Preconditioners for ill-conditioned Toeplitz matrices *

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Abstract.

This paper is concerned with the solution of systems of linear equations $\mathbf{A}_N \mathbf{x} = \mathbf{b}$, where $\{\mathbf{A}_N\}_{N \in \mathbb{N}}$ denotes a sequence of positive definite Hermitian ill-conditioned Toeplitz matrices arising from a (real-valued) nonnegative generating function $f \in C_{2\pi}$ with zeros. We construct positive definite Hermitian preconditioners \mathbf{M}_N such that the eigenvalues of $\mathbf{M}_N^{-1}\mathbf{A}_N$ are clustered at 1 and the corresponding PCG-method requires only $\mathcal{O}(N\log N)$ arithmetical operations to achieve a prescribed precision. We sketch how our preconditioning technique can be extended to symmetric Toeplitz systems, doubly symmetric block Toeplitz systems with Toeplitz blocks and non-Hermitian Toeplitz systems.

Numerical tests confirm the theoretical expectations.

AMS subject classification: 65F10, 65F15, 65T10.

 $Key\ words:$ Ill-conditioned Toeplitz matrices , CG-method, clusters of eigenvalues, preconditioners.

1 Introduction.

Systems of linear equations

$$\boldsymbol{A}_{N}\boldsymbol{x} = \boldsymbol{b}$$

with positive definite Hermitian Toeplitz matrices A_N arise in a variety of applications in mathematics and engineering (see [11] and the references therein). Along with stabilization techniques for direct fast and superfast Toeplitz solvers, preconditioned conjugate gradient methods (PCG–methods) and other iterative methods have attained much attention during the last years. As essential computational effort, the CG–method requires the multiplication of a vector with the matrix A_N in each iteration step. For Toeplitz matrices A_N , the multiplication with a vector can be computed with $\mathcal{O}(N\log N)$ arithmetical operations by fast Fourier transforms (FFT). The number of iteration steps of the CG–method depends on the distribution of the eigenvalue of A_N . In particular, it holds (see [1, p.573]

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THEOREM 1.1. Let A_N be a positive definite Hermitian (N, N)-matrix which has p and q isolated large and small eigenvalues, respectively:

$$0 < \lambda_1 \le \lambda_2 \le \dots \le \lambda_q \quad < \quad a \le \lambda_{q+1} \le \dots \lambda_{N-p} \le b$$

$$(1.1) \quad < \quad \lambda_{N-p+1} \le \lambda_{N-p+2} \le \dots \le \lambda_N \quad (0 < a < b < \infty).$$

Let $\lceil x \rceil$ denote the smallest integer $\geq x$. Then the CG-method for the solution of $\mathbf{A}_N \mathbf{x} = \mathbf{b}$ requires at most

$$n = \left[\left(\ln \frac{2}{\tau} + \sum_{k=1}^{q} \frac{b}{\lambda_k} \right) / \ln \frac{1 + (\frac{a}{b})^{1/2}}{1 - (\frac{a}{b})^{1/2}} \right] + p + q$$

iteration steps to achieve precision τ , i.e.

$$\frac{||\boldsymbol{x}_n - \boldsymbol{x}||_A}{||\boldsymbol{x}_0 - \boldsymbol{x}||_A} \le \tau ,$$

where $||x||_A := \sqrt{\bar{x}' A_N x}$ and where x_n denotes the numerical solution after n iteration steps.

In the sequel, we denote by $C_{2\pi}$ the space of 2π -periodic, real-valued continuous functions.

Let $\{\sigma_k^N\}_{k=1}^N$ be a sequence of real numbers and let $\gamma_N(\varepsilon)$ denote the number of those among σ_k^N $(k=1,\ldots,N)$ which are outside the interval $(p-\varepsilon,p+\varepsilon)$. If $\gamma_N(\varepsilon) < K(\varepsilon)$, where $K(\varepsilon)$ is independent of N, then we say that the values σ_k^N are clustered at p [32]. If the eigenvalues of a sequence of (N,N)-matrices A_N are clustered at 1, then the CG-method converges superlinearly (see [13]).

For a sequence of (N, N)-Toeplitz matrices $A_N = A_N(f)$ $(N \in \mathbb{N})$ generated by a function $f \in C_{2\pi}$, it is well-known that the eigenvalues are distributed as f [32, 17]. Let

$$f_{\min} \ := \min\{f(x) \ : \ x \in [0,2\pi)\} \,, \quad f_{\max} \ := \max\{f(x) \ : \ x \in [0,2\pi)\} \,.$$

Then the eigenvalues of $A_N(f)$ are contained in $[f_{\min}, f_{\max}]$. If f > 0, then by Theorem 1.1 the number of iteration steps of the CG-method to achieve a prescribed precision is independent of N and the CG-method requires only $\mathcal{O}(N \log N)$ arithmetical operations.

The situation changes completely, if we allow $f \geq 0$ to have zeros. In this case, the CG-method converges very slow with increasing N. To accelerate the convergence of the CG-method, several authors proposed preconditioners for Toeplitz systems. Clearly, the multiplication of any vector with the preconditioned matrix should also only require $\mathcal{O}(N\log N)$ arithmetical operations. Therefore, two types of preconditioners were mainly exploited for linear Toeplitz systems, namely so-called "Strang-preconditioners" [13, 30, 14]

(1.2)
$$\boldsymbol{M}_{N}(\mathcal{S}_{N}f, \boldsymbol{F}_{N}) := \boldsymbol{F}_{N} \operatorname{diag}\left((\mathcal{S}_{N}f)(\frac{2\pi j}{N})\right)_{j=0}^{N-1} \bar{\boldsymbol{F}}_{N},$$

where $S_N f$ denotes the (N-1)-th Fourier sum of f and optimal preconditioners [15]

(1.3)
$$\boldsymbol{M}_{N}^{\mathcal{O}}(\boldsymbol{F}_{N}) := \boldsymbol{F}_{N} \, \delta(\bar{\boldsymbol{F}}_{N} \, \boldsymbol{A}_{N} \, \boldsymbol{F}_{N}) \, \bar{\boldsymbol{F}}_{N},$$

where $\delta(\mathbf{A}) := \operatorname{diag}(a_{kk})_{k=0}^{N-1}$ and a_{kk} are the diagonal entries of \mathbf{A} . Here \mathbf{F}_N denotes the N-th Fourier matrix

$$\boldsymbol{F}_N := \frac{1}{\sqrt{N}} \left(\mathrm{e}^{-2\pi \mathrm{i} j k/N} \right)_{j,k=0}^{N-1}.$$

If f > 0, then both preconditioners \mathbf{M}_N are positive definite and the eigenvalues of the preconditioned matrices $\mathbf{M}_N^{-1} \mathbf{A}_N$ are clustered at 1. The same holds if we replace \mathbf{F}_N by other unitary matrices, for example by the product of \mathbf{F}_N with a unitary diagonal matrix which leads to ω -circulant preconditioners [10, 19] or, if \mathbf{A}_N is real-valued, by unitary trigonometric matrices as the sine-I transform [5] which results in so-called τ -preconditioners, the Hartley transform [7] or other trigonometric transforms [8, 21].

Unfortunately, if $f \geq 0$ has zeros, then the above preconditioners do not work in general. The Strang-preconditioners are not positive definite for arbitrary $f \in C_{2\pi}$. The convergence of the PCG-method with the above optimal preconditioners is not independet of N also in the τ -case, if f has zeros of higher order [6, 4]. An alternative choice are banded preconditioners belonging to the Toeplitz or to the τ -class which lead to satisfactory results [5, 9, 10, 26, 4], multigrid methods [16] or "improved circulants" [31].

In this paper, we propose simple positive definite ω -circulant preconditioners. In particular, if $f(2\pi j/N) > 0$ for all $j = 0, \ldots, N-1$, then we obtain our preconditioners by replacing $\mathcal{S}_N f$ in (1.2) by f. In Section 3, we prove that our preconditioners lead to superlinear convergence of the corresponding PCG-method and that the number of PCG-iterations for reaching a fixed tolerance is independent of N.

Our idea can be extended to (real) symmetric Toeplitz matrices, non–Hermitian Toeplitz matrices and doubly symmetric block Toepliz matrices with Toeplitz blocks. We sketch various generalizations in Section 4. Writing this paper, we became aware of the preprint [20] of T. Huckle located at his home page, where the author suggests a trigonometric preconditioner with respect to the discrete sine transform of type I which is similar to our trigonometric preconditioners in Section 4. However, our initial approach in the complex case and our proofs are different from [20].

Numerical tests for Hermitian and symmetric Toeplitz matrices as well as for non–symmetric Toeplitz matrices and doubly symmetric block Toeplitz matrices with Toeplitz blocks in Section 5 demonstrate the quality of our new preconditioners.

2 Construction of preconditioners

Let $C_{2\pi}$ and $L_{2\pi}^p$ $(1 \leq p < \infty)$ denote the Banach spaces of 2π -periodic continuous functions and of 2π -periodic Lebesgue measurable functions with

finite integral $\int_{0}^{2\pi} |f(x)|^p dx$, respectively. By o_N , we denote the vector consisting of N zeros and by I_N the (N, N)-identity matrix.

We are interested in the solution of Hermitian Toeplitz systems

(2.1)
$$\mathbf{A}_N(f) \mathbf{x} = \mathbf{b}, \quad \mathbf{A}_N(f) := (a_{j-k})_{i,k=0}^{N-1},$$

where the sequence $\{A_N(f)\}_{N=1}^{\infty}$ of Toeplitz matrices is generated by a nonnegative function $f \in C_{2\pi}$, i.e.

$$a_k = a_k(f) := \frac{1}{2\pi} \int_0^{2\pi} f(x) e^{-ikx} dx$$
.

Then we obtain for $\boldsymbol{u}=(u_j)_{j=0}^{N-1}\in\mathbb{C}^N$ that

(2.2)
$$\bar{\boldsymbol{u}}' \boldsymbol{A}_{N}(f) \boldsymbol{u} = \sum_{j=0}^{N-1} \sum_{k=0}^{N-1} \bar{u}_{j} u_{k} a_{j-k}$$

$$= \frac{1}{2\pi} \sum_{j=0}^{N-1} \sum_{k=0}^{N-1} \bar{u}_{j} u_{k} \int_{0}^{2\pi} f(x) e^{-i(j-k)x} dx$$

$$= \frac{1}{2\pi} \int_{0}^{2\pi} |\sum_{k=0}^{N-1} u_{k} e^{ikx}|^{2} f(x) dx \geq 0$$

such that the Toeplitz matrices $A_N(f)$ are positive semidefinite. Moreover, if f > 0 on a set of positive Lebesgue measure, then following lemma states that the matrices $A_N(f)$ are positive definite such that (2.1) can be solved by the CG-method.

LEMMA 2.1. Let $f \in L^1_{2\pi}$ be a nonnegative function, where the set $\{x \in [0, 2\pi] : f(x) > 0\}$ has a positive Lebesgue measure. Then the corresponding Toeplitz matrices $\mathbf{A}_N(f)$ are positive definite.

Lemma 2.1 was proved in [9]. However, the proof is very short such that we include it in this paper.

PROOF. Let $N \in \mathbb{N}$ be fixed. By the above considerations, it remains to show that 0 is not eigenvalue of $A_N(f)$. Assume that $A_N(f)$ has eigenvalue 0. Then there exists $u \in \mathbb{C}^N$ $u \neq o_N$ such that

$$ar{m{u}}' \, m{A}_N(f) \, m{u} \; = \; rac{1}{2\pi} \, \int_0^{2\pi} \, | \sum_{k=0}^{N-1} \, u_k \mathrm{e}^{\mathrm{i} k x} |^2 \, f(x) \, \mathrm{d} x \; = 0 \; .$$

Since the integrand is nonnegative almost everywhere, the integrand must be zero almost everywhere. Consequently,

$$|\sum_{k=0}^{N-1} u_k \mathrm{e}^{\mathrm{i}kx}| = 0$$

on the set $\{x \in [0, 2\pi] : f(x) > 0\}$ of positive Lebesgue measure. But this implies the contradiction $u = o_N$. \square

By Theorem 1.1, the convergence of the CG-method depends on the distribution of the eigenvalues of $A_N(f)$. Unfortunately, if the generating $f \in C_{2\pi}$ has zeros, then the CG-method converges very slow. To accelerate the convergence of the CG-method we are looking for suitable preconditioners $M_N(f)$ of $A_N(f)$. Having Theorem 1.1 in mind, we want to find a Hermitian positive definite matrix $M_N(f)$ such that the eigenvalues of $M_N(f)^{-1}A_N(f)$ are bounded from below by a positive constant independent of N and the number of isolated eigenvalues of $M_N(f)^{-1}A_N(f)$ is independent of N.

For the construction of $M_N(f)$ we consider (2.2). In the following, we assume that f has only a finite number of zeros. Then we can choose an equispaced grid

$$x_l := \frac{2\pi l}{N} + w \quad (w \in [0, \frac{2\pi}{N}) \; ; \; l = 0, \dots, N - 1)$$

such that

$$(2.3) f(x_l) > 0 (l = 0, ..., N-1).$$

Approximating the integral on the right-hand side of (2.2) by the trapezoidal rule with respect to the above grid, we obtain

(2.4)
$$\bar{\boldsymbol{u}}' \boldsymbol{A}_{N}(f) \boldsymbol{u} = \frac{1}{2\pi} \int_{0}^{2\pi} |\sum_{k=0}^{N-1} u_{k} e^{ikx}|^{2} f(x) dx$$

$$\approx \frac{1}{N} \sum_{l=0}^{N-1} |\sum_{k=0}^{N-1} u_{k} e^{ikx_{l}}|^{2} f(x_{l})$$

$$= \sum_{l=0}^{N-1} f(x_{l}) \frac{1}{\sqrt{N}} \left(\sum_{j=0}^{N-1} \bar{u}_{j} e^{-2\pi i l j/N} e^{-ijw} \right) \times \frac{1}{\sqrt{N}} \left(\sum_{k=0}^{N-1} u_{k} e^{2\pi i k l/N} e^{ikw} \right)$$

$$= (\boldsymbol{F}_{N} \boldsymbol{W}_{N} \bar{\boldsymbol{u}})' \boldsymbol{D}_{N} \bar{\boldsymbol{F}}_{N} \boldsymbol{W}_{N} \boldsymbol{u}$$

$$= \bar{\boldsymbol{u}}' \boldsymbol{M}_{N}(f) \boldsymbol{u}$$

with the diagonal matrices

$$oldsymbol{W}_N \ := \ \operatorname{diag}\left(\mathrm{e}^{-\mathrm{i}kw}
ight)_{k=0}^{N-1} \ , \quad oldsymbol{D}_N \ := \ \operatorname{diag}\left(f(x_l)
ight)_{l=0}^{N-1}$$

and with

(2.5)
$$M_N(f) = M_N(f, F_N) := W_N F_N D_N \bar{F}_N \bar{W}_N.$$

By (2.3), the matrix $\mathbf{M}_N(f)$ is Hermitian and positive definite. A matrix of the form (2.5) is called an α -circulant matrix and in the special case that $w = \pi/N$ a skew-circulant matrix. Setting $\mathbf{v} := \mathbf{M}_N(f)^{1/2} \mathbf{u}$, we get

$$ar{m{v}}' \, m{M}_N(f)^{-1/2} \, m{A}_N(f) \, m{M}_N(f)^{-1/2} \, m{v} \, pprox \, \, ar{m{v}}' m{v}$$

such that by properties of the Rayleigh quotient, $M_N(f)$ seems to be a good preconditioner of $A_N(f)$. Indeed, using FFT, the multiplication with

$$M_N(f)^{-1} = W_N F_N D_N^{-1} \bar{F}_N \bar{W}_N$$

takes only $\mathcal{O}(N \log N)$ arithmetical operations. In the next section, we prove that the eigenvalues of $\mathbf{M}_N(f)^{-1} \mathbf{A}_N(f)$ are clustered at 1.

We mention that our preconditioner $M_N(f)$ is closely related to the Strang-preconditioner $M_N(\mathcal{S}_N f) = M_N(\mathcal{S}_N f, \mathbf{F}_N)$ in (1.2). By orthogonality of the functions e^{ijx} $(j \in \mathbb{Z})$ in $L_{2\pi}^2$, it is easy to check that (2.2) can be replaced by

$$ar{m{u}}' \, m{A}_N(f) \, m{u} \; = \; rac{1}{2\pi} \, \int_0^{2\pi} \, | \sum_{k=0}^{N-1} \, u_k \, \mathrm{e}^{\mathrm{i} \, k x} |^2 \, (\mathcal{S}_N f)(x) \, \, \mathrm{d} x$$

with

$$(\mathcal{S}_N f)(x) \ := \ \sum_{j=-(N-1)}^{N-1} \, a_j \, \mathrm{e}^{\mathrm{i} j x} \, .$$

Now the above quadrature formula (2.4) with w=0 and with $\mathcal{S}_N f$ instead of f leads to the Strang-preconditioner. Clearly, if f is a trigonometric polynomial of degree $\langle N \rangle$ and if $f(2\pi l/N) > 0$ ($l=0,\ldots,N-1$), then $\mathbf{M}_N(\mathcal{S}_N f) = \mathbf{M}_N(f)$.

However, for arbitrary nonnegative functions $f \in C_{2\pi}$, the matrix $\mathbf{M}_N(\mathcal{S}_N f)$ may be not positive definite. This is one reason for the introduction of $\mathbf{M}_N(f)$.

3 Clustering of the eigenvalues of $M_N(f)^{-1}A_N(f)$

We rewrite (2.4) as

(3.1)
$$\bar{\boldsymbol{u}}' \, \boldsymbol{A}_{N}(f) \, \boldsymbol{u} = \sum_{j=0}^{N-1} \sum_{k=0}^{N-1} \bar{u}_{j} \, u_{k} \, a_{j-k}$$

$$\approx \sum_{j=0}^{N-1} \sum_{k=0}^{N-1} \bar{u}_{j} \, u_{k} \, \tilde{a}_{j-k} = \bar{\boldsymbol{u}}' \, \boldsymbol{M}_{N}(f) \, \boldsymbol{u}$$

with

$$\tilde{a}_k = \tilde{a}_k(f) := \frac{1}{N} \sum_{l=0}^{N-1} f(x_l) e^{-2\pi i l k/N} e^{-ikw}$$

and ask for the approximation error. Assume that $f \in C_{2\pi}$ is a function of bounded variation. Replacing $f(x_l)$ by the Fourier series of f at x_l , we obtain

(3.2)
$$\tilde{a}_k = \frac{1}{N} \sum_{l=0}^{N-1} \sum_{j \in \mathbb{Z}} a_j e^{ijx_l} e^{-2\pi i lk/N} e^{-ikw}$$

$$= \sum_{j=0}^{N-1} a_j e^{-iwk} e^{iwj} \left(\frac{1}{N} \sum_{l=0}^{N-1} e^{-2\pi i lk/N} e^{2\pi i lj/N} \right)$$

$$+ \sum_{j=0}^{N-1} \sum_{r \in \mathbb{Z} \setminus \{0\}} a_{j+rN} e^{-iwk} e^{iw(j+rN)} \left(\frac{1}{N} \sum_{l=0}^{N-1} e^{-2\pi i lk/N} e^{2\pi i lj/N} \right)$$

$$= a_k + \sum_{r \in \mathbb{Z} \setminus \{0\}} a_{k+rN} e^{iwrN} .$$

This is the well-known aliasing effect. Set

(3.3)
$$b_k = b_k(f) := \sum_{r \in \mathbb{Z} \setminus \{0\}} a_{k+rN}(f) e^{iwrN}.$$

Then it follows by (3.2) that

(3.4)
$$A_N(f) = M_N(f) + B_N(f), \quad B_N(f) := -(b_{j-k})_{j,k=0}^{N-1}.$$

Thus

(3.5)
$$M_N(f)^{-1} A_N(f) = I_N + M_N(f)^{-1} B_N(f) .$$

Note that

$$b_k(\mathcal{S}_N f) = \begin{cases} a_{k-N}(f) & k = 1, \dots, N-1, \\ a_{k+N}(f) & k = -1, \dots, 1-N, \\ 0 & k = 0, \end{cases}$$

which describes the approximation error in case of the Strang-preconditioner.

Lemma 3.1. Let p_s be a nonnegative, real-valued trigonometric polynomial of degree $\leq s$, where $2s \leq N$. Then at most 2s eigenvalues of $\mathbf{M}_N(p_s)^{-1}\mathbf{A}_N(p_s)$ differ from 1.

PROOF. By (3.3), it follows that $b_k = 0$ for $|k| \le N - 1 - s$. Consequently, $\mathbf{B}_N(f)$ has rank 2s. Now the assertion follows by (3.5). \square

For the proof of our main theorem we need the following

Lemma 3.2. Let $g \in C_{2\pi}$ be a nonnegative function, where the set $\{x \in [0, 2\pi] : g(x) > 0\}$ has a positive Lebesgue measure. Furthermore, let $h \in C_{2\pi}$ be a positive function with $h_{\min} > 0$ and let f := g h. Then, for any $N \in \mathbb{N}$, the eigenvalues of $\mathbf{A}_N(g)^{-1}\mathbf{A}_N(f)$ lie in the interval $[h_{\min}, h_{\max}]$.

Lemma 3.2 was proved for example in [5]. For a more sophisticated version see [28, 27]. We want to give the following very simple proof.

Proof. Applying the theorem of mean in

$$ar{m{u}}' \, m{A}_N(f) \, m{u} \; = \; rac{1}{2\pi} \, \int_0^{2\pi} \, | \sum_{k=0}^{N-1} \, u_k \, \mathrm{e}^{\mathrm{i} k x} |^2 \, f(x) \, \mathrm{d} x \; ,$$

we obtain that

$$ar{m{u}}' \, m{A}_N(f) \, m{u} \; = \; h_* \; rac{1}{2\pi} \, \int_0^{2\pi} \, | \sum_{k=0}^{N-1} \, u_k \, \mathrm{e}^{\mathrm{i} \, kx} |^2 \, g(x) \, \, \mathrm{d} x$$

with $h_* \in [h_{\min}, h_{\max}]$. This can be rewritten as

$$\bar{\boldsymbol{u}}' \boldsymbol{A}_N(f) \boldsymbol{u} = h_* \bar{\boldsymbol{u}}' \boldsymbol{A}_N(q) \boldsymbol{u}$$
.

By Lemma 2.1, the matrix $A_N(g)$ is positive definite such that for $u \neq o_N$

$$h_* = \frac{\bar{\boldsymbol{u}}' \, \boldsymbol{A}_N(f) \, \boldsymbol{u}}{\bar{\boldsymbol{u}}' \, \boldsymbol{A}_N(g) \, \boldsymbol{u}}.$$

By properties of the Rayleigh quotient this yields the assertion.

In the following, we restrict our attention to nonnegative functions $f \in C_{2\pi}$ having a zero of even order 2s $(s \in \mathbb{N})$ in x = 0. The clustering of the eigenvalues of $M_N(f)^{-1}A_N(f)$ for arbitrary functions

$$f(x) = (x - x_1)^{2s_1} \dots (x - x_m)^{2s_m} \tilde{f}(x), \quad (\tilde{f} > 0)$$

follows in a similar way.

With $f \in C_{2\pi}$ or better with the order 2s of the zero x = 0 of f, we associate the nonnegative trigonometric polynomial

$$(3.6) p_s(x) := (2 - 2\cos x)^s = (2 - e^{ix} - e^{-ix})^s$$

of degree s which has a zero of the same order 2s in x = 0.

Now we can prove our main result.

Theorem 3.3. Let $f \in C_{2\pi}$ be a nonnegative function with a zero of order 2s $(s \in \mathbb{N})$ in x = 0. Let $A_N(f)$ denote the corresponding Toeplitz matrices with preconditioners $\mathbf{M}_N(f)$ defined by (2.5). Then the matrices $\mathbf{M}_N(f)^{-1}\mathbf{A}_N(f)$ have the following properties:

- i) The eigenvalues of $\mathbf{M}_N(f)^{-1}\mathbf{A}_N(f)$ are bounded from below by a positive constant independent of N.
- ii) Let p_s denote the associated trigonometric polynomial (3.6) of f and let h := f/p_s . Then, for $N\geq 2s$, at most 2s eigenvalues of $oldsymbol{M}_N(f)^{-1}oldsymbol{A}_N(f)$ are not contained in the interval $[\frac{h_{\min}}{h_{\max}}, \frac{h_{\max}}{h_{\min}}]$.

 iii) The eigenvalues of $\boldsymbol{M}_N(f)^{-1}\boldsymbol{A}_N(f)$ are clustered at 1.

Proof. In this proof, we denote by $\mathbf{R}_N(m)$ arbitrary (N, N)-matrices of rank m.

1. To prove ii), we use the decomposition

$$\frac{\bar{\boldsymbol{u}}'\,\boldsymbol{A}_N(f)\,\boldsymbol{u}}{\bar{\boldsymbol{u}}'\,\boldsymbol{M}_N(f)\,\boldsymbol{u}} \;=\; \frac{\bar{\boldsymbol{u}}'\,\boldsymbol{A}_N(f)\,\boldsymbol{u}}{\bar{\boldsymbol{u}}'\,\boldsymbol{A}_N(p_s)\,\boldsymbol{u}} \;\; \frac{\bar{\boldsymbol{u}}'\,\boldsymbol{A}_N(p_s)\,\boldsymbol{u}}{\bar{\boldsymbol{u}}'\,\boldsymbol{M}_N(f)\,\boldsymbol{u}} \quad \; (\boldsymbol{u}\neq\boldsymbol{o}_N)\;.$$

By Lemma 3.2 and since $A_N(p_s)$ and $M_N(f)$ are positive definite, it follows that

$$(3.7) h_{\min} \frac{\bar{\boldsymbol{u}}' \, \boldsymbol{A}_N(p_s) \, \boldsymbol{u}}{\bar{\boldsymbol{u}}' \, \boldsymbol{M}_N(f) \, \boldsymbol{u}} \leq \frac{\bar{\boldsymbol{u}}' \, \boldsymbol{A}_N(f) \, \boldsymbol{u}}{\bar{\boldsymbol{u}}' \, \boldsymbol{M}_N(f) \, \boldsymbol{u}} \leq h_{\max} \frac{\bar{\boldsymbol{u}}' \, \boldsymbol{A}_N(p_s) \, \boldsymbol{u}}{\bar{\boldsymbol{u}}' \, \boldsymbol{M}_N(f) \, \boldsymbol{u}}.$$

By (3.4) and Lemma 3.1, we conclude that

$$\boldsymbol{A}_N(p_s) = \boldsymbol{M}_N(p_s) + \boldsymbol{R}_N(2s)$$

and consequently

$$rac{ar{oldsymbol{u}}' oldsymbol{A}_N(f) oldsymbol{u}}{ar{oldsymbol{u}}' oldsymbol{M}_N(f) oldsymbol{u}} \ \le \ h_{ ext{max}} rac{ar{oldsymbol{u}}' oldsymbol{M}_N(p_s) oldsymbol{u}}{ar{oldsymbol{u}}' oldsymbol{M}_N(f) oldsymbol{u}} \ + \ h_{ ext{max}} rac{ar{oldsymbol{u}}' oldsymbol{R}_N(2s) oldsymbol{u}}{ar{oldsymbol{u}}' oldsymbol{M}_N(f) oldsymbol{u}}$$

By construction of $M_N(f)$ this can be rewritten as

$$\frac{\bar{\boldsymbol{u}}'\left(\boldsymbol{A}_N(f) - h_{\max}\,\boldsymbol{R}_N(2s)\right)\boldsymbol{u}}{\bar{\boldsymbol{u}}'\,\boldsymbol{M}_N(f)\,\boldsymbol{u}} \, \leq \, \frac{h_{\max}}{h_{\min}} \quad (\boldsymbol{u} \neq \boldsymbol{o}_N) \, .$$

Assume that $\mathbf{R}_N(2s)$ has s_1 positive eigenvalues. Then, by properties of the Rayleigh quotient and by Weyl's theorem [18, p.184] at most s_1 eigenvalues of $\mathbf{M}_N(f)^{-1}\mathbf{A}_N(f)$ are larger than $\frac{h_{\max}}{h_{\min}}$. Similarly, we obtain that by consideration of the left-hand side of (3.7) that at most $2s-s_1$ eigenvalues of $\mathbf{M}_N(f)^{-1}\mathbf{A}_N(f)$ are smaller than $\frac{h_{\min}}{h_{\max}}$. Thus, at most 2s eigenvalues of $\mathbf{M}_N(f)^{-1}\mathbf{A}_N(f)$ are not contained in $\left[\frac{h_{\min}}{h_{\max}}, \frac{h_{\max}}{h_{\min}}\right]$.

2. To prove i), we use the decomposition (see [4, 6])

$$\frac{\bar{\boldsymbol{u}}'\,\boldsymbol{A}_N(f)\,\boldsymbol{u}}{\bar{\boldsymbol{u}}'\,\boldsymbol{M}_N(f)\,\boldsymbol{u}} \;=\; \frac{\bar{\boldsymbol{u}}'\,\boldsymbol{A}_N(f)\,\boldsymbol{u}}{\bar{\boldsymbol{u}}'\,\boldsymbol{A}_N(p_s)\,\boldsymbol{u}} \;\; \frac{\bar{\boldsymbol{u}}'\,\boldsymbol{M}_N(p_s)\,\boldsymbol{u}}{\bar{\boldsymbol{u}}'\,\boldsymbol{M}_N(f)\,\boldsymbol{u}} \;\; \frac{\bar{\boldsymbol{u}}'\,\boldsymbol{A}_N(p_s)\,\boldsymbol{u}}{\bar{\boldsymbol{u}}'\,\boldsymbol{M}_N(p_s)\,\boldsymbol{u}} \quad (\boldsymbol{u}\neq\boldsymbol{o}_N)\;.$$

By Lemma 3.2 and construction of $M_N(f)$ we see that

$$rac{ar{oldsymbol{u}}'oldsymbol{A}_N(f)oldsymbol{u}}{ar{oldsymbol{u}}'oldsymbol{M}_N(f)oldsymbol{u}}\,\geq\,rac{h_{\min}}{h_{\max}}\,rac{ar{oldsymbol{u}}'oldsymbol{A}_N(p_s)oldsymbol{u}}{ar{oldsymbol{u}}'oldsymbol{M}_N(p_s)oldsymbol{u}}\,.$$

Since $A_N(p_s)$ and $M_N(p_s)$ are positive definite, it remains to show that there exists $c < \infty$ such that

$$\frac{\bar{\boldsymbol{u}}'\,\boldsymbol{A}_N(p_s)\,\boldsymbol{u}}{\bar{\boldsymbol{u}}'\,\boldsymbol{M}_N(p_s)\,\boldsymbol{u}} \,\geq\, \frac{1}{c} > 0 \,.$$

By (3.4) this this can be rewritten as

$$\frac{\bar{\boldsymbol{u}}'\left(\boldsymbol{A}_{N}(p_{s})-\boldsymbol{B}_{N}(p_{s})\right)\boldsymbol{u}}{\bar{\boldsymbol{u}}'\boldsymbol{A}_{N}(p_{s})\boldsymbol{u}} \leq c$$

$$1+\frac{\bar{\boldsymbol{u}}'\left(-\boldsymbol{B}_{N}(p_{s})\right)\boldsymbol{u}}{\bar{\boldsymbol{u}}'\boldsymbol{A}_{N}(p_{s})\boldsymbol{u}} \leq c.$$

The rest of the proof follows the same lines as the proof of Theorem 4.3 in [4], which was formulated for so-called τ -preconditioners.

3. By definition, $h = f/p_s$ is a continuous positive function. Since the trigonometric polynomials are dense in $C_{2\pi}$, for all $\varepsilon > 0$, there exist a positive trigonometric polynomial q of degree $n = n(\varepsilon)$ such that

(3.8)
$$q(x) - \frac{1}{2} \varepsilon h_{\min} \leq h(x) \leq q(x) + \frac{1}{2} \varepsilon h_{\min}$$

for all $x \in [0, 2\pi)$. Thus, since $p_s \geq 0$,

$$(3.9) q p_s - \frac{1}{2} \varepsilon h_{\min} p_s \leq f \leq q p_s + \frac{1}{2} \varepsilon h_{\min} p_s .$$

Regarding (2.2), we obtain by the inequality of the right-hand side

$$ar{m{u}}' \, m{A}_N(f) \, m{u} \; \leq \; ar{m{u}}' \, m{A}_N(q \, p_s) \, m{u} \; + \; rac{1}{2} \, arepsilon h_{\min} \, ar{m{u}}' \, m{A}_N(p_s) \, m{u} \; ,$$

and further, since $\boldsymbol{M}_N(f)$ is positive definite, for all $\boldsymbol{u} \in \mathbb{C}^N$ $(\boldsymbol{u} \neq \boldsymbol{o}_N)$

$$(3.10) \qquad \frac{\bar{\boldsymbol{u}}' \, \boldsymbol{A}_N(f) \, \boldsymbol{u}}{\bar{\boldsymbol{u}}' \, \boldsymbol{M}_N(f) \, \boldsymbol{u}} \, \leq \, \frac{\bar{\boldsymbol{u}}' \, \boldsymbol{A}_N(q \, p_s) \, \boldsymbol{u}}{\bar{\boldsymbol{u}}' \, \boldsymbol{M}_N(f) \, \boldsymbol{u}} \, + \, \frac{1}{2} \, \varepsilon h_{\min} \, \frac{\bar{\boldsymbol{u}}' \, \boldsymbol{A}_N(p_s) \, \boldsymbol{u}}{\bar{\boldsymbol{u}}' \, \boldsymbol{M}_N(f) \, \boldsymbol{u}}$$

Now it holds by (3.4) and Lemma 3.1 that

$$(3.11) \boldsymbol{A}_N(p_s) = \boldsymbol{M}_N(p_s) + \boldsymbol{R}_N(2s) .$$

Moreover, we have by [3] that

$$\boldsymbol{A}_N(q\,p_s) = \boldsymbol{A}_N(q)\,\boldsymbol{A}_N(p_s) + \boldsymbol{R}_N(2n+2s).$$

By (3.11), this can be written as

$$\mathbf{A}_{N}(q p_{s}) = (\mathbf{M}_{N}(q) + \mathbf{R}_{N}(2n)) (\mathbf{M}_{N}(p_{s}) + \mathbf{R}_{N}(2s)) + \mathbf{R}_{N}(2n+2s)$$

$$(3.12) = \mathbf{M}_{N}(q) \mathbf{M}_{N}(p_{s}) + \mathbf{R}_{N}(m)$$

with a Hermitian matrix $\mathbf{R}_N(m)$ of rank $m \leq 4n+4s+\min\{2n,2s\}$. Substituting (3.11) and (3.12) in (3.10), we obtain

$$\begin{array}{lll} \frac{\bar{\boldsymbol{u}}'\,\boldsymbol{A}_N(f)\,\boldsymbol{u}}{\bar{\boldsymbol{u}}'\,\boldsymbol{M}_N(f)\,\boldsymbol{u}} & \leq & \frac{\bar{\boldsymbol{u}}'\,\boldsymbol{M}_N(q)\,\boldsymbol{M}_N(p_s)\,\boldsymbol{u}}{\bar{\boldsymbol{u}}'\,\boldsymbol{M}_N(f)\,\boldsymbol{u}} \,+\, \frac{\bar{\boldsymbol{u}}'\,\boldsymbol{R}_N(m)\,\boldsymbol{u}}{\bar{\boldsymbol{u}}'\,\boldsymbol{M}_N(f)\,\boldsymbol{u}} \\ & + & \frac{1}{2}\,\varepsilon h_{\min}\,\frac{\bar{\boldsymbol{u}}'\,\boldsymbol{M}_N(p_s)\,\boldsymbol{u}}{\bar{\boldsymbol{u}}'\,\boldsymbol{M}_N(f)\,\boldsymbol{u}} \,+\, \frac{1}{2}\,\varepsilon h_{\min}\,\frac{\bar{\boldsymbol{u}}'\,\boldsymbol{R}_N(2s)\,\boldsymbol{u}}{\bar{\boldsymbol{u}}'\,\boldsymbol{M}_N(f)\,\boldsymbol{u}} \end{array}$$

and since

$$rac{oldsymbol{ar{u}}' oldsymbol{M}_N(p_s) oldsymbol{u}}{ar{oldsymbol{u}}' oldsymbol{M}_N(f) oldsymbol{u}} \ \le \ rac{1}{h_{\min}}$$

further

$$\frac{\bar{\boldsymbol{u}}'\left[\boldsymbol{A}_{N}(f)-\boldsymbol{R}_{N}(\tilde{m})\right]\boldsymbol{u}}{\bar{\boldsymbol{u}}'\boldsymbol{M}_{N}(f)\boldsymbol{u}}\leq\frac{\bar{\boldsymbol{u}}'\boldsymbol{M}_{N}(q)\boldsymbol{M}_{N}(p_{s})\boldsymbol{u}}{\bar{\boldsymbol{u}}'\boldsymbol{M}_{N}(f)\boldsymbol{u}}\;+\;\frac{1}{2}\,\varepsilon$$

with $\tilde{m} \leq m+2s$. Setting $\boldsymbol{v}:=\boldsymbol{M}_N(p_s)^{1/2}\boldsymbol{u}$ and using that $\boldsymbol{M}_N(f)=\boldsymbol{M}_N(h)\,\boldsymbol{M}_N(p_s)$, we get

(3.13)
$$\frac{\bar{\boldsymbol{u}}'\left[\boldsymbol{A}_{N}(f)-\boldsymbol{R}_{N}(\tilde{m})\right]\boldsymbol{u}}{\bar{\boldsymbol{u}}'\boldsymbol{M}_{N}(f)\boldsymbol{u}} \leq \frac{\bar{\boldsymbol{v}}'\boldsymbol{M}_{N}(q)\boldsymbol{v}}{\bar{\boldsymbol{v}}'\boldsymbol{M}_{N}(h)\boldsymbol{v}} + \frac{1}{2}\varepsilon.$$

Finally, we have by (3.8) and by definition of M_N , for all $v \in \mathbb{C}^N$ ($v \neq o_N$) that

$$ar{oldsymbol{v}}' \, oldsymbol{M}_N(q) \, oldsymbol{v} \; \leq \; ar{oldsymbol{v}}' \, oldsymbol{M}_N(h) \, oldsymbol{v} \; + \; rac{1}{2} arepsilon \, h_{\min} \, ar{oldsymbol{v}}' \, oldsymbol{v}$$

and further since $0 < \frac{\bar{\boldsymbol{v}}' \, \boldsymbol{v}}{\bar{\boldsymbol{v}}' \, \boldsymbol{M}_N(h) \, \boldsymbol{v}} \leq \frac{1}{h_{\min}}$ that

$$\frac{\bar{\boldsymbol{v}}'\,\boldsymbol{M}_N(q)\,\boldsymbol{v}}{\bar{\boldsymbol{v}}'\,\boldsymbol{M}_N(h)\,\boldsymbol{v}} \;\leq\; 1 + \; \frac{1}{2}\varepsilon\;.$$

Using the above inequality in (3.13), we obtain

$$\frac{\bar{{\pmb u}}' \, [{\pmb A}_N(f) - {\pmb R}_N(\tilde{m})] \, {\pmb u}}{\bar{{\pmb u}}' \, {\pmb M}_N(f) \, {\pmb u}} \, \, \leq \, \, 1 \, \, + \, \, \varepsilon \, .$$

Similarly, we conclude from the left-hand inequality of (3.9) that

$$\frac{\bar{\boldsymbol{u}}' \left[\boldsymbol{A}_N(f) - \boldsymbol{R}_N(\tilde{\boldsymbol{m}}) \right] \boldsymbol{u}}{\bar{\boldsymbol{u}}' \, \boldsymbol{M}_N(f) \, \boldsymbol{u}} \, \geq \, 1 \, - \, \varepsilon \, .$$

Consequently, at most \tilde{m} eigenvalues of $M_N(f)^{-1}A_N(f)$ are not contained in $[1-\varepsilon, 1+\varepsilon]$. This completes the proof. \square

By Theorem 3.3, Theorem 1.1 and construction of $M_N(f)$, our PCG-method converges superlinearly and requires only $\mathcal{O}(N \log N)$ arithmetical operations to achieve a prescribed precision.

Remark 3.1. Unfortunately, we cannot find a similar proof for nonnegative functions $f \in C_{2\pi}$ having not only zeros of even order. The reason therefore is that there does not exist a nonnegative trigonometric polynomial which has a zero of odd order in x = 0. Consequently, we cannot produce an equivalent of (3.6). Our numerical tests show that our preconditioners work well also in the odd case. However, for the matrices $A_N(f)$ generated by the function

$$f(x) = \sqrt{2 - 2\cos x} = |2\sin\frac{x}{2}|,$$

the number n of eigenvalues of $M_N^{-1}(f)A_N(f)$ which are not contained in the interval $(1 - \varepsilon, 1 + \varepsilon)$ grows as follows:

N	32	64	128	256	512
$\varepsilon = 10^{-3}$	7	8	9	10	11
$\varepsilon = 10^{-5}$	10	12	13	15	17

At first glance it seems that the eigenvalues of $\mathbf{M}_N(f)^{-1}\mathbf{A}_N(f)$ are not clustered at 1.

4 Generalizations of the preconditioning technique

In this section, we sketch how our preconditioners can be generalized to the following settings:

- $A_N(f)$ are (real) symmetric Toeplitz matrices,
- $A_N(f)$ are non-Hermitian Toeplitz matrices,
- $A_{M,N}(f)$ are doubly symmetric block Toeplitz matrices with Toeplitz blocks.

4.1 Preconditioners for symmetric Toeplitz matrices

First, we suppose in addition to Section 2 that the generating function $f \in C_{2\pi}$ of the matrices $A_N(f)$ is even. Then

$$a_k = a_k(f) = \frac{2}{\pi} \int_0^{\pi} f(x) \cos kx \, \mathrm{d}x$$

and the Toeplitz matrices $A_N(f) \in \mathbb{R}^{N,N}$ are symmetric. In this case, the multiplication of a vector with $A_N(f)$ can be realized using fast trigonometric transforms instead of fast Fourier transforms. See Remark 4.1. In this way, complex arithmetic can be completely avoided in the iterative solution of (2.1). This is one of the reasons to look for preconditioners of type (2.5), where the Fourier matrix F_N is replaced by trigonometric matrices corresponding to fast trigonometric transforms.

In practice, four discrete sine transforms (DST) and four discrete cosine transforms (DCT) were applied (see [33]). Any of these eight trigonometric transforms can be realized with $\mathcal{O}(N\log N)$ arithmetical operations (see for example [2], [29]). Likewise, we can define preconditioners with respect to any of these transforms. Here we refer to the extensive examinations in [23]. For the case $f \geq 0$, interesting results concerning τ -preconditioners which are related to the sine-I transform are contained in [6, 4]. In particular, Di Benedetto suggested a banded preconditioner of the form $\mathbf{M}_N(p_s)$ with respect to the sine-I transform.

In this paper, we restrict our attention to the so-called DST-II and DCT-II, which are determined by the following transform matrices:

$$\begin{array}{lll} \text{DCT-II} & : & \boldsymbol{C}_N^{II} \ := \ \left(\frac{2}{N}\right)^{1/2} \ \left(\varepsilon_j^N \cos \frac{j(2k+1)\pi}{2N}\right)_{j,k=0}^{N-1} \in \mathbb{R}^{N,N}, \\ \\ \text{DST-II} & : & \boldsymbol{S}_N^{II} \ := \ \left(\frac{2}{N}\right)^{1/2} \ \left(\varepsilon_{j+1}^N \sin \frac{(j+1)(2k+1)\pi}{2N}\right)_{j,k=0}^{N-1} \in \mathbb{R}^{N,N}, \end{array}$$

where $\varepsilon_k^N:=2^{-1/2}$ (k=0,N) and $\varepsilon_k^N:=1$ $(k=1,\ldots,N-1)$. Moreover, we use the DCT–I with transform matrix

$$\tilde{\boldsymbol{C}}_{N+1}^{I} := \left((\varepsilon_k^N)^2 \cos \frac{jk\pi}{N} \right)_{j,k=0}^{N}.$$

The matrices $m{C}_N^{II}$ and $m{S}_N^{II}$ are orthogonal and $m{ ilde{C}}_{N+1}^{I}$ satisfies

(4.1)
$$\tilde{\boldsymbol{C}}_{N+1}^{I} \, \tilde{\boldsymbol{C}}_{N+1}^{I} = \frac{N}{2} \, \boldsymbol{I}_{N+1} \,.$$

The eight trigonometric transforms are closely related to Toeplitz matrices [24]. In particular, it holds for the DCT-II and the DST-II:

Lemma 4.1. Let stoep \mathbf{a}' and shank \mathbf{a}' denote a symmetric Toeplitz matrix and a persymmetric Hankel matrix with first row \mathbf{a}' , respectively. Then there exist the following relations between trigonometric transforms and symmetric Toeplitz matrices:

$$\left(m{C}_{N}^{II}
ight)' \, m{D}_{1} \, m{C}_{N}^{II} = rac{1}{2} \operatorname{stoep}(a_{0}, \ldots, a_{N-1}) \, + \, rac{1}{2} \operatorname{shank}(a_{1}, \ldots, a_{N-1}, 0) \, , \\ \left(m{S}_{N}^{II}
ight)' \, \, m{D}_{2} \, m{S}_{N}^{II} = rac{1}{2} \operatorname{stoep}(a_{0}, \ldots, a_{N-1}) \, - \, rac{1}{2} \operatorname{shank}(a_{1}, \ldots, a_{N-1}, 0) \, .$$

with

$$egin{array}{lll} m{D}_1 &:=& \mathrm{diag}(d_0,\ldots,d_{N-1})'\,, \; m{D}_2 := \mathrm{diag}(d_1,\ldots,d_N)'\,, \ m{d} &=& (d_0,\ldots,d_N)'\,:= m{ ilde{C}}_{N+1}^I \; (a_0,\ldots,a_{N-1},0)'\,. \end{array}$$

For the proof see [24].

Remark 4.1. By Lemma 4.1, it follows that

$$\operatorname{stoep}(a_0,\ldots,a_{N-1}) \,=\, \left(oldsymbol{C}_N^{II}
ight)' oldsymbol{D}_1 \, oldsymbol{C}_N^{II} \,+\, \left(oldsymbol{S}_N^{II}
ight)' oldsymbol{D}_2 \, oldsymbol{S}_N^{II} \,.$$

Thus, if the vector \mathbf{d} is precomputed by the DCT-I, then the multiplication of a vector with a symmetric Toeplitz matrix of size (N,N) requires two DCT-II, two DST-II and 2N real multiplications and can therefore be realized with $\mathcal{O}(N\log N)$ arithmetical operations (see also [24]).

Since for even $f \in C_{2\pi}$, the (N-1)-th Fourier sum can be written as

$$(S_N f)(x) = 2 \sum_{k=0}^{N-1} (\varepsilon_k^N)^2 a_k \cos(kx),$$

we obtain by Lemma 4.1 that

$$\mathbf{A}_{N}(f) = (\mathbf{C}_{N}^{II})'(2\mathbf{D}) \, \mathbf{C}_{N}^{II} - \operatorname{shank}(a_{1}, \dots, a_{N-1}, 0)
(4.2) = (\mathbf{C}_{N}^{II})' \operatorname{diag} \left((\mathcal{S}_{N} f)(\frac{j\pi}{N}) \right)_{j=0}^{N-1} \, \mathbf{C}_{N}^{II} - \operatorname{shank}(a_{1}, \dots, a_{N-1}, 0) ,
\mathbf{A}_{N}(f) = (\mathbf{S}_{N}^{II})'(2\tilde{\mathbf{D}}) \, \mathbf{S}_{N}^{II} + \operatorname{shank}(a_{1}, \dots, a_{N-1}, 0)
(4.3) = (\mathbf{S}_{N}^{II})' \operatorname{diag} \left((\mathcal{S}_{N} f)(\frac{j\pi}{N}) \right)_{j=1}^{N} \, \mathbf{S}_{N}^{II} + \operatorname{shank}(a_{1}, \dots, a_{N-1}, 0) .$$

Consequently, we introduce the Strang-type-preconditioners by [25]:

$$\begin{array}{lll} \operatorname{DCT} - \operatorname{II} : & \boldsymbol{M}_{N}(\mathcal{S}_{N} f, \boldsymbol{C}_{N}^{II}) & := & (\boldsymbol{C}_{N}^{II})' \operatorname{diag}\left(\mathcal{S}_{N} f(\frac{j\pi}{N})\right)_{j=0}^{N-1} \boldsymbol{C}_{N}^{II}, \\ (4.4) & \operatorname{DST} - \operatorname{II} : & \boldsymbol{M}_{N}(\mathcal{S}_{N} f, \boldsymbol{S}_{N}^{II}) & := & (\boldsymbol{S}_{N}^{II})' \operatorname{diag}\left(\mathcal{S}_{N} f(\frac{j\pi}{N})\right)_{j=1}^{N} \boldsymbol{S}_{N}^{II}. \end{array}$$

See also [21]. Again, if f has zeros, then it can not be assured that the Strang-type-preconditioners are positive definite. Therefore, we define similar to (2.5) the preconditioners

$$\begin{array}{lll} \operatorname{DCT}-\operatorname{II}: & \boldsymbol{M}_{N}(f,\boldsymbol{C}_{N}^{II}) &:= & (\boldsymbol{C}_{N}^{II})' \operatorname{diag}\left(f(\frac{j\pi}{N})\right)_{j=0}^{N-1} \boldsymbol{C}_{N}^{II}, \\ (4.5) & \operatorname{DST}-\operatorname{II}: & \boldsymbol{M}_{N}(f,\boldsymbol{S}_{N}^{II}) &:= & (\boldsymbol{S}_{N}^{II})' \operatorname{diag}\left(f(\frac{j\pi}{N})\right)_{j=1}^{N} \boldsymbol{S}_{N}^{II}. \end{array}$$

If $f(j\pi/N)>0$ for all $j=0,\ldots,N-1$, then $\boldsymbol{M}_N(f,\boldsymbol{C}_N^{II})$ is positive definite. If $f(j\pi/N)>0$ for all $j=1,\ldots,N$, then $\boldsymbol{M}_N(f,\boldsymbol{S}_N^{II})$ is positive definite.

Note that independent of our results, T. Huckle [20] suggested a preconditioner of type (4.5) with respect to the DST-I.

Clearly, if f is a trigonometric polynomial of degree < N, then the Strang-type-preconditioners (4.4) coincide with our preconditioners (4.5). Moreover, we have by (4.2) and (4.3) for trigonometric polynomials f = p of degree $\le s$ (2s < N) that

$$A_N(p) = M_N(p, C_N^{II}) - R_N(2s) = M_N(p, S_N^{II}) + R_N(2s)$$
.

Thus, we can prove in a completely similar way as in Section 3 the following

THEOREM 4.2. Let $f \in C_{2\pi}$ be an even nonnegative function with a zero of order 2s $(s \in \mathbb{N})$ in x = 0. Let $A_N(f)$ denote the corresponding Toeplitz matrices with preconditioners $M_N(f) = M_N(f, S_N^{II})$ defined by (4.4). Then the matrices $M_N(f)^{-1}A_N(f)$ have the following properties:

- i) The eigenvalues of $\mathbf{M}_N(f)^{-1}\mathbf{A}_N(f)$ are clustered at 1.
- ii) Let p_s denote the associated trigonometric polynomial (3.6) of f and let $h:=f/p_s$. Then, for $N\geq 2s$, at most 2s eigenvalues of $\boldsymbol{M}_N(f)^{-1}\boldsymbol{A}_N(f)$ are not contained in the interval $\left[\frac{h_{\min}}{h_{\max}},\frac{h_{\max}}{h_{\min}}\right]$.

The PCG-method with our preconditioners can be realized in a more efficient way than the PCG-method with banded Toeplitz matrices as preconditioners [22, 26]:

Remark 4.2. Our PCG-method requires only two DCT-II, two DST-II and $\mathcal{O}(N)$ real multiplications in each iteration step. This can be seen for the preconditioner $\mathbf{M}_N(f, \mathbf{C}_N^{II})$ as follows: Instead of

$$(oldsymbol{C}_N^{II})'oldsymbol{E}^{-1}oldsymbol{C}_N^{II}\left((oldsymbol{C}_N^{II})'oldsymbol{D}oldsymbol{C}_N^{II}+(oldsymbol{S}_N^{II})'oldsymbol{ ilde{D}}oldsymbol{S}_N^{II}
ight)oldsymbol{x}=(oldsymbol{C}_N^{II})'oldsymbol{E}^{-1}oldsymbol{C}_N^{II}oldsymbol{b}$$

with
$$m{E} := \mathrm{diag}\left(f(rac{j\pi}{N})
ight)_{j=0}^{N-1}$$
, we solve
$$m{E}^{-1}\left(m{D} + m{C}_N^{II}(m{S}_N^{II})'m{ ilde{D}}m{S}_N^{II}(m{C}_N^{II})'
ight)m{ ilde{x}} = m{ ilde{b}}$$

with $\tilde{\boldsymbol{x}} := \boldsymbol{C}_N^{II} \boldsymbol{x}$ and $\tilde{\boldsymbol{b}} := \boldsymbol{E}^{-1} \boldsymbol{C}_N^{II} \boldsymbol{b}$. The vectors \boldsymbol{d} , $\tilde{\boldsymbol{b}}$ and \boldsymbol{x} can be precomputed and postcomputed, respectively. See also [19, 20].

4.2 Preconditioners for non-Hermitian Toeplitz matrices

Next, we are interested in the solution of systems of linear equations $\mathbf{A}_N(f)\mathbf{x} = \mathbf{b}$ with regular, but non-Hermitian Toeplitz matrices $\mathbf{A}_N(f)$. We intend to solve the normal equation

(4.6)
$$\bar{\boldsymbol{A}}'_{N}(f)\boldsymbol{A}_{N}(f)\boldsymbol{x} = \bar{\boldsymbol{A}}'_{N}(f)\boldsymbol{b}$$

using the PCG-method. By [3], it holds that

$$\bar{\boldsymbol{A}}'_{N}(f)\boldsymbol{A}_{N}(f) = \boldsymbol{A}_{N}(|f|^{2}) + \boldsymbol{R}_{N} + \boldsymbol{U}_{N},$$

with a low rank matrix \mathbf{R}_N and a matrix \mathbf{U}_N of small spectral norm. If f=p is a trigonometric polynomial of degree $\leq s$ $(2s \leq N)$, then

$$\bar{\boldsymbol{A}}'_N(f)\boldsymbol{A}_N(f) = \boldsymbol{A}_N(|f|^2) + \boldsymbol{R}_N(2s).$$

Assume that $|f| \in C_{2\pi}$ has only a finite number of zeros. If $A_N(|f|^2)$ is Hermitian and if $|f(\frac{2\pi j}{N}+w)| > 0$ for a suitable $w \in [0, 2\pi/N)$ for all $j = 0, \ldots, N-1$, then we define our preconditioners by

$$m{M}_N(|f|^2, m{F}_N) := m{W}_N \, m{F}_N \, \operatorname{diag} \left(|f(rac{2\pi j}{N} + w)|^2
ight)_{i=0}^{N-1} \, ar{m{F}}_N \, ar{m{W}}_N \, .$$

If $A_N(|f|^2)$ is symmetric and if $|f(\frac{2\pi j}{N})| > 0$ for all $j = 0, \ldots, N-1$ or $|f(\frac{2\pi j}{N})| > 0$ for all $j = 1, \ldots, N$, then we use

$$\begin{aligned} \boldsymbol{M}_{N}(|f|^{2},\boldsymbol{C}_{N}^{II}) &:= & (\boldsymbol{C}_{N}^{II})' \operatorname{diag}\left(|f(\frac{\pi j}{N})|^{2}\right)_{j=0}^{N-1} \boldsymbol{C}_{N}^{II}, \\ \boldsymbol{M}_{N}(|f|^{2},\boldsymbol{S}_{N}^{II}) &:= & (\boldsymbol{S}_{N}^{II})' \operatorname{diag}\left(|f(\frac{\pi j}{N})|^{2}\right)_{j=1}^{N} \boldsymbol{S}_{N}^{II} \end{aligned}$$

as preconditioners, respectively.

4.3 Preconditioners for doubly symmetric block Toeplitz matrices with Toeplitz blocks

Finally, the generalization of our results to doubly symmetric block–Toeplitz systems with Toeplitz blocks is straightforward. We consider systems of linear equations

$$A_{M.N}x = b$$

where $A_{M,N}$ denotes a positive definite doubly symmetric block–Toeplitz matrix with Toeplitz blocks (BTTB matrix), i.e.

$$A_{M,N} := (A_{r-s})_{r,s=0}^{M-1}$$
 with $A_r := (a_{r,j-k})_{j,k=0}^{N-1}$

and $a_{r,j} = a_{|r|,|j|}$. We assume that the matrices $A_{M,N}$ are generated by a real-valued 2π -periodic continuous even function in two variables, i.e.

$$a_{j,k} := rac{1}{4\pi^2}\int\limits_0^{2\pi}\int\limits_0^{2\pi} arphi(s,t)\,\mathrm{e}^{-\mathrm{i}(sj+tk)}\,\mathrm{d} s\,\mathrm{d} t\,.$$

Lemma 4.1 can be extended to BTTB matrices as follows:

$$\begin{array}{lll} \boldsymbol{A}_{M,N} & = & (\boldsymbol{C}_{M}^{II} \otimes \boldsymbol{C}_{N}^{II})' \, \boldsymbol{D}_{1} \, (\boldsymbol{C}_{M}^{II} \otimes \boldsymbol{C}_{N}^{II}) + (\boldsymbol{S}_{M}^{II} \otimes \boldsymbol{C}_{N}^{II})' \, \boldsymbol{D}_{2} \, (\boldsymbol{S}_{M}^{II} \otimes \boldsymbol{C}_{N}^{II}) \\ & + & (\boldsymbol{C}_{M}^{II} \otimes \boldsymbol{S}_{N}^{II})' \, \boldsymbol{D}_{3} \, (\boldsymbol{C}_{M}^{II} \otimes \boldsymbol{S}_{N}^{II}) + (\boldsymbol{S}_{M}^{II} \otimes \boldsymbol{S}_{N}^{II})' \, \boldsymbol{D}_{4} \, (\boldsymbol{S}_{M}^{II} \otimes \boldsymbol{S}_{N}^{II}) \end{array}$$

with

$$m{D}_1 := \operatorname{diag}\left(\operatorname{col}(ilde{a}_{r,j})_{j,r=0}^{N-1,M-1}
ight) \,, \qquad m{D}_2 := \operatorname{diag}\left(\operatorname{col}(ilde{a}_{r,j})_{j=0,r=1}^{N-1,M}
ight) \,, \ m{D}_3 := \operatorname{diag}\left(\operatorname{col}(ilde{a}_{r,j})_{j=1,r=0}^{N,M-1}
ight) \,, \qquad m{D}_4 := \operatorname{diag}\left(\operatorname{col}(ilde{a}_{r,j})_{j=1,r=1}^{N,M}
ight) \,,$$

$$(ilde{a}_{r,j})_{j,r=0}^{N,M} \ := \ ilde{m{C}}_{M+1}^{I} \ \left((a_{r,j})_{j,r=0}^{N,M}
ight) (ilde{m{C}}_{N+1}^{I})' \ ,$$

 $a_{r,N}:=0\ (r=0,\ldots,M)$ and $a_{M,j}:=0\ (j=0,\ldots,N).$ Here col: $\mathbb{R}^{N,M}\to\mathbb{R}^{MN}$ is defined by

col
$$(x_{j,k})_{i=0,k=0}^{N-1,M-1} := (x_r)_{r=0}^{MN-1}$$
 with $x_{kN+j} := x_{j,k}$.

Consequently, the multiplication of a vector with a BTTB matrix requires only $\mathcal{O}(MN\log(MN))$ arithmetical operations. For details see [25]. We define our so-called "level-2" preconditioners by

$$\begin{split} \boldsymbol{M}_{N}(\varphi, \boldsymbol{C}_{M}^{II} \otimes \boldsymbol{C}_{N}^{II})) &:= & (\boldsymbol{C}_{M}^{II} \otimes \boldsymbol{C}_{N}^{II})' \operatorname{diag}(\operatorname{col}\left(\varphi(\frac{r\pi}{M}, \frac{j\pi}{N})\right)_{j,k=0}^{N-1,M-1}) \times \\ & & (\boldsymbol{C}_{M}^{II} \otimes \boldsymbol{C}_{N}^{II}) \,, \\ \boldsymbol{M}_{N}(\varphi, \boldsymbol{S}_{M}^{II} \otimes \boldsymbol{S}_{N}^{II})) &:= & (\boldsymbol{S}_{M}^{II} \otimes \boldsymbol{S}_{N}^{II})' \operatorname{diag}(\operatorname{col}\left(\varphi(\frac{r\pi}{M}, \frac{j\pi}{N})\right)_{j,k=1}^{N,M}) \times \\ & & (\boldsymbol{S}_{M}^{II} \otimes \boldsymbol{S}_{N}^{II}) \,. \end{split}$$

Using the same arguments as in the Remark 4.2, we see that our PCG–method requires per iteration step only MN multiplications more than the conventional CG–method.

5 Numerical Examples

In this section, we show the efficiency of our new preconditioning technique by various numerical examples. The fast computation of the preconditioners and the PCG-method were implemented in MATLAB, where the C-programs for the fast trigonometric transforms were included by cmex. The algorithms were tested on a Sun SPARCstation 20.

As transform length we choose $N=2^n$ and as right-hand side \boldsymbol{b} of (2.1) the vector consisting of N entries "1". The PCG-method started with the zero vector and stopped if $\|\boldsymbol{r}^{(j)}\|_2/\|\boldsymbol{r}^{(0)}\|_2 < 10^{-7}$, where $\boldsymbol{r}^{(j)}$ denotes the residual vector after j iterations.

It is remarkable, that the number of iterations also depends on roundoff-errors. Computation by the PCG-method which incorporates the FFT for the fast matrix-vector multiplications leads to another number of iteration steps than the same computation without FFT-techniques, i.e. with straightforward matrix-vector multiplications.

We begin with Hermitian ill–conditioned Toeplitz matrices $\boldsymbol{A}_N(f)$ arising from the generating function

i)
$$f(x) = (x/2 - \pi/4)^4$$
 $(x \in [0, 2\pi))$.

The second column of Table 5.1 shows the number of iterations of the CG-method without preconditioning. The columns 3 and 4 contain the numbers of iterations of the PCG-method with the optimal preconditioner $\boldsymbol{M}_{N}^{\mathcal{O}}(\boldsymbol{F}_{N})$ given by (1.3) and with our preconditioner $\boldsymbol{M}_{N}(f,\boldsymbol{F}_{N})$ defined by (2.5) with $w := \pi/N$, respectively.

n	I_N	$oldsymbol{M}_N^{\mathcal{O}}(oldsymbol{F}_N)$	$oldsymbol{M}_N(f,oldsymbol{F}_N)$
4	26	17	11
5	85	36	13
6	349	67	15
7	1570	154	20
8	> 3000	377	23
9	> 3000	995	25
10	> 3000	2220	32

Table 5.1: $f(x) = (x/2 - \pi/4)^4$ $(x \in [0, 2\pi))$

Next, we consider symmetric Toeplitz matrices A_N . We compare the Strang-type-preconditioners (4.4), our preconditioners (2.5) and (4.5) and the optimal trigonometric preconditioners defined by

$$\begin{array}{lll} \text{DCT-II:} & \boldsymbol{M}_{N}^{\mathcal{O}}(\boldsymbol{C}_{N}^{II}) & := & (\boldsymbol{C}_{N}^{II})' \; \delta(\boldsymbol{C}_{N}^{II} \; \boldsymbol{A}_{N} \; (\boldsymbol{C}_{N}^{II})') \; \boldsymbol{C}_{N}^{II}, \\ \text{DST-II:} & \boldsymbol{M}_{N}^{\mathcal{O}}(\boldsymbol{S}_{N}^{II}) & := & (\boldsymbol{S}_{N}^{II})' \delta(\boldsymbol{S}_{N}^{II} \; \boldsymbol{A}_{N} \; (\boldsymbol{S}_{N}^{II})') \; \boldsymbol{S}_{N}^{II}. \end{array}$$

See for example [8, 12, 24]. Our test matrices correspond to the following generating functions:

ii) (see [26]):
$$f(x) := (x^2 - 1)^2$$
 $(x \in [-\pi, \pi))$.

In (2.5), we set $w := \pi/N$.

iii) (see [26, 9, 10]):
$$f(x) := x^4 \quad (x \in [-\pi, \pi))$$
.

In (2.5), we set
$$w := \pi/N$$
.

The Tables 5.2 and 5.3 present the number of iteration steps for different preconditioners. The asterix emphasizes that the corresponding preconditioners are not positive definite. Our new preconditioners lead to the best results. Compare also with [26, 9, 10]. Note that by the Remark 4.2, our PCG-method requires per iteration step only few arithmetical operations more than the conventional CG-method.

		$oldsymbol{M}_N(\mathcal{S}_N$	$_{N}f,oldsymbol{O}_{N})$	$oldsymbol{M}_N^{\mathcal{O}}$	(\boldsymbol{O}_N)	$M_N(j)$	$f, oldsymbol{O}_N)$
n	I_N	$oldsymbol{C}_{N}^{II}$	$oldsymbol{S}_N^{II}$	$oldsymbol{C}_{N}^{II}$	$oldsymbol{S}_N^{II}$	$oldsymbol{S}_N^{II}$	$oldsymbol{F}_N$
5	25	9*	8*	17	10	5	5
6	69	9*	8*	21	11	5	6
7	190	10*	10*	26	14	7	7
8	457	10*	10*	33	16	8	8
9	> 1000	11	9	43	19	9	9
10	> 1000	10*	10*	59	24	7	7

Table 5.2: $f(x) = (x^2 - 1)^2$ $(x \in [-\pi, \pi))$

Our next test is related to non–Hermitian Toeplitz systems. As generating function of $A_N(f)$ we choose

iv) (see [24]):
$$f(x) = x^2 e^{ix}$$
 ($x \in [-\pi, \pi)$).

Then, the matrices $A_N(f)$ have real entries such that we restrict our attention to trigonometric preconditioners. Table 5.5 compares the PCG-method applied to the normal equation (4.6) with

- the optimal preconditioner of $\mathbf{A}'_{N}(f)\mathbf{A}_{N}(f)$ (see [24])

$$\boldsymbol{M}_{N}^{\mathcal{O}_{1}} := \boldsymbol{O}_{N}' \ \delta(\boldsymbol{O}_{N} \boldsymbol{A}_{N}'(f) \boldsymbol{A}_{N}(f) \boldsymbol{O}_{N}') \ \boldsymbol{O}_{N},$$

- the optimal preconditioner of $\boldsymbol{A}_N(|f|^2)$

$$oldsymbol{M}_N^{\mathcal{O}_2} := oldsymbol{O}_N' \; \delta(oldsymbol{O}_N oldsymbol{A}_N(|f|^2) oldsymbol{O}_N') \; oldsymbol{O}_N \, ,$$

		$m{M}_N(\mathcal{S}_N f, m{O}_N)$		$oldsymbol{M}_N^{\mathcal{O}}(oldsymbol{O}_N)$		$oldsymbol{M}_N(f, oldsymbol{O}_N)$	
n	$oldsymbol{I}_N$	$oldsymbol{C}_{N}^{II}$	$oldsymbol{S}_N^{II}$	$oldsymbol{C}_{N}^{II}$	$oldsymbol{S}_N^{II}$	$oldsymbol{S}_N^{II}$	$oldsymbol{F}_N$
5	33	12*	10*	18	10	6	6
6	116	18*	15*	30	13	7	6
7	487	27*	21*	54	16	8	8
8	>1000	40*	33*	155	19	9	10
9	>1000	115*	63*	376	25	9	10
10	>1000	218*	165*	>1000	32	10	11

Table 5.3: $f(x) = x^4$ $(x \in [-\pi, \pi))$

- the Strang-type-preconditioner $\boldsymbol{M}_N(\mathcal{S}_N(|f|^2),\boldsymbol{O}_N)$ and our preconditioner $\boldsymbol{M}_N(|f|^2,\boldsymbol{S}_N^{II})$ defined by (4.7).

Finally, let us turn to BTTB matrices $A_{N,N}$. In our two examples, the matrices $A_{N,N}$ are generated by the functions

v) (see [22]):
$$\varphi(s,t) = s^2 t^4$$
 and $\psi(s,t) = (s^2 + t^2)^2$ $(s,t \in [-\pi,\pi))$.

Both matrices are ill-conditioned and the CG-method without preconditioning, with Strang-type-preconditioning or with optimal trigonometric preconditioning converges very slow (see [22, 25]). Our preconditioning determined by (4.7) leads to the number of iterations in Table 5.5. Again, our PCG-method requires per iteration step only few arithmetical operations more than the conventional CG-method.

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I_N	$oldsymbol{M}_N^{\mathcal{O}_1}(oldsymbol{C}_N^{II})$	$oldsymbol{M}_N^{\mathcal{O}_1}(oldsymbol{S}_N^{II})$	$oldsymbol{M}_N^{\mathcal{O}_2}(oldsymbol{C}_N^{II})$	$oldsymbol{M}_N^{\mathcal{O}_2}(oldsymbol{S}_N^{II})$	$oldsymbol{M}_N^{\mathcal{O}_1}(oldsymbol{C}_N^{II}) egin{array}{c c c c c c c c c c c c c c c c c c c $	$oldsymbol{M}_N(\mathcal{S}_N(f ^2), oldsymbol{S}_N^{II})$	$oldsymbol{M}_N(f ^2,oldsymbol{S})$
84	29	21	34	18	22*	19*	
311	52	26	64	22	32*	26*	I
1226	116	33	139	27	56*	44*	T
5220	256	40	324	39	96*	76*	Ī
>10000	664	74	865	55	200*	157*	Ī
>10000	1758	101	2546	78	466*	357*	

Table 5.4: $f(x) := x^2 e^{ix}$ $(x \in [-\pi, \pi))$

N	$m{M}_N(arphi,m{S}_N^{II}\otimesm{S}_N^{II})$	$m{M}_N(\psi, m{S}_N^{II} \otimes m{S}_N^{II})$
8	13	9
16	16	12
32	22	14
64	29	19
128	36	25
256	43	35
512	52	49

Table 5.5: $\varphi(s,t) = s^2 t^4$ and $\psi(s,t) = (s^2 + t^2)^2$ $(s,t \in [-\pi,\pi))$

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