoptimal preconditioners by Tyrtyshnikov, computed examples that illustrate their performance are presented in Section 3, and concluding remarks can be found in Section 4.

2 Generalized superoptimal preconditioners

A generalized circulant matrix can be diagonalized by the product of the Fourier matrix and a suitable unitary diagonal matrix; see, e.g., [6,11].

Proposition 2.1 *An $\{e^{i\theta}\}$-circulant matrix $\tilde{C} \in \mathbf{C}^{n\times n}$, whose entries satisfy (2), has the spectral factorization*

$$\tilde{C} = F_\theta D F_\theta^H, \tag{7}$$

where $F_\theta \in \mathbf{C}^{n\times n}$ is the unitary generalized Fourier matrix with entries

$$[F_\theta]_{h+1,k+1} = \frac{1}{\sqrt{n}} e^{-i\frac{2\pi h}{n}(k-\frac{\theta}{2\pi})}, \qquad 0 \le h,k < n, \tag{8}$$

and the diagonal matrix $D \in \mathbf{C}^{n\times n}$ is independent of θ. The superscript ^{H} denotes transposition and complex conjugation.

The spectral factorization (7) can be computed with the aid of the fast Fourier transform in $\mathcal{O}(n\log n)$ flops, and can be applied to evaluate $\tilde{C}^{-1}y$ for any $y \in \mathbf{C}^n$ in $\mathcal{O}(n\log n)$ flops, assuming that $\tilde{C}^{-1}$ exists.

We are interested in determining the nonsingular generalized circulant $\tilde{C}$ that solves

$$\min_{\tilde{C}\in\mathbb{C}'_{n,\theta}} \|I - \tilde{C}^{-1}A_n\|_F, \tag{9}$$

where $\mathbb{C}'_{n,\theta}$ stands for the subset of nonsingular matrices in $\mathbb{C}_{n,\theta}$. We denote the generalized circulant that solves (9) by $\tilde{T}_{n,\theta}$ and refer to it as a superoptimal $\{e^{i\theta}\}$-circulant preconditioner. The special case when $\theta = 0$ yields the superoptimal preconditioner proposed by Tyrtyshnikov [19].

Theorem 2.2 *Let $A_n \in \mathbf{C}^{n\times n}$ be a nonsingular Toeplitz matrix (1). The superoptimal $\{e^{i\theta}\}$-circulant preconditioner $\tilde{T}_{n,\theta}$ for A_n is given by*

$$\tilde{T}_{n,\theta} = F_\theta D_\theta F_\theta^H,$$

where

$$D_\theta = \mathrm{diag}\left[\frac{w_1(\theta)}{\bar{u}_1(\theta)}, \frac{w_2(\theta)}{\bar{u}_2(\theta)}, \ldots, \frac{w_n(\theta)}{\bar{u}_n(\theta)}\right] \in \mathbf{C}^{n\times n}, \tag{10}$$

$$u_k(\theta) = [F_\theta^H A_n F_\theta]_{kk}, \quad w_k(\theta) = [F_\theta^H A_n A_n^H F_\theta]_{kk}, \quad k = 1, 2, \ldots, n, \tag{11}$$

and F_θ is the generalized Fourier matrix defined by (8). The bar in (10) denotes complex conjugation.

Proof. The result can be shown by generalizing the proof of Theorem 2.12 in [2]. Any nonsingular $\{\mathrm{e}^{\mathrm{i}\theta}\}$-circulant can be represented by

$$C_\theta = F_\theta \Lambda F_\theta^H,$$

where

$$\Lambda = \mathrm{diag}[\lambda_1, \lambda_2, \ldots, \lambda_n] \in \mathbf{C}^{n\times n}$$

is nonsingular. Therefore,

$$\min_{C_\theta \in \mathbb{C}'_{n,\theta}} \|I - C_\theta A_n\|_F^2 = \min_{\lambda_1,\lambda_2,\ldots,\lambda_n} \sum_{k=1}^{n} (1 - \lambda_k u_k(\theta) - \bar{u}_k(\theta)\bar{\lambda}_k + \lambda_k w_k(\theta)\bar{\lambda}_k). \tag{12}$$

We observe that the quotients

$$\lambda_k = \bar{u}_k(\theta)/w_k(\theta), \quad k = 1, 2, \ldots, n,$$

minimize (12). Substituting the matrix

$$D_\theta = \mathrm{diag}\left[\lambda_1^{-1}, \lambda_2^{-1}, \ldots, \lambda_n^{-1}\right] \in \mathbf{C}^{n\times n}$$

into (7) yields the superoptimal $\{\mathrm{e}^{\mathrm{i}\theta}\}$-circulant preconditioner $\tilde{T}_{n,\theta} = C_\theta^{-1}$. $\square$

Corollary 2.3 *Let $A_n \in \mathbf{C}^{n\times n}$ be a nonsingular Toeplitz matrix (1). The superoptimal $\{\mathrm{e}^{\mathrm{i}\theta}\}$-circulant preconditioner $\tilde{T}_{n,\theta}$ for A_n is given by*

$$\tilde{T}_{n,\theta} = c_\theta(A_n A_n^H) c_\theta(A_n^H)^{-1},$$

where $c_\theta(M)$ denotes the best $\{\mathrm{e}^{\mathrm{i}\theta}\}$-circulant approximation of $M \in \mathbf{C}^{n\times n}$ in the Frobenius norm.

Proof. We obtain from Theorem 2.2 that

$$\tilde{T}_{n,\theta} = F_\theta W_\theta U_\theta^{-H} F_\theta^H = F_\theta W_\theta F_\theta^H F_\theta U_\theta^{-H} F_\theta^H,$$

where

$$U_\theta = \mathrm{diag}[u_1(\theta), u_2(\theta), \ldots, u_n(\theta)], \quad W_\theta = \mathrm{diag}[w_1(\theta), w_2(\theta), \ldots, w_n(\theta)].$$

Finding $c_\theta(A_n^H)$ means minimizing $\|C - A_n^H\|_F = \|F_\theta D F_\theta^H - A_n^H\|_F$ and, since the Frobenius norm is unitarily invariant, this is equivalent to the minimization of $\|D - F_\theta^H A_n^H F_\theta\|_F$ over all diagonal matrices $D \in \mathbf{C}^{n\times n}$. The solution of the latter problem is the diagonal part of $F_\theta^H A_n^H F_\theta$; see [2, Theorem 2.7(i)]. Therefore, $c_\theta(A_n^H)^{-1}$ is equal to $F_\theta U_\theta^{-H} F_\theta^H$. Analogously, $c_\theta(A_n A_n^H) = F_\theta W_\theta F_\theta^H$. $\square$

It is easy to see that when the Toeplitz matrix A_n is Hermitian, so is $\tilde{T}_{n,\theta}$. If, in addition, A_n is positive definite, then $\tilde{T}_{n,\theta}$ is as well. We refer to the generalized circulant preconditioner $\tilde{C} \in \mathbb{C}_n'$, that satisfies

$$\|I - \tilde{C}^{-1} A_n\|_F = \min_{C \in \mathbb{C}_n'} \|I - C^{-1} A_n\|_F$$

as the optimal superoptimal generalized circulant preconditioner, where $\mathbb{C}_n'$ denotes the subset of the nonsingular matrices in $\mathbb{C}_n$.

Corollary 2.4 *The optimal superoptimal generalized circulant preconditioner lives in $\mathbb{C}_{n,\theta^*}$, where $\theta^* \in (-\pi, \pi]$ satisfies*

$$\sum_{k=1}^{n} \left(1 - \frac{|u_k(\theta^*)|^2}{w_k(\theta^*)}\right) = \min_{\theta \in (-\pi,\pi]} \sum_{k=1}^{n} \left(1 - \frac{|u_k(\theta)|^2}{w_k(\theta)}\right) \tag{13}$$

with $u_k(\theta)$ and $w_k(\theta)$ defined by (11).

Proof. The result follows by considering the minimization problem (12). Let $\lambda_k = \lambda_k(\theta)$, $k = 1, 2, \ldots, n$, be the minimizers of the sum (12) for fixed θ. Then the sum simplifies to (13). $\square$

The matrix-matrix products in (11) between the matrices F_θ^H and any $n \times n$ matrix can be evaluated in $\mathcal{O}(n^2 \log n)$ flops for each value of θ. Therefore the quantities $u_k(\theta)$ and $w_k(\theta)$, $k = 1, 2, \ldots, n$, can be computed in $\mathcal{O}(n^2 \log n)$ flops for each θ in a straightforward manner. Additionally, the Toeplitz structure of A_n can be exploited to accelerate the computation. Efficient algorithms that partition A_n into the sum of lower and upper triangular Toeplitz matrices [19] or, alternatively, when $\theta \in \{0, \pi\}$, partition A_n into the sum of a circulant and a skew-circulant matrix [3] require the evaluation of the fast Fourier transform of just a few n-vectors and, hence, $\mathcal{O}(n \log n)$ flops for each value of θ. When $\theta \notin \{0, \pi\}$, the partitioning used in [3] should be replaced by (14) below.

When a large number of linear systems of equations with a fixed Toeplitz matrix A_n and different right-hand sides are to be solved, then it is meaningful to compute a fairly accurate solution of the minimization problem (13). However, if the preconditioner is to be applied just a few times, then one may consider to reduce the computational effort required to solve this minimization problem by only minimizing the right-hand side of (13) over a small set of equidistant angles θ.

Application of Krylov subspace methods to the preconditioned linear systems of equations (4) with $C = \tilde{T}_{n,\theta}$ requires the computation of matrix-vector products with the matrix $\tilde{T}_{n,\theta}^{-1} A_n$. We evaluate these matrix-vector products without forming the matrix. Instead, we split A_n into two generalized circulants, one of which is an $\{\mathrm{e}^{\mathrm{i}\theta}\}$-circulant, as described by the following result.

Proposition 2.5 ([13]) *The Toeplitz matrix A_n can be expressed as*

$$A_n = \hat{C}_\theta + \check{C}_\psi, \tag{14}$$

where $\hat{C}_\theta$ is an $\{\mathrm{e}^{\mathrm{i}\theta}\}$-circulant and $\check{C}_\psi$ is an $\{\mathrm{e}^{\mathrm{i}\psi}\}$-circulant, for any $-\pi < \theta \neq \psi \leq \pi$.

The special case of (14) when $\theta = 0$ is discussed, e.g., in [11]. The splitting (14) and the factorizations

$$\hat{C}_\theta = F_\theta \hat{\Lambda} F_\theta^H, \quad \check{C}_\psi = F_\psi \check{\Lambda} F_\psi^H,$$

yield, with the notation of the proof of Theorem 2.2, that

$$\tilde{T}_{n,\theta}^{-1} = C_\theta = F_\theta \Lambda F_\theta^H$$

and

$$C_\theta(\hat{C}_\theta + \check{C}_\psi) = F_\theta \Lambda \hat{\Lambda} F_\theta^H + F_\theta \Lambda F_\theta^H F_\psi \check{\Lambda} F_\psi^H.$$

The preconditioned linear system of equations (4) with $C = \tilde{T}_{n,\theta}$ therefore can be expressed in the form

$$\Lambda(\hat{\Lambda} + F_\theta^H F_\psi \check{\Lambda} F_\psi^H F_\theta) y = \Lambda F_\theta^H b, \qquad x = F_\theta y. \tag{15}$$

We use this form in the computations. The normal equations associated with (4) are transformed to a form analogous to (15) before solution with the CG method.

3 Computed examples

This section illustrates the performance of the superoptimal generalized circulant preconditioners. In all computed examples, the initial approximate solution x_0 is the zero vector and the iterations are terminated as soon as an iterate x_k that satisfies

$$\frac{\|b - A_n x_k\|}{\|b\|} \leq 1 \cdot 10^{-10} \tag{16}$$

has been computed. In the first three examples the right-hand side vector b is chosen so that the system (3) has the solution $x = [1, 1, \ldots, 1]^T \in \mathbb{C}^n$. These choices of stopping criterion and right-hand side are the same as for computed examples reported in [2,11].

When comparing $\{e^{i\theta}\}$-circulant preconditioners, we consider a preconditioner to be the "best" if the preconditioned system requires the fewest number of matrix-vector product evaluations to satisfy the stopping criterion (16) with the chosen Krylov subspace method; if several preconditioners require the same smallest number of matrix-vector product evaluations, then the preconditioner that yields the smallest residual error is considered the "best" one. All computations were carried out in MATLAB with about 15 significant decimal digits.

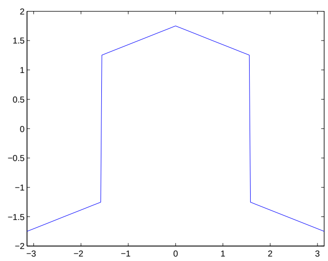

Fig. 1. Example 1: Graph of the generating function (17) with $\varepsilon = 1/256$.

n	$\tilde{S}_n$	residual	$\tilde{C}_n$	residual	$\tilde{T}_n$	residual
32	6	$5.7 \cdot 10^{-13}$	6	$4.5 \cdot 10^{-12}$	5	$4.1 \cdot 10^{-11}$
64	6	$1.7 \cdot 10^{-12}$	6	$1.6 \cdot 10^{-11}$	6	$4.6 \cdot 10^{-13}$
128	6	$2.9 \cdot 10^{-12}$	7	$3.6 \cdot 10^{-12}$	6	$1.1 \cdot 10^{-12}$
256	6	$3.5 \cdot 10^{-11}$	7	$5.9 \cdot 10^{-12}$	6	$1.8 \cdot 10^{-11}$
512	6	$9.0 \cdot 10^{-11}$	7	$4.7 \cdot 10^{-12}$	6	$7.5 \cdot 10^{-11}$
1024	7	$6.1 \cdot 10^{-13}$	7	$2.1 \cdot 10^{-11}$	7	$4.1 \cdot 10^{-13}$

Table 1
Example 1: Number of iterations and relative residual norm for the GMRES method with the generalized circulant Strang preconditioner $\tilde{S}_n$, the optimal generalized circulant preconditioner $\tilde{C}_n$, and the superoptimal generalized circulant preconditioner $\tilde{T}_n$ with $\theta = \pi$. The parameter n shows the order of the matrices.

Example 1. Let the sequence of real symmetric Toeplitz matrices A_n be determined by the real-valued, even, 2π-periodic, continuous symbol $f(x)$ defined on $[-\pi, \pi]$ by

$$f(x) = \begin{cases} \frac{7}{4} - \frac{x}{\pi - 2\varepsilon}, & 0 \le x < \frac{\pi}{2} - \varepsilon, \\ \frac{5}{4} - \frac{5}{4\varepsilon}(x - \frac{\pi}{2} + \varepsilon), & |x - \frac{\pi}{2}| \le \varepsilon, \\ -\frac{5}{4} - \frac{1}{\pi - 2\varepsilon}(x - \frac{\pi}{2} - \varepsilon), & \frac{\pi}{2} + \varepsilon < x \le \pi, \\ f(-x), & -\pi \le x < 0; \end{cases} \tag{17}$$

see Figure 1 for a graph of the function. The eigenvalues of A_n are distributed like $f(-\pi + \frac{2\pi j}{n+1})$, $j = 1, 2, \ldots, n$, for n large; see, e.g., [8, Chapter 5]. We let $\varepsilon = 1/n$. Then the spectrum of A_n is "clustered" in the intervals $[-\frac{7}{4}, -\frac{5}{4}]$ and $[\frac{5}{4}, \frac{7}{4}]$ when n is large.

The Fourier coefficients of the function (17) are given by

$$a_k = \begin{cases} \frac{1}{\pi k^2}\left(\frac{2}{\pi-2\varepsilon} - (-1)^{\frac{k-1}{2}}\left(\frac{2}{\pi-2\varepsilon} - \frac{5}{2\varepsilon}\right)\sin(k\varepsilon)\right), & k = \pm 1, \pm 3, \pm 5, \ldots\ , \\ 0, & k = 0, \pm 2, \pm 4, \ldots\ . \end{cases}$$

They are absolutely summable and, therefore, the function f is in the Wiener class. However, since the matrices A_n are indefinite, this does not guarantee that the spectra of the preconditioned matrices "cluster" at 1 as n is increased. Nevertheless, preconditioning can reduce the number of iterations required significantly. Table 1 compares the superoptimal generalized circulant preconditioner $\tilde{T}_n$ to the generalized circulant Strang preconditioner $\tilde{S}_n$ described in [13], and the optimal generalized circulant preconditioner $\tilde{C}_n$ discussed in [7,12]. We have $\theta^* = \pi$ defined by (13). This yields real preconditioners. The optimal superoptimal generalized circulant preconditioner $\tilde{T}_n$ is best in the sense defined above for all orders n. The "standard" optimal circulant and Strang preconditioners for matrices A_n of even order are singular and cannot be used. Therefore, also the "standard" superoptimal preconditioner cannot be applied.

The "standard" Strang, optimal, and superoptimal preconditioners are nonsingular for matrices of odd order. We therefore compared these preconditioners to their generalized counterparts for the orders $n = 31, 63, 127, \ldots, 1023$. In all these examples the superoptimal generalized circulant preconditioners were the best ones, either because they required the least number of iterations or because they delivered the smallest residual error for the same number of iterations. □

n	$\tilde{S}_n^{NE}$	residual	$\tilde{C}_n$	residual	$\tilde{T}_n$	residual
1024	16	$5.2 \cdot 10^{-12}$	8	$4.9 \cdot 10^{-12}$	7	$7.8 \cdot 10^{-11}$
2048	16	$1.1 \cdot 10^{-11}$	8	$3.5 \cdot 10^{-12}$	7	$5.4 \cdot 10^{-11}$
4096	17	$2.2 \cdot 10^{-11}$	8	$2.4 \cdot 10^{-12}$	7	$3.8 \cdot 10^{-11}$

Table 2

Example 2: Number of iterations and relative residual norm for the preconditioned conjugate gradient method applied to the normal equations associated with (4) with the generalized circulant Strang preconditioner (column $\tilde{S}_n^{NE}$), for GMRES preconditioned by the optimal generalized circulant preconditioner (column $\tilde{C}_n$), and for GMRES preconditioned by the superoptimal generalized circulant preconditioner (column $\tilde{T}_n$) with $\theta = \pi$ for linear systems of equations of even order n.

Example 2. The Toeplitz matrices A_n in this example are non-Hermitian and nonsingular with coefficients

$$a_k = \begin{cases} -\frac{(n-k)^3}{n^3}, & k > 0, \\ 1, & k = 0, \\ \frac{n+k}{n}, & k < 0. \end{cases}$$

Table 2 shows results for the generalized Strang preconditioner $\tilde{S}_n$ used in the normal equations and solved by CG, and for GMRES preconditioned by the optimal and superoptimal generalized circulant preconditioners $\tilde{C}_n$ and $\tilde{T}_n$. The Strang and generalized Strang preconditioners do not perform well when applied to a general non-Hermitian Toeplitz matrix; we therefore applied these preconditioners to the normal equations. We have $\theta^* = \pi$. This is the optimal angle also for the other two generalized preconditioners. The optimal superoptimal generalized circulant preconditioner is seen to perform the best for all orders. Solution of the preconditioned normal equations by the conjugate gradient method is not competitive, because it requires many more iterations than preconditioned GMRES and, additionally, the number of matrix-vector product evaluations is twice the number of iterations, since each iteration requires a matrix-vector product evaluation with the matrix and with its conjugate transpose. When considering matrices A_n of the odd orders $n = 1023, 2047, 4095$, we also found the superoptimal generalized circulant preconditioner to be "best" when compared with the "standard" Strang, optimal, superoptimal preconditioners, and the generalized Strang and optimal preconditioners. We omit tables for the latter results. □

n	$\tilde{S}_n^{NE}$	residual	$\tilde{C}_n$	residual	$\tilde{T}_n$	residual
1024	11	$3.0 \cdot 10^{-11}$	12	$4.4 \cdot 10^{-12}$	11	$2.9 \cdot 10^{-11}$
2048	12	$8.3 \cdot 10^{-13}$	12	$3.0 \cdot 10^{-11}$	12	$2.1 \cdot 10^{-12}$
4096	12	$1.7 \cdot 10^{-12}$	13	$3.3 \cdot 10^{-12}$	12	$1.8 \cdot 10^{-11}$

Table 3
Example 3: Number of iterations and relative residual norm for the preconditioned conjugate gradient method applied to the normal equations associated with (4) with the generalized Strang preconditioner (column $\tilde{S}_n^{NE}$), for GMRES preconditioned by the optimal generalized circulant preconditioner (column $\tilde{C}_n$), and for GMRES preconditioned by the superoptimal generalized circulant preconditioner (column $\tilde{T}_n$) with $\theta = \pi$ for linear systems of equations of even order n.

Example 3. We consider Toeplitz matrices determined by the symbol

$$f(x) = \mathrm{i}e^{\mathrm{i}x/2} + \frac{1}{2}, \quad -\pi < x \le \pi,$$

with Fourier coefficients

$$\begin{cases} a_0 = -\frac{2}{\pi(1-2k)} + \frac{1}{2}, \\ a_k = -\frac{2}{\pi(1-2k)}, \quad k = \pm 1, \pm 2, \pm 3, \ldots \ . \end{cases}$$

The origin is in the convex hull of the spectrum. We have $\theta^* = \pi$ for all n. This is the optimal angle also for the other two generalized preconditioners. The iterative methods used are the same as in Example 2. Table 3 displays the performance of the generalized preconditioners for n even. Note that while the number of iterations required when solving the normal equations using the generalized Strang preconditioner $\tilde{S}_n^{NE}$ reported in Table 3 is competitive, the number of matrix-vector product evaluations is twice this number and therefore much larger than for the other methods. The optimal superoptimal generalized circulant preconditioner is seen to perform the best. □

Example 4. Consider the family of Toeplitz matrices defined by

$$A_n(t) = t\hat{C}_{-3\pi/4} + (1-t)\hat{C}_{\pi/4}, \quad t \in [0,1], \tag{18}$$

where the $\{e^{-3i\pi/4}\}$-circulant $\hat{C}_{-3\pi/4}$ and the $\{e^{i\pi/4}\}$-circulant $\hat{C}_{\pi/4}$ of order $n = 256$ are constructed by means of random diagonal matrices and the generalized Fourier matrix; cf. (7) and (14). Figure 2 shows $\|I - \tilde{T}_{n,\theta}^{-1} A_n(t)\|_F$ as a function of θ for different values of t. The figure indicates that when $t = 0.1$ the superoptimal generalized circulant preconditioner with $\theta = \pi/4$ might perform well and when $t = 0.9$ the superoptimal generalized circulant preconditioner with $\theta = -3\pi/4$ might yield fast convergence. This is confirmed by Table 4, which displays the number of iterations required for several superoptimal generalized circulant preconditioners. The optimal superoptimal generalized circulant preconditioner with θ^* chosen according to Corollary 2.4 requires the smallest number of iterations for any t-value. Column entries "-" mark that GMRES did not determine an acceptable approximate solution within 256 iterations. Note that without preconditioner GMRES did not converge within 256 iterations for any of the Toeplitz matrices considered. □

The examples of this section show that superoptimal generalized circulant preconditioners can be attractive to apply to the solution of (3) when the matrix A_n is Hermitian indefinite or a general non-Hermitian Toeplitz matrix. We remark that when A_n is Hermitian positive definite, the use of optimal or Strang-type circulant or generalized circulant preconditioners generally is preferable, because these preconditioners are cheaper to compute than superoptimal circulant or generalized circulant preconditioners and perform well for this kind of Toeplitz matrix.

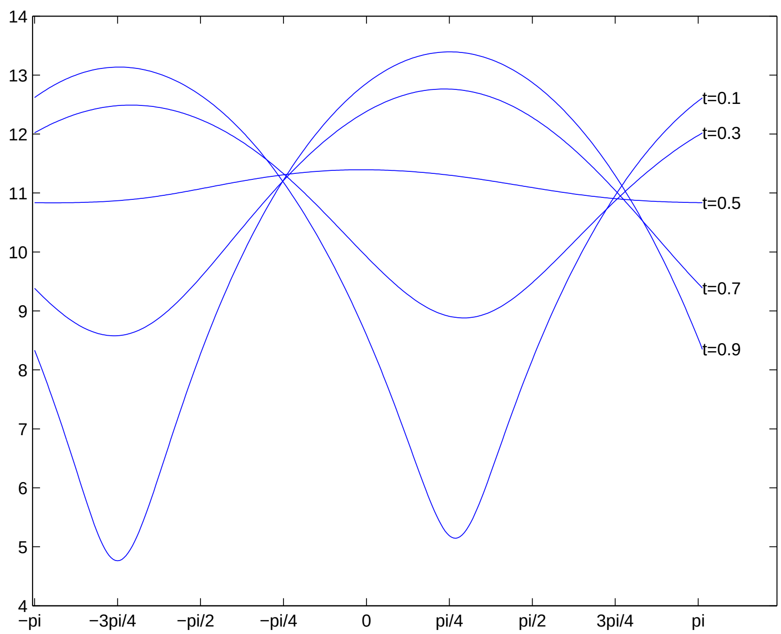

Fig. 2. Example 4: $\|I - \tilde{T}_{256,\theta}^{-1} A_{256}(t)\|_F$ depending on θ for $t = 0.1, 0.3, 0.5, 0.7, 0.9$.

t	I	$\tilde{T}_{-3\pi/4}$	$\tilde{T}_0$	$\tilde{T}_{\pi/4}$	$\tilde{T}_{\theta^*}$
0.1	–	–	155	61	61
0.3	–	–	201	159	157
0.5	–	238	245	243	231
0.7	–	167	254	–	164
0.9	–	49	–	–	49

Table 4
Example 4: Number of iterations for unpreconditioned GMRES, for GMRES preconditioned by superoptimal generalized circulant preconditioners (columns labelled $\tilde{T}_{-3\pi/4}$, $\tilde{T}_{\pi/4}$, and $\tilde{T}_{\theta^*}$). The optimal angle θ^* is defined by (13). The column labelled $\tilde{T}_0$ shows results for the superoptimal circulant preconditioner defined by (6).

4 Conclusion

Properties of superoptimal preconditioners based on generalized circulants are investigated. The numerical examples show that these preconditioners can be competitive for the solution of linear systems of equations with a Hermitian indefinite or a non-Hermitian Toeplitz matrix. The angle θ can be chosen to minimize a suitable quantity such as (13), or to avoid the preconditioner being singular. In the real case, one may avoid the solution of the minimization problem (13) by just considering circulants and skew-circulants. The computed examples suggest that the application of superoptimal generalized circulant preconditioners, and therefore the solution of the minimization problem (13) for the optimal angle θ^*, can be worthwhile when many Toeplitz systems with the same matrix and different right-hand sides have to be solved.

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