

Circulant/Skewcirculant Matrices as Preconditioners for Hermitian Toeplitz Systems

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Abstract. We study the solutions of Hermitian positive definite Toeplitz systems $T_n x = b$ by the preconditioned conjugate gradient method. For preconditioner A_n the convergence rate is known to be governed by the distribution of the eigenvalues of the preconditioned matrix $A_n^{-1}T_n$. New properties of the circulant preconditioners introduced by Strang, R. Chan, T. Chan, Szegö/Grenander and Tyrtysnikov are derived concerning the positive definiteness of A_n and the spectrum of $A_n^{-1}T_n$. Furthermore, we introduce a new class of Toeplitz matrices, similar to the Wiener class. For this class we consider new preconditioners as products of circulant and skewcirculant matrices C_n and S_n , that are best approximations of T_n in the Frobenius norm, and study the spectra of the preconditioned matrices.

Key Words. Toeplitz matrix, circulant matrix, preconditioned conjugate gradient method.

AMS(MOS) Subject Classifications. 65F10,65F15

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0. Introduction

Systems of linear equations

$$T_n x = b \tag{1}$$

with Hermitian positive definite Toeplitz matrices

$$T_n := T_n(t_0, t_1, \dots, t_{n-1}) := \begin{pmatrix} t_0 & t_1 & \cdots & \cdots & t_{n-1} \\ \bar{t}_1 & t_0 & t_1 & & \vdots \\ \vdots & \bar{t}_1 & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & t_1 \\ \bar{t}_{n-1} & \cdots & \cdots & \bar{t}_1 & t_0 \end{pmatrix} \tag{2}$$

arise in many applications such as time series analysis and digital signal processing. Direct fast and superfast methods for solving (1) are based on Schur algorithm or Szegő recursion and need $O(n^2)$, resp. $O(n \log^2(n))$, operations [15,18,10,1,2]. More recently, Strang [17] proposed to use the preconditioned conjugate gradient method, and since that time, the design of effective preconditioners M has received much attention [3,4,19,5]. The pcg-method requires that M is positive definite, linear equations $Mx = y$ are fast computable, and the spectrum of $M^{-1}T_n$ should be clustered around 1. First, circulant matrices are used as preconditioners [6,7,20], and later also skewcirculant matrices [11,12]. In [13,14], Kuo and Ku introduced new approximations to T_n which are Hankel plus Toeplitz matrices and submatrices of circulant matrices.

Linear equations with circulant matrices [8]

$$C := \begin{pmatrix} c_0 & c_1 & c_2 & \cdots & c_{n-1} \\ c_{n-1} & c_0 & c_1 & \cdots & c_{n-2} \\ c_{n-2} & c_{n-1} & c_0 & \cdots & c_{n-3} \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ c_1 & \cdots & c_{n-2} & c_{n-1} & c_0 \end{pmatrix} \tag{3}$$

can be solved by Fast Fourier Transformation in $O(n \log(n))$. This is a consequence of the eigendecomposition

$$C = F_n^H \Lambda F_n \tag{4}$$

with Λ a diagonal matrix and

$$F_n^H = \frac{1}{\sqrt{n}} \left(e^{2\pi i k j / n} \right)_{k,j=0}^{n-1} =$$

$$= \frac{1}{\sqrt{n}} \begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & w & w^2 & \cdots & w^{n-1} \\ 1 & w^2 & w^4 & \cdots & w^{2(n-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & w^{n-1} & w^{2(n-1)} & \cdots & w^{(n-1)(n-1)} \end{pmatrix}, \quad w = e^{2\pi i/n}, \quad (5)$$

the Fourier matrix of order n . Thereby, F_n is complex symmetric, unitary, and fulfills the equation $\bar{F}_n = F_n^H$. Hence, the eigenvalues of a given circulant matrix (3) are

$$\lambda_j = \sum_{k=0}^{n-1} c_k w^{jk} = p(w^j), \quad j = 0, \dots, n-1 \quad (6)$$

where

$$p(z) = c_0 + c_1 z + \cdots + c_{n-1} z^{n-1}$$

is the polynomial associated with C . The corresponding eigenvectors are

$$u_j = (1, w^j, \dots, w^{j(n-1)})^T, \quad j = 0, \dots, n-1.$$

With the notation (2) for Hermitian circulant C , (3) can be written in the form

$$C := \begin{cases} T_n(c_0, c_1, \dots, c_{k-1}, c_k, c_{k-1}, \dots, c_1) & \text{for even } n \\ T_n(c_0, c_1, \dots, c_k, c_k, \dots, c_1) & \text{for odd } n \end{cases}, \quad k = \lfloor n/2 \rfloor.$$

Skewcirculant matrices differ from circulant matrices by a change of the sign in the subdiagonalelements. Thus, skewcirculant matrices are of the form

$$S := \begin{pmatrix} s_0 & s_1 & s_2 & \cdots & s_{n-1} \\ -s_{n-1} & s_0 & s_1 & \cdots & s_{n-2} \\ -s_{n-2} & -s_{n-1} & s_0 & \cdots & s_{n-3} \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ -s_1 & \cdots & -s_{n-2} & s_{n-1} & s_0 \end{pmatrix}. \quad (7)$$

Using the unitary diagonal matrix

$$\Omega := \text{diag}(1, \sigma, \dots, \sigma^{n-1}), \quad \sigma = e^{i\pi/n}, \quad (8)$$

$\bar{\Omega} S \Omega$ is circulant for every skewcirculant matrix S . Because of (4) and (5), the eigenvalues and eigenvectors of S are given by

$$\lambda_j = p(\sigma w^j), \quad u_j = (1, \sigma w^j, \dots, (\sigma w^j)^{n-1})^T, \quad j = 0, \dots, n-1, \quad (9)$$

with

$$p(z) = s_0 + s_1 z + \cdots + s_{n-1} z^{n-1}.$$

In connection with Toeplitz matrices it is often assumed, that the Hermitain matrices T_n are finite sections of a fixed singly infinite Toeplitz matrix $T = T(t_0, t_1, \dots)$. Then, every matrix T is associated with a function

$$f(\theta) = \sum_{k=-\infty}^{\infty} t_k e^{ik\theta} \quad , \quad \theta \in [0, 2\pi] ;$$

f is said to be in the Wiener class if the sequence t_k , $k = \dots, -1, 0, 1, \dots$, is in l_1 , and therefore

$$\sum_{k=0}^{\infty} |t_k| < \infty .$$

If $f(\theta) > 0$, then T is positive definite, and thus the same holds for all T_n , $n = 1, 2, \dots$.

The preconditioners of Strang and of Szegö/Grenander

For a given Toeplitz matrix T_n Strang [17] proposed the circulant matrix

$$C_S = T_n(t_0, t_1, t_2, \dots, \bar{t}_2, \bar{t}_1)$$

as preconditioner for (1). C_S is obtained by preserving the central half diagonals of T_n and using them to form a circulant matrix. In the same way you get the skewcirculant matrix

$$S_S = T_n(t_0, t_1, \dots, -\bar{t}_2, -\bar{t}_1) .$$

It has been shown by R. Chan and Strang [6], that the spectrum of $C_S^{-1}T_n$ is clustered around 1, except a finite number of outliers, for Toeplitz matrices generated by positive functions in the Wiener class. The same is true for $S_S^{-1}T_n$ [11]. Intuitively, it is clear that for a near circulant matrix T_n one choses C_S as preconditioner and S_S for a near skewcirculant T_n . To get a better criterion let us consider another elementary proof [4] for the clustering property of the spectrum of $C_S^{-1}T_n$, with T_n belonging to a positive function in the Wiener class. Let us assume $n = 2k$. Then there exists an integer m such that for a given ϵ it holds

$$\sum_{k=m+1}^{\infty} |t_k| \leq \epsilon .$$

Set $\Delta(\epsilon)$ the matrix that you get by removing the last m columns and rows of $C_S - T_n$. Because of

$$\gamma_m := |t_{k-1} - t_{k+1}| + \dots + |t_{m+1} - t_{n-m-1}| \leq \sum_{k=m+1}^{\infty} |t_k| \leq \epsilon \quad (10)$$

all row sums of $\Delta(\epsilon)$ are bounded by ϵ . Then, the Theorem of Gershgorin states that the $n - m$ eigenvalues of $\Delta(\epsilon)$ lie in the interval $[-\epsilon, \epsilon]$. $\Delta(\epsilon)$ is a principal submatrix of

$C_S - T_n$ and thus, in view of the interlace property [16], the ϵ -neighbourhood of 0 contains at least $n - 2m$ eigenvalues of $C_S - T_n$. Note, that m is independent of n , and hence, the eigenvalues of $C_S^{-1}T_n$ are clustered around 1 for large n .

For the skewcirculant matrix S_S instead of (10) we get

$$\sigma_m := |t_{k-1} + t_{k+1}| + \cdots + |t_{m+1} + t_{n-m-1}| \leq \sum_{k=m+1}^{\infty} |t_k| \leq \epsilon \quad (10)'$$

Now, (10) and (10)' give a criterion for choosing the preconditioner. For given n and ϵ let m_c (m_s) be the maximal index with $\gamma_{m_c} \leq \epsilon$, resp. $\sigma_{m_s} \leq \epsilon$. Then, at least $n - 2m_c$ eigenvalues of $C_S - T_n$ lie in $[-\epsilon, \epsilon]$ and at least $n - 2m_s$ eigenvalues of $S_S - T_n$. Hence, we use C_S as preconditioner if $m_c \geq m_s$ for a small ϵ . If, for example, all t_k have the same sign, then the left side of (10) is smaller than the left side in (10)' and thus C_S leads to a better clustering.

In [9] Szegő and Grenander introduced another class of circulant approximations to T_n . For $1 \leq p \leq n$ set

$$d_k = \sum_{j=-p}^p t_j \left(1 - \frac{|j|}{p}\right) w^{jk} \quad , \quad k = 0, 1, \dots, n-1 \quad , \quad (11)$$

D_p the diagonal matrix with elements d_k , and $C_p = F_n^H D_p F_n$. In order to analyse the convergence of the sequence C_p for $n \rightarrow \infty$, they considered the norm

$$|T_n|^2 = \frac{1}{n} \sum_{j=1}^n \lambda_j(T_n)^2 = \frac{1}{n} \|T_n\|_F^2 \quad , \quad (12)$$

where $\|A\|_F$ denotes the Frobeniusnorm of A . For the circulant matrices C_p we prove

Theorem 1. *The eigenvalues of T_n and C_p fulfill the inequalities*

$$\lambda_{\min}(T_n) \leq \lambda_{\min}(T_p) \leq \lambda_{\min}(C_p) \leq \lambda_{\max}(C_p) \leq \lambda_{\max}(T_p) \leq \lambda_{\max}(T_n) \quad .$$

Proof: It holds

$$\sum_{j=-p+1}^{p-1} (p - |j|) t_j w^j = u^H T_p u \quad \text{with} \quad u = (1, w, \dots, w^{p-1})^T \quad , \quad |w| = 1 \quad .$$

Hence, the eigenvalues of C_p are contained in the range of the leading principal submatrix T_p of T_n . #

Remarks: 1. Theorem 1 guarantees that for positive definite T_n the approximations C_p are positive definite, too. Therefore, C_p can be used as preconditioner.

2. C_p with its eigenvalues (11) is different from the best Frobeniusnorm approximation \tilde{C}_p

to $T_n(t_0, t_1, \dots, t_{p-1}, 0, \dots, 0)$. From (6) it follows that the eigenvalues of \tilde{C}_p are (see also (13) in the next section)

$$\sum_{j=-p+1}^{p-1} \left(1 - \frac{|j|}{n}\right) t_j w^{jk} \quad , \quad k = 0, 1, \dots, n-1 \quad .$$

3. In view of (7)-(9), the corresponding skewcirculant approximation is given by

$$S_p = \Omega * C_p(\bar{\Omega} T_n \Omega) * \bar{\Omega} \quad .$$

2. The optimal and superoptimal Frobenius norm approximation

The optimal circulant preconditioner C_F was first considered by T. Chan [7]. C_F is defined as the best circulant approximation to T_n in the Frobenius norm and thus, is given by

$$C_F = T_n\left(t_0, \frac{(n-1)t_1 + \bar{t}_{n-1}}{n}, \dots, \frac{t_{n-1} + (n-1)\bar{t}_1}{t_1}\right) . \quad (13)$$

Here, we will consider a more general approach to this approximation problem. For a given unitary matrix U we set

$$M_U := \{U^H \Lambda U \mid \Lambda \text{ diagonal matrix over } \mathbf{C}\} .$$

Then it holds (see [5] for the circulant case $U = F_n$)

Theorem 2. *For a matrix A the solution of*

$$\min_{D \in M_U} \|D - A\|_F$$

is given by

$$F_U(A) = U^H \text{diag}(U A U^H) U \quad .$$

If A is Hermitian then the eigenvalues of $F_U(A)$ lie in the interval $[\lambda_{\min}(A), \lambda_{\max}(A)]$. Furthermore, the operator F_U has the following properties:

- (i) F_U is a linear mapping of the Banach algebra of complex $n \times n$ matrices in the subalgebra M_U .
- (ii) $\text{lub}_F(F_U) = \text{lub}_2(F_U) = 1$.
- (iii) $F_U(D * A) = D * F_U(A) = F_U(A) * D = F_U(A * D)$ for all matrices $D \in M_U$.

Proof: With the notation $B = U A U^H$, for an element $D = U^H \Lambda U \in M_U$ the expression

$$\|D - A\|_F = \|\Lambda - U A U^H\|_F \quad ,$$

takes its minimal value if Λ is the diagonal of B .
Furthermore, it holds

$$\text{lub}_2(F_U) = \max_{B \neq 0} \frac{\|\text{diag}(B)\|}{\|B\|} \leq \max_{B \neq 0} \frac{|b_{i,i}|_{max}}{\sigma_{max}(B)} \leq 1,$$

$$\text{lub}_F(F_U) = \max_{B \neq 0} \frac{\|\text{diag}(B)\|_F}{\|B\|_F} \leq 1,$$

and $F_U(I) = I$. Thereby, σ_{max} denotes the maximal singular value of B . #

As a Corollary of Theorem 2 we get, that, for a given Hermitian Toeplitz matrix T_n , C_F of (13) is equal to

$$C_F = F_n^H \text{diag}(F_n T_n F_n^H) F_n$$

and the skewcirculant approximation S_F fulfills

$$S_F = \Omega F_n^H \text{diag}(F_n \bar{\Omega} T_n \Omega F_n^H) F_n \bar{\Omega}$$

with F_n and Ω defined in (5) and (8). In addition, from Theorem 2 it is obvious, that for positive definite T_n , C_F and S_F are positive definite, too.

The same analysis can be applied to Tyrtyshnikovs superoptimal preconditioner [20,5]

$$C_T = C_F (T_n^H)^{-1} * C_F (T_n T_n^H),$$

the solution of

$$\min \|I - C^{-1} T_n\|_F \quad \text{over all circulant matrices } C.$$

With the set M_U defined as above, we can prove

Theorem 3. (a) For a given nonsingular matrix A the solution of

$$\min_{D \in M_U} \|I - DA\|_F$$

is given by

$$D = G_U(A) := (F_U(AA^H))^{-1} * F_U(A^H) = F_U(A^H) * (F_U(AA^H))^{-1}.$$

The eigenvalues of $F_U(A)$ and $G_U(A)$ can be ordered such that

$$|\lambda_i(G_U(A))|^{-1} \geq |\lambda_i(F_U(A))| \quad \text{or} \quad \lambda_i(G_U(A)) = \lambda_i(F_U(A)) = 0.$$

Furthermore, it holds

$$G_U(D * A) = D^{-1} * G_U(A), \quad D \in M_U.$$

(b) For an Hermitian positive definite A , $G_U(A)$ is nonsingular. Therefore, we can define

$$H_U(A) := G_U(A)^{-1}$$

Then, the eigenvalues λ of $H_U(A)$ fulfill

$$\lambda_{\min}(A) \leq \lambda_{\min}(F_U(A)) \leq \lambda \leq \lambda_{\max}(A),$$

and with an appropriate numbering

$$\lambda_i(H_U(A)) \geq \lambda_i(F_U(A)).$$

Proof: Let $D = U^H \Lambda U$ and $B = UAU^H = (b_1, \dots, b_n)^T$. Then, the solution of

$$\min \|I - DA\|_F = \min \|I - \Lambda B\|_F$$

is given by

$$\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n) \quad \text{and} \quad \lambda_i = \frac{\bar{b}_{i,i}}{\|b_i\|^2}. \quad (14)$$

Because of

$$\Lambda = \text{diag}(B^H) * \text{diag}(BB^H)^{-1}$$

it follows

$$G_U(A) = U^H \Lambda U = U^H (\text{diag}(UA^H U^H) \text{diag}(UAA^H U^H)^{-1}) U = F_U(A^H) F_U(AA^H)^{-1}.$$

The eigenvalues of $F_U(A)$ are the numbers $b_{i,i}$. Hence, (14) shows that either $b_{i,i} = 0$ or

$$\left| \frac{1}{\lambda_i(G_U(A))} \right| \geq |b_{i,i}| = |\lambda_i(F_U(A))|.$$

If A is Hermitian positive definite, then B has a orthonormal basis of eigenvectors and thus, $B = Q^H \Delta Q$ with $Q^H Q = I$ and $\Delta = \text{diag}(\delta_1, \dots, \delta_n) > 0$. Therefore, it holds

$$\lambda_i(H_U(A)) = \frac{(BB^H)_{i,i}}{b_{i,i}} = \frac{q_i^H |\Delta|^2 q_i}{q_i^H \Delta q_i} = \frac{\sum_{j=1}^n \delta_j^2 |q_{j,i}|^2}{\sum_{j=1}^n \delta_j^2 |q_{j,i}|^2 (1/\delta_j)}.$$

This proves

$$\lambda_{\min}(A) \leq \lambda_i(H_U(A)) \leq \lambda_{\max}(A)$$

and

$$\lambda_i(H_U(A)) = \frac{(BB^H)_{i,i}}{b_{i,i}} \geq b_{i,i} = \lambda_i(F_U(A)).$$

#

Remarks:

1. Part (a) of Theorem 3 remains true if we replace the assumption that A is nonsingular by the condition $u_i A \neq 0$ for each row u_i of U , because then it also follows $\|b_i\| > 0$. If this condition is not fulfilled, then the solution is no more unique.

2. The operator H_U is not linear. Moreover, the eigenvalues of $H_U(A + \alpha I)$ are given by

$$\frac{\|b_i\|^2 + |\alpha|^2 + 2\operatorname{Re}(\alpha \bar{b}_{i,i})}{\bar{b}_{i,i} + \bar{\alpha}}.$$

If for an Hermitian indefinite matrix A there exists a number α with

$$|b_{i,i}| < \alpha \leq \frac{\|b_i\|^2}{|b_{i,i}|} \quad \text{for all } b_{i,i} \leq 0,$$

then for this α the matrix

$$H_U(A + \alpha I) - \alpha I \tag{15}$$

is positive definite. We can assume, that with $H_U(A + \alpha I)^{-1} * (A + \alpha I)$ also $(H_U(A + \alpha I) - \alpha I)^{-1} * A$ will be a good approximation to the identity matrix. Hence, for fixed U the matrix (15) seems to be a good choice for a preconditioner in the indefinite case.

As a direct conclusion from Theorem 3 we get

Corollary 1. *For an Hermitian positive definite Toeplitz matrix T_n the superoptimal circulant, resp. skewcirculant, Frobenius norm approximation has the form*

$$C_T = C_F(T_n)^{-1} * C_F(T_n^2) \quad \text{and} \quad S_T = S_F(T_n)^{-1} * S_F(T_n^2).$$

With an appropriate numbering the eigenvalues of C_T and S_T fulfill

$$\lambda_i(C_T) \geq \lambda_i(C_F) \quad \text{and} \quad \lambda_i(S_T) \geq \lambda_i(S_F)$$

$$0 \leq \lambda_{\min}(T_n) \leq \lambda_{\min}(C_F) \leq \lambda_{\min}(C_T) \quad \text{and} \quad \lambda_{\max}(C_F) \leq \lambda_{\max}(C_T) \leq \lambda_{\max}(T_n)$$

$$0 \leq \lambda_{\min}(T_n) \leq \lambda_{\min}(S_F) \leq \lambda_{\min}(S_T) \quad \text{and} \quad \lambda_{\max}(S_F) \leq \lambda_{\max}(S_T) \leq \lambda_{\max}(T_n).$$

Hence, for positive definite T_n , C_T and S_T are positive definite, too.

3. New classes of optimal circulant approximations

In [9] Szegö and Grenander proved that for T_n , associated with an l_2 -function f defined on the circle with radius 1, the approximations (11) converge to T_n if p and n tend to infinity with respect to the norm (12). This is also obvious for the circulant and skewcirculant approximations C_S , S_S , C_F , S_F , C_T , and S_T if $n \rightarrow \infty$. The convergence in the norm (12) is equivalent to the following property:

For every given positive ϵ the numbers $N(\epsilon, n)$ of eigenvalues $\lambda_i(C_n - T_n)$ with absolute values exceeding ϵ fulfill

$$\frac{N(\epsilon, n)}{n} \rightarrow 0 \quad \text{for } n \rightarrow \infty.$$

If we strengthen the conditions on T_n and consider Toeplitz matrices associated with functions out of the Wiener class, then Strang and R. Chan showed, that the eigenvalues of $C_S - T_n$ are asymptotically clustered around 0 and therefore, $N(\epsilon, n)$ is bounded by a constant M [6].

Let us introduce a new class by defining

$$f \in l'_2 \leftrightarrow \sum_{i=1}^{\infty} i|t_i|^2 \leq M < \infty. \quad (16)$$

Then it is easy to verify that

$$\begin{aligned} l_1 &\subset l_2 \quad \text{and} \quad l'_2 \subset l_2, \\ l_1 &\not\subset l'_2 \quad \text{and} \quad l'_2 \not\subset l_1. \end{aligned}$$

All l_1 -test examples that appear in the literature on circulant preconditioners are elements of l'_2 , too. For T_n associated with a function $f \in l'_2$ from (16) it follows

$$\sum_{j=1}^n \lambda_j^2(C_S - T_n) = \|C_S - T_n\|_F^2 = 2 \sum_{i=1}^n i|t_i|^2 \leq 2M.$$

Hence the eigenvalues of $C_S - T_n$ are clustered around 0 for $n \rightarrow \infty$. This gives an elementary proof for the clustering property of $M^{-1}T_n$ for at most all known circulant and skewcirculant preconditioners. For the following we will assume that T_n is associated with a function $f \in l'_2$.

In order to reduce the number of iterations in the pcg-algorithm, it seems to be worthwhile, to spend more computational effort in finding better preconditioners. One approach is the use of approximations that are submatrices of circulant $2n \times 2n$ matrices [13,14]. Here, we will propose other approximations that use both circulant and skewcirculant matrices. To get a symmetric positive definite approximation of a positive definite Toeplitz matrix T_n we will consider

$$M := C_F^\alpha S_F^\beta C_F^\alpha. \quad (17)$$

We can find an optimal choice of α and β by the following

Lemma 1. *Let T_n be a sequence of Hermitian positive definite Toeplitz matrices that fulfill (16). Then, with*

$$C_F = F_n^H \Lambda F_n \quad \text{and} \quad T_n = V^H \Delta V$$

it holds that also the eigenvalues of

$$C_F^\alpha - T_n^\alpha = F_n^H \Lambda^\alpha F_n - V^H \Delta^\alpha V$$

are clustered around 0 for $n \rightarrow \infty$.

Proof: Let us consider only the nontrivial case $\alpha \neq 0$. With the notation $U = VF_n^H = (u_1, \dots, u_n)$ we only have to show that

$$\|C_F^\alpha - T_n^\alpha\|_F = \|\Lambda^\alpha - U^H \Delta^\alpha U\|_F$$

is bounded for $n \rightarrow \infty$. In view of

$$\sum_{i,j=1}^n u_i^H \Delta u_j u_j^H \Delta u_i = \sum_{i=1}^n u_i^H \Delta^2 u_i = \text{spur}(U^H \Delta^2 U) = \text{spur}(\Delta^2) = \sum_{i=1}^n \delta_i^2$$

and

$$\sum_{i,j=1}^n (\delta_i^2 - \delta_j^2) |u_{i,j}|^2 = 0$$

it holds

$$\begin{aligned} \|C_F - T_n\|_F^2 &= \sum_{i,j=1}^n |u_i^H \Delta u_j|^2 - \sum_{i=1}^n |u_i^H \Delta u_i|^2 + \sum_{i=1}^n (\lambda_i - u_i^H \Delta u_i)^2 = \\ &= \sum_{i=1}^n (\delta_i^2 + \lambda_i^2 - 2\lambda_i u_i^H \Delta u_i) = \\ &= \sum_{i,j=1}^n (\delta_j^2 + \lambda_i^2 - 2\lambda_i \delta_j) |u_{i,j}|^2 = \\ &= \sum_{i,j=1}^n (\delta_j - \lambda_i)^2 |u_{i,j}|^2. \end{aligned}$$

In the same way we get

$$\|C_F^\alpha - T_n^\alpha\|_F^2 = \sum_{i,j=1}^n (\delta_j^\alpha - \lambda_i^\alpha)^2 |u_{i,j}|^2.$$

Now, δ_j and λ_i are contained in the interval $[\lambda_{\min}(T_n), \lambda_{\max}(T_n)]$. Therefore, it exists a positive number M with

$$(\delta_j^\alpha - \lambda_i^\alpha)^2 \leq M * (\delta_j - \lambda_i)^2 \text{ for } i, j = 1, 2, \dots, n.$$

Hence, it follows

$$\|C_F^\alpha - T_n^\alpha\|_F^2 \leq M * \|C_F - T_n\|_F^2 < \infty.$$

#

For all preconditioner (17) we get that $M^{-1}T_n$ has the same spectrum as

$$\begin{aligned} S_F^{-\beta/2} C_F^{-\alpha} T_n C_F^{-\alpha} S_F^{-\beta/2} &= \\ &= S_F^{-\beta/2} C_F^{-\alpha} (T_n - C_F) C_F^{-\alpha} S_F^{-\beta/2} + S_F^{-\beta/2} (C_F^{1-2\alpha} - S_F^{1-2\alpha}) S_F^{-\beta/2} + S_F^{1-2\alpha-\beta}. \end{aligned}$$

Hence, in view of Lemma 1 and the Theorem of Courant-Fischer [16], the eigenvalues of $M^{-1}T_n$ are in general clustered around 1 only if $2\alpha + \beta = 1$. Thus, without further information the optimal choice is $\beta = 1/2$ and $\alpha = 1/4$, because then the circulant and the skewcirculant part have the same weight. All in all, we get

Theorem 4. Let T_n be an Hermitian positive definite Toeplitz matrix, associated with a function $f \in l'_2$, and C_F, S_F the best Frobeniusnorm approximations to T_n . Then the preconditioner

$$M = C_F^{1/4} S_F^{1/2} C_F^{1/4} \quad (18)$$

is Hermitian positive definite, uniformly bounded, and the spectrum of $M^{-1}T_n$ is asymptotically clustered around 1.

Remarks: 1. In the same way one can define a preconditioner $S_F^{1/4} C_F^{1/2} S_F^{1/4}$, or replace C_F and S_F by other circulant/skewcirculant approximations, e.g. by C_S and S_S .
2. In every step of the preconditioned conjugate gradient method the number of operations doubles if we use the approximation (18) instead of C_S . In each iteration we have in addition to solve one circulant and one skewcirculant linear equation.

In order to improve the approximation, we can replace (18) by

$$M = C_F^{1/4} \tilde{S} C_F^{1/4}, \quad (19)$$

where S solves a new Frobeniusnorm approximation problem. A possible choice, for example, is

$$\|\tilde{S} - C_F^{-1/4} T_n C_F^{-1/4}\|_F = \min_{S \text{ skewcirculant}} \|S - C_F^{-1/4} T_n C_F^{-1/4}\|_F. \quad (20)$$

The solution of (20) is given by

$$\tilde{S} = S_F(C_F^{-1/4} T_n C_F^{-1/4}),$$

and is positive definite and uniformly bounded for T_n in the class (16). $M - T_n$ with M defined in (20) has a smaller Frobenius norm than the approximation (18). Hence, the spectrum of $M^{-1}T_n$ is again clustered around 1.

Similar approximations of the form (19) we get by solving

$$\min_{S \text{ skewcirculant}} \|I - S^{-1} C_F^{-1/4} T_n C_F^{-1/4}\|_F, \quad (21)$$

$$\min_{S \text{ skewcirculant}} \|S C_F^{1/4} - C_F^{-1/4} T_n\|_F, \quad (22)$$

or

$$\min_{S \text{ skewcirculant}} \|C_F^{1/4} S C_F^{1/4} - T_n\|_F. \quad (23)$$

The solutions of (20)-(23) can be computed explicitly, but the number of operations for that is in general much too large in comparison with the case of using $M = C_F$. Hence, the preconditioner (18) seems to be the most competitive one in this class of approximations, because one has to compute only both C_F and S_F .

4. Numerical examples

For comparing the different preconditioners we consider the following examples:

1. $t_j = 1/(j+1)^2$ for $j = 0, 1, \dots, n-1$ [17,7].
2. $t_j = \cos(j)/(j+1)$ $j = 0, 1, \dots, n-1$ [7]; the associated function is neither in l_1 nor in l'_2 .
3. $t_0 = 2$ and $t_j = \frac{1+i}{(1+j)^{1.1}}$ for $j = 1, 2, \dots, n-1$ [4,5].

First, for example 1 and 2 we will display the spectrum of $M^{-1}T_n$ for the preconditioners (18) and (20)-(23). Thereby, $C^{\wedge}(-1)$ denotes C_F , and $MA1 - MA5$ denote (18), (20)-(23).

Fig. 1. Example 1 with $n = 16$

Fig. 2. Example 2 with $n = 16$

The following tables display the number of iterations in the preconditioned conjugate gradient method for solving a positive definite Toeplitz system. Thereby, the start vector is e_1 , and the algorithm stops, if the residuum is smaller than 10^{-7} .

Example 2	$n = 16$	$n = 32$	$n = 64$	$n = 128$	$n = 256$
C_F	7	8	8	9	9
S_F	7	8	8	8	9
$C_F^{1/4} S_F^{1/2} C_F^{1/4}$	6	6	6	6	6
(20)	5	6	6	6	6

Table 1. Iterations of the pcg-algorithm for example 2

Example 1	$n = 16$	$n = 32$	$n = 64$	$n = 128$	$n = 256$
C_F	6	5	6	6	6
S_F	6	6	6	6	6
$C_F^{1/4} S_F^{1/2} C_F^{1/4}$	5	5	4	4	4

Table 2. Iterations of the pcg-algorithm for example 1

Example 3	$n = 16$	$n = 32$	$n = 64$	$n = 128$	$n = 256$
C_F	7	7	7	7	7
S_F	7	8	7	7	8
$C_F^{1/4} S_F^{1/2} C_F^{1/4}$	7	6	6	6	6

Table 3. Iterations of the pcg-algorithm for example 3

The following table shows for example 2 with $n = 16$ the behaviour of the pcg-algorithm for all preconditioners introduced in the previous section.

M :	C_F	S_F
Number of iterations:	7	7

$C_F^{1/4} S_F^{1/2} C_F^{1/4}$	(20)	(21)	(22)	(23)
6	5	5	5	5

Table 4. Iterations of the pcg-algorithm for example 2

This examples show that preconditioners of the form $M = CSC$ reduce the number of iterations in the pcg-algorithm. The advantage is largest if the associated function is not in l_1 .

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