

Preconditioners for ill-conditioned Toeplitz systems constructed from positive kernels

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Abstract. In this paper, we are interested in the iterative solution of ill-conditioned Toeplitz systems generated by continuous non-negative real-valued functions f with a finite number of zeros. We construct new w -circulant preconditioners without explicit knowledge of the generating function f by approximating f by its convolution $f * K_N$ with a suitable positive reproducing kernel K_N . By the restriction to positive kernels we obtain positive definite preconditioners. Moreover, if f has only zeros of even order $\leq 2s$, then we can prove that the property $\int_{-\pi}^{\pi} t^{2k} K_N(t) dt \leq CN^{-2k}$ ($k = 0, \dots, s$) of the kernel is necessary and sufficient to ensure the convergence of the PCG-method in a number of iteration steps independent of the dimension N of the system. Our theoretical results were confirmed by numerical tests.

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1 Introduction

In this paper, we are concerned with the iterative solution of sequences of “mildly” ill-conditioned Toeplitz systems

$$\mathbf{A}_N \mathbf{x}_N = \mathbf{b}_N,$$

where $\mathbf{A}_N \in \mathbb{C}^{N,N}$ are positive definite Hermitian Toeplitz matrices generated by a continuous non-negative function f which has only a finite number of zeros. Often these systems are obtained by discretization of continuous problems (partial differential equation, integral equation with weakly singular kernel) and the dimension N is related to the grid parameter of the discretization. For further applications see [12] and the references therein.

Iterative solution methods for Toeplitz systems, in particular the conjugate gradient method (CG-method), have attained much attention during the last years. The reason for this is that the essential computational effort per iteration step, namely the multiplication of a vector with the Toeplitz matrix \mathbf{A}_N , can be reduced to $\mathcal{O}(N \log N)$ arithmetical operations by fast Fourier transforms (FFT). However, the number of iteration steps depends on the distribution of the eigenvalues of \mathbf{A}_N . If we allow the generating function f to have isolated zeros, then the condition numbers of the related Toeplitz matrices grow polynomial with N and the CG-method converges very slow [8, 28, 45]. Therefore, the really task consists in the construction of suitable preconditioners \mathbf{M}_N of \mathbf{A}_N so that the number of iteration steps of the corresponding preconditioned CG-method (PCG-method) becomes independent of N . Here it is useful to recall a result of O. Axelsson [1, p. 573] relating the spectrum of the coefficient matrix to the number of iteration steps to achieve a prescribed precision:

Theorem 1.1. Let \mathbf{A} be a positive definite Hermitian (N, N) -matrix which has p and q isolated large and small eigenvalues, respectively:

$$\begin{aligned} 0 < \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_q < a \leq \lambda_{q+1} \leq \dots \leq \lambda_{N-p} \leq b \\ < \lambda_{N-p+1} \leq \lambda_{N-p+2} \leq \dots \leq \lambda_N \quad (0 < a < b < \infty). \end{aligned}$$

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

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

iteration steps to achieve precision τ , i.e.

$$\frac{\|\mathbf{x}_n - \mathbf{x}\|_A}{\|\mathbf{x}_0 - \mathbf{x}\|_A} \leq \tau,$$

where $\|\mathbf{x}\|_A := \sqrt{\mathbf{x}' \mathbf{A} \mathbf{x}}$ and where \mathbf{x}_n denotes the numerical solution after n iteration steps.

In literature two kinds of preconditioners were mainly exploited, namely banded Toeplitz matrices and matrices arising from a matrix algebra $\mathcal{A}_{\mathbf{O}_N} := \{\bar{\mathbf{O}}'_N(\text{diag } \mathbf{d})\mathbf{O}_N : \mathbf{d} \in \mathbb{C}^N\}$, where \mathbf{O}_N denotes a unitary matrix.

For another approach by multigrid methods see for example [23].

Various banded Toeplitz preconditioners were examined [10, 5, 40, 36, 41]. It was proved that the corresponding PCG-methods converge in a number of iteration steps independent of N . However, there is the significant constraint that the cost per iteration of the proposed procedure should be upper-bounded by $\mathcal{O}(N \log N)$. This implies some conditions on the growth of the bandwidth of the banded Toeplitz preconditioners [41].

The above constraint is trivially fulfilled if we chose preconditioners from matrix algebras, where the unitary matrix \mathbf{O}_N has to allow an efficient multiplication with a vector in $\mathcal{O}(N \log N)$ arithmetical operations. Up to now, the only preconditioners of the matrix algebra class which

ensure the desired convergence of the corresponding PCG–method are the preconditioners proposed in [31, 25]. Unfortunately, the construction of these preconditioners requires the explicit knowledge of the generating function f .

Extensive examinations were done with natural and optimal Tau preconditioners [6, 3]. Only for sufficiently smooth functions, where the necessary smoothness depends on the order of the zeros of f , the natural Tau preconditioners become positive definite and lead to the desired location of the eigenvalues of the preconditioned matrices. The optimal Tau preconditioner is in general a bad choice if f has zeros of order > 2 . The reason for this will become clear in the following sections.

In this paper, we combine our approach in [31] with the approximation of f by its convolution with a reproducing kernel K_N . The kernel approach was given in [15] for positive generating functions. Interesting tests with B –spline kernels were performed by R. Chan et al. in [14]. The advantage of the kernel approach is that it does not require the explicit knowledge of the generating function. However, only for our *theoretical* proofs we need some knowledge about the location of the zeros of the generating function f . See remarks at the end of this section. We restrict our attention to positive kernels. This ensures that our preconditioners are positive definite. Suppose that f has only zeros of even order $\leq 2s$. Then we prove that under the “*moment condition*”

$$\int_{-\pi}^{\pi} t^{2k} K_N(t) dt \leq CN^{-2k} \quad (k = 0, \dots, s)$$

on the kernels K_N , the eigenvalues of $\mathbf{M}_N^{-1} \mathbf{A}_N$ are contained in some interval $[a, b]$ ($0 < a \leq b < \infty$) except for a fixed number (independent of N) of eigenvalues falling into $[b, \infty)$ so that PCG converges in $\mathcal{O}(1)$ steps.

Note that the above kernel property with $s = 1$ implies for sufficiently smooth f the Jackson result

$$\|f - K_N * f\|_{\infty} \leq N^{-2} \omega(f^{(2)}, 1/N),$$

where ω denotes the modulus of continuity. On the other hand, the classical saturation result of P. P. Korovkin [29, 21] states that we cannot expect a convergence speed of $\|f - K_N * f\|_{\infty}$ better than N^{-2} even in the presence of very regular functions f .

This paper is organized as follows: In Section 2, we introduce our w –circulant positive definite preconditioners. We show how the corresponding PCG–method can be implemented with only $\mathcal{O}(N)$ arithmetical operations per step more than the original CG–method. Section 3 is concerned with the location of the eigenvalues of the preconditioned matrices. We will see that under some assumptions on the kernel the number of CG–iterations is independent of N . Special kernels as Jackson kernels and B –spline kernels are considered in Section 5. In Section 6, we sketch how our ideas can be extended to (real) symmetric Toeplitz matrices with trigonometric preconditioners and to doubly symmetric block Toeplitz matrices with Toeplitz blocks. Finally, Section 7 contains numerical results.

After sending our manuscript to SIAM J. Sci. Comput., R. H. Chan informed us that his group has got similar results as in our preprint. See [16] and for a refined version [17]. The construction of circulant preconditioners of R. H. Chan et al. is based on Jackson kernels and the proofs are different from ours. In [16], the authors prove convergence of the corresponding PCG–method in $\mathcal{O}(\log N)$ iteration steps. By a trick (see [16, Theorem 4.2]), which can also be applied to our w –circulant preconditioners, the R. H. Chan et al. need no knowledge about the location of the zeros of f .

2 Preconditioners from kernels

Let $C_{2\pi}$ denote the Banach space of 2π -periodic real-valued continuous functions with norm

$$\|f\|_\infty := \max_{x \in [-\pi, \pi]} |f(x)|.$$

We are interested in the solution of Hermitian Toeplitz systems

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

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

generated by a non-negative function $f \in C_{2\pi}$ which has only a finite number of zeros. By [10], the matrices $\mathbf{A}_N(f)$ are positive definite such that (2.1) can be solved by the CG-method. Unfortunately, since the generating function $f \in C_{2\pi}$ has zeros, the related Toeplitz matrices are asymptotically ill-conditioned and the CG-method converges very slow. To accelerate the convergence of the CG-method, we are looking for suitable preconditioners of \mathbf{A}_N , where we do not suppose the explicit knowledge of the generating function f . To reach our aim, we use reproducing kernels. This method was originally proposed for Toeplitz matrices arising from positive functions $f \in C_{2\pi}$ in [15].

In [14], R. Chan et al. showed by numerical tests that preconditioners from special kernels related to B -splines can improve the convergence of the CG-method also if $f \geq 0$ has zeros of various order. A theoretical proof of R. Chan's results was open up to now.

In this paper, we restrict our attention to even trigonometric polynomials

$$K_N(x) := c_{N,0} + 2 \sum_{k=1}^{N-1} c_{N,k} \cos kx, \quad c_{N,k} = a_k(K_N). \quad (2.2)$$

If

$$\frac{1}{2\pi} \int_0^{2\pi} K_N(x) dx = c_{N,0} = 1 \quad (2.3)$$

and $K_N \geq 0$, then K_N is called a *positive* (trigonometric) *kernel*. As main examples of such kernels we consider generalized Jackson polynomials and B -spline kernels in Section 4. For $f \in C_{2\pi}$, let f_N denote the *convolution of f with K_N* , i.e.

$$f_N(x) = (f * K_N)(x) := \frac{1}{2\pi} \int_0^{2\pi} f(t) K_N(x-t) dt \quad (2.4)$$

or equivalently in the Fourier domain

$$f_N(x) = \sum_{k=-(N-1)}^{N-1} a_k(f) c_{N,k} e^{ikx}. \quad (2.5)$$

We consider so-called *reproducing kernels* K_N ($N \in \mathbb{N}$) with the property that

$$\lim_{N \rightarrow \infty} \|f - f_N\|_\infty = 0 \quad (2.6)$$

for all $f \in C_{2\pi}$.

We chose grids G_N ($N \in \mathbb{N}$) consisting of equispaced nodes

$$x_{N,l} := w_N + \frac{2\pi l}{N} \quad (l = 0, \dots, N-1; w_N \in [0, \frac{2\pi}{N})) \quad (2.7)$$

such that $f(x_{N,l}) \neq 0$ for all $l = 0, \dots, N-1$. Note that the choice of the grids requires some preliminary information about the location of the zeros of f . By a trick (cf. [16]) this restriction can be neglected if we accept some more outliers. We consider matrices of the form

$$\mathbf{M}_N(f) := \mathbf{W}_N \mathbf{F}_N \mathbf{D}_N(f) \bar{\mathbf{F}}_N \bar{\mathbf{W}}_N \quad (2.8)$$

with

$$\mathbf{F}_N := \frac{1}{\sqrt{N}} \left(e^{-2\pi i j k / N} \right)_{j,k=0}^{N-1}, \quad \mathbf{W}_N := \text{diag} \left(e^{-ikw_N} \right)_{k=0}^{N-1}, \quad \mathbf{D}_N(f) = \text{diag} \left(f(x_{N,l}) \right)_{l=0}^{N-1}.$$

Obviously, the matrices \mathbf{M}_N can be written as

$$\mathbf{M}_N(f) = \begin{pmatrix} \tilde{a}_0 & \tilde{a}_{N-1} e^{iNw_N} & \dots & \tilde{a}_1 e^{iNw_N} \\ \tilde{a}_1 & \tilde{a}_0 & & \\ \vdots & & \ddots & \vdots \\ \tilde{a}_{N-1} & \dots & \dots & \tilde{a}_0 \end{pmatrix}$$

with

$$\tilde{a}_k = \tilde{a}_k(f) := \frac{1}{N} \sum_{l=0}^{N-1} f(x_{N,l}) e^{-ikw_N} e^{-2\pi i k l / N}. \quad (2.9)$$

These are (e^{iNw_N}) -*circulant matrices* (see [20]). In particular, we obtain circulant matrices for $w_N = 0$ and skew-circulant matrices for $w_N = \frac{\pi}{N}$.

As preconditioners for (2.1), we suggest matrices of the form

$$\mathbf{M}_N := \mathbf{M}_N(f_N) \quad (2.10)$$

with suitable positive reproducing kernels K_N . By (2.5), the construction of these preconditioners requires only the knowledge of the Toeplitz matrices \mathbf{A}_N . It is not necessary to know the generating function f explicitly. However, for the theoretical results in this paper, we must have some information about the location of the zeros of f . Note that by a trick in [16] this information is also superfluous. Here we point out that the auxiliary nontrivial problem of finding some crucial analytic properties of the generating function f has been treated and partially solved in [40].

Moreover, our preconditioners have the following desirable properties:

1. Since $f \geq 0$ with a finite number of zeros and K_N is a positive kernel, it follows by (2.4) that $f_N > 0$. Thus, the matrices $\mathbf{M}_N(f_N)$ are positive definite.

2. In the following section, we will prove that under certain conditions on the kernels K_N the eigenvalues of $\mathbf{M}_N^{-1}\mathbf{A}_N$ are bounded from below by a positive constant independent of N and that the number of isolated eigenvalues of $\mathbf{M}_N^{-1}\mathbf{A}_N$ is independent of N . Then, by Theorem 1.1, the number of PCG–steps to achieve a fixed precision is independent of N .
3. By construction (2.8), the multiplication of \mathbf{M}_N with a vector requires only $\mathcal{O}(N \log N)$ arithmetical operations by using FFT–techniques. By a technique presented in [26] it is possible to implement a PCG–method with preconditioner \mathbf{M}_N which takes only $\mathcal{O}(N)$ instead of $\mathcal{O}(N \log N)$ arithmetical operations per iteration step more than the original CG–method with respect to \mathbf{A}_N .

3 Eigenvalues of $\mathbf{M}_N^{-1}\mathbf{A}_N$

In this section, we prove that under certain assumptions on the kernels K_N the eigenvalues of $\mathbf{M}_N^{-1}\mathbf{A}_N$ are bounded from below by a positive constant independent of N and that the number of isolated eigenvalues of $\mathbf{M}_N^{-1}\mathbf{A}_N$ is independent of N . For the proof of our main result, we need some preliminary lemmata.

Lemma 3.1 Let $p \in C_{2\pi}$ be a non–negative function which has only a finite number of zeros. Let $h \in C_{2\pi}$ be a positive function with

$$h_{\min} := \min_{x \in [0, 2\pi]} h(x), \quad h_{\max} := \max_{x \in [0, 2\pi]} h(x).$$

Then, for $f := ph$ and any $N \in \mathbb{N}$, the eigenvalues of $\mathbf{A}_N^{-1}(p)\mathbf{A}_N(f)$ lie in the interval $[h_{\min}, h_{\max}]$.

The proof can be found for example in [5, 10, 31]. A more sophisticated version for $f, g \in L^1$ was proved in [38, 37].

Lemma 3.2 Let p be a real–valued non–negative trigonometric polynomial of degree $\leq s$. Let $N \geq 2s$. Then at most $2s$ eigenvalues of $\mathbf{M}_N(p)^{-1}\mathbf{A}_N(p)$ differ from 1.

Proof: For arbitrary $f \in C_{2\pi}$ with pointwise convergent Fourier series, we obtain by replacing $f(x_{N,l})$ in (2.9) by the Fourier series of f at $x_{N,l}$

$$\begin{aligned} \tilde{a}_k &= \frac{1}{N} \sum_{l=0}^{N-1} \sum_{j \in \mathbb{Z}} a_j e^{ijx_{N,l}} e^{-2\pi ilk/N} e^{-ikw_N} \\ &= \sum_{j=0}^{N-1} a_j e^{-iw_N k} e^{iw_N j} \left(\frac{1}{N} \sum_{l=0}^{N-1} e^{-2\pi ilk/N} e^{2\pi ilj/N} \right) \\ &\quad + \sum_{j=0}^{N-1} \sum_{r \in \mathbb{Z} \setminus \{0\}} a_{j+rN} e^{-iw_N k} e^{iw_N(j+rN)} \left(\frac{1}{N} \sum_{l=0}^{N-1} e^{-2\pi ilk/N} e^{2\pi ilj/N} \right) \\ &= a_k + \sum_{r \in \mathbb{Z} \setminus \{0\}} a_{k+rN} e^{iw_N r N}. \end{aligned}$$

This is well-known as *aliasing effect*. Then it follows that

$$\mathbf{A}_N(f) = \mathbf{M}_N(f) - \mathbf{B}_N(f), \quad (3.1)$$

where

$$\mathbf{B}_N(f) := (b_{j-k}(f))_{j,k=0}^{N-1}, \quad b_k(f) := \sum_{r \in \mathbb{Z} \setminus \{0\}} a_{k+rN}(f) e^{iw_N r N}.$$

We consider $f = p$. Since p is of degree smaller than $s \leq \frac{N}{2}$, we have that $b_k(p) = 0$ for $|k| \leq N - 1 - s$. Consequently, $\mathbf{B}_N(p)$ is of rank $\leq 2s$. Now the assertion follows by (3.1). ■

In the sequel, we restrict our attention to Toeplitz matrices having a non-negative generating function $f \in C_{2\pi}$ with a zero of even order $2s$ ($s \in \mathbb{N}$) at $x = 0$.

We use the trigonometric polynomial

$$p_s(x) := (2 - 2 \cos x)^s = (2 \sin \frac{x}{2})^{2s} = \sum_{k=0}^s \alpha_k \cos kx \quad (s \geq 1) \quad (3.2)$$

of degree s which has also a zero of order $2s$ at $x = 0$.

The convergence of our PCG-method is related to the behavior of the grid functions

$$q_{s,N}(x) := \frac{p_{s,N}(x)}{p_s(x)} \quad (x \in G_N), \quad (3.3)$$

where $p_{s,N}(x) := (p_s * K_N)(x)$. More precisely, for the proof of our main theorem, we need that $\{q_{s,N}(x)\}_{N \in \mathbb{N}}$ is bounded for all $x \in G_N$ from above and below by positive constants independent of N . This will be the content of the following lemmata.

First, we see that the above property follows immediately for all grid points $x \in G_N$ having some distance independent of N from the zero of f :

Lemma 3.3 Let G_N be defined by (2.7) with $w_N \neq 0$. Let $\{K_N\}_{N \in \mathbb{N}}$ be a sequence of positive even reproducing kernels and let $q_{s,N}$ be given by (3.3). Then, for $x_N \in G_N \cap [a, b]$ ($[a, b] \subset (0, 2\pi)$) and for every $\varepsilon > 0$ there exists $N(\varepsilon)$ such that

$$1 - \varepsilon \leq q_{s,N}(x_N) \leq 1 + \varepsilon$$

for all $N \geq N(\varepsilon)$.

Proof: Since $x_N \in [a, b]$ ($N \in \mathbb{N}$) for some $a > 0, b < 2\pi$, we have that

$$p_s(x_N) \geq \min\{p_s(a), p_s(b)\} > 0.$$

Further, we obtain by (2.6) that for every $\varepsilon > 0$ there exists $N(\varepsilon)$ such that

$$|p_s(x) - p_{s,N}(x)| \leq \varepsilon \min\{p_s(a), p_s(b)\} \quad (x \in [0, 2\pi))$$

for all $N \geq N(\varepsilon)$. By rewriting (3.3) in the form

$$q_{s,N}(x_N) = 1 + \frac{p_{s,N}(x_N) - p_s(x_N)}{p_s(x_N)}$$

we obtain the assertion. ■

By Lemma 3.3, it remains to consider the sequences $\{q_{s,N}(x_N)\}_{N \in \mathbb{N}}$ for $x_N \in G_N$ with $x_N \rightarrow 0$ for $N \rightarrow \infty$ or with $x_N \rightarrow 2\pi$ for $N \rightarrow \infty$. Since both cases require the same ideas, we consider $x_N \in G_N$ with

$$\lim_{N \rightarrow \infty} x_N = 0.$$

The existence of a lower bound of $\{q_{s,N}(x_N)\}_{N \in \mathbb{N}}$ does also not require additional properties of the kernel K_N :

Lemma 3.4 Let G_N be defined by (2.7) with $w_N \neq 0$. Let $\{K_N\}_{N \in \mathbb{N}}$ be a sequence of positive even reproducing kernels and let $q_{s,N}$ be given by (3.3). Then, for $x_N \in G_N$ with $\lim_{N \rightarrow \infty} x_N = 0$, there exists a constant $\alpha > 0$ independent of N such that

$$\alpha \leq q_{s,N}(x_N).$$

Proof: By definition of $q_{s,N}$ and $p_{s,N}$, we have that

$$q_{s,N}(x_N) = \frac{1}{2\pi} \int_0^{2\pi} \frac{p_s(t)}{p_s(x_N)} K_N(x_N - t) dt$$

and since $p_s \geq 0$ and $K_N \geq 0$, we obtain for $x_N < \pi$ that

$$q_{s,N}(x_N) \geq \frac{1}{2\pi} \int_{x_N}^{\pi} \frac{p_s(t)}{p_s(x_N)} K_N(x_N - t) dt.$$

The polynomial p_s is monotonely increasing on $[0, \pi]$. Thus

$$q_{s,N}(x_N) \geq \frac{1}{2\pi} \int_{x_N}^{\pi} K_N(x_N - t) dt.$$

Since K_N is even and fulfills (2.3), we get for any sequence $x_N \in G_N$ ($x_N < \pi$) with $\lim_{N \rightarrow \infty} x_N = 0$ that

$$q_{s,N}(x_N) \geq \frac{1}{2\pi} \int_0^{\pi-x_N} K_N(t) dt \geq \text{const.} \quad \blacksquare$$

It remains to examine if

$$q_{s,N}(x_N) = \frac{p_{s,N}(x_N)}{p_s(x_N)} \leq \beta$$

for any $x_N \in G_N$ with $\lim_{N \rightarrow \infty} x_N = 0$. Here the ‘‘moment property’’ comes into the play.

Lemma 3.5 Let G_N ($n \in \mathbb{N}$) be defined by (2.7) with

$$0 < w \leq w_N N \leq \tilde{w} < 2\pi. \quad (3.4)$$

Let $\{K_N\}_{N \in \mathbb{N}}$ be a sequence of positive even kernels and let $q_{s,N}$ ($s \geq 1$) be given by (3.3). Then there exists a constant $\beta < \infty$ independent of N such that

$$q_{s,N}(x_N) \leq \beta$$

for all $x_N \in G_N$ with $\lim_{N \rightarrow \infty} x_N = 0$ if and only if K_N fulfills the ‘‘moment property’’

$$\int_{-\pi}^{\pi} t^{2k} K_N(t) dt = \mathcal{O}(N^{-2k}) \quad (k = 0, \dots, s). \quad (3.5)$$

Note that the restriction (3.4) on the grids G_N means that we have for any $x_N \in G_N$ that $w/N \leq x_N$.

Proof: Since $\sin^2 x \leq x^2$ for all $x \in \mathbb{R}$, we obtain by (3.2) that

$$p_s(x) \leq x^{2s} \quad (x \in \mathbb{R}). \quad (3.6)$$

Similarly, we have for any fixed $0 \leq y \leq \pi/2$ that

$$\sin^2 x \geq \left(\frac{2}{\pi} \frac{\frac{\pi}{2} - y}{\frac{\pi}{2} + y} \right)^2 x^2 \quad (x \in [-\frac{\pi}{2} - y, \frac{\pi}{2} + y])$$

and hence

$$p_s(x) \geq \left(\frac{2}{\pi} \right)^{2s} \left(\frac{\frac{\pi}{2} - y}{\frac{\pi}{2} + y} \right)^{2s} x^{2s} \quad (x \in [-\pi - 2y, \pi + 2y]). \quad (3.7)$$

Using (3.6), we conclude by $K_N \geq 0$ that

$$\begin{aligned} p_{s,N}(x) &= \frac{1}{2\pi} \int_{-\pi}^{\pi} p_s(x-t) K_N(t) dt \\ &\leq \frac{1}{2\pi} \int_{-\pi}^{\pi} (x-t)^{2s} K_N(t) dt \\ &= \frac{1}{2\pi} \sum_{k=0}^{2s} \binom{2s}{k} (-1)^k x^{2s-k} \int_{-\pi}^{\pi} t^k K_N(t) dt \quad (x \in [-\pi, \pi]) \end{aligned}$$

and since K_N is even

$$p_{s,N}(x) \leq \frac{1}{2\pi} \sum_{k=0}^s \binom{2s}{2k} x^{2s-2k} \int_{-\pi}^{\pi} t^{2k} K_N(t) dt.$$

Let K_N satisfy (3.5). Then

$$p_{s,N}(x) \leq \frac{c}{2\pi} \sum_{k=0}^s \binom{2s}{2k} x^{2s-2k} N^{-2k}.$$

By (3.4), we have for any grid sequence $x_N \in G_N$ that $x_N \geq w/N$. Consequently,

$$p_{s,N}(x_N) \leq C x_N^{2s}.$$

By (3.7) this implies that there exists $\beta < \infty$ independent of N so that $q_{s,N}(x_N) \leq \beta$. On the other hand, we see by (3.7) with $y := \pi/4$ that

$$\begin{aligned} p_{s,N}(x) &= \frac{1}{2\pi} \int_{-\pi}^{\pi} p_s(x-t) K_N(t) dt \\ &\geq \frac{1}{2\pi} \left(\frac{2}{3\pi}\right)^{2s} \sum_{k=0}^s \binom{2s}{2k} x^{2s-2k} \int_{-\pi}^{\pi} t^{2k} K_N(t) dt \quad (x \in [-\frac{\pi}{2}, \frac{\pi}{2}]). \end{aligned}$$

By definition of G_N , there exists a grid sequence $\{x_N\}_{N \in \mathbb{N}}$ so that x_N approaches zero as N^{-1} ($N \rightarrow \infty$). Assume that K_N does not fulfill (3.5). Then we obtain for the above sequence that $p_{s,N}(x_N) \geq c N^{-2s+\varepsilon}$ ($\varepsilon > 0$), while we have by (3.6) that $p_s(x_N) = \mathcal{O}(N^{-2s})$. Thus $q_{s,N}(x_N)$ cannot be bounded from above. This completes the proof. \blacksquare

By Lemma 3.3 – Lemma 3.5, we obtain that for grids G_N defined by (2.7) and (3.4) and for even positive reproducing kernels with (3.5) there exist

$$\begin{aligned} 0 < \alpha &:= \inf\{q_{s,N}(x) : x \in G_N; N \in \mathbb{N}\} \\ \infty > \beta &:= \sup\{q_{s,N}(x) : x \in G_N; N \in \mathbb{N}\} \end{aligned} \quad (3.8)$$

Now we can prove our main theorem.

Theorem 3.6 Let $\{\mathbf{A}_N(f)\}_{N \in \mathbb{N}}$ be a sequence of Toeplitz matrices generated by a non-negative function $f \in C_{2\pi}$ which has only a zero of order $2s$ ($s \in \mathbb{N}$) at $x = 0$. Let the grids G_N be defined by (2.7) and (3.4). Assume that $\{K_N\}_{N \in \mathbb{N}}$ is a sequence of even positive reproducing kernels satisfying (3.5). Finally, let $\mathbf{M}_N(f_N)$ be defined by (2.10). Then we have:
i) The eigenvalues of $\mathbf{M}_N^{-1}(f_N) \mathbf{A}_N(f)$ are bounded from below by a positive constant independent of N .
ii) For $N \geq 2s$, at most $2s$ eigenvalues of $\mathbf{M}_N(f_N)^{-1} \mathbf{A}_N(f)$ are not contained in the interval $[\frac{h_{\min}}{\beta h_{\max}}, \frac{h_{\max}}{\alpha h_{\min}}]$. Here α, β are given by (3.8) and h_{\min}, h_{\max} are defined as in Lemma 3.1, where $h := f/p_s$.

Proof: 1. To show ii), we consider the Rayleigh quotient

$$\frac{\bar{\mathbf{u}}' \mathbf{A}_N(f) \mathbf{u}}{\bar{\mathbf{u}}' \mathbf{M}_N(f_N) \mathbf{u}} = \frac{\bar{\mathbf{u}}' \mathbf{A}_N(f) \mathbf{u}}{\bar{\mathbf{u}}' \mathbf{A}_N(p_s) \mathbf{u}} \frac{\bar{\mathbf{u}}' \mathbf{A}_N(p_s) \mathbf{u}}{\bar{\mathbf{u}}' \mathbf{M}_N(f_N) \mathbf{u}} \quad (\mathbf{u} \neq \mathbf{o}_N). \quad (3.9)$$

By Lemma 3.1, we have that

$$\frac{\bar{\mathbf{u}}' \mathbf{A}_N(f) \mathbf{u}}{\bar{\mathbf{u}}' \mathbf{A}_N(p_s) \mathbf{u}} \in [h_{\min}, h_{\max}]$$

and thus, since the second factor on the right-hand side of (3.9) is positive

$$h_{\min} \frac{\bar{\mathbf{u}}' \mathbf{A}_N(p_s) \mathbf{u}}{\bar{\mathbf{u}}' \mathbf{M}_N(f_N) \mathbf{u}} \leq \frac{\bar{\mathbf{u}}' \mathbf{A}_N(f) \mathbf{u}}{\bar{\mathbf{u}}' \mathbf{M}_N(f_N) \mathbf{u}} \leq h_{\max} \frac{\bar{\mathbf{u}}' \mathbf{A}_N(p_s) \mathbf{u}}{\bar{\mathbf{u}}' \mathbf{M}_N(f_N) \mathbf{u}}. \quad (3.10)$$

By Lemma 3.2, we know that

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

with a matrix $\mathbf{R}_N(2s)$ of rank $2s$ and consequently

$$\frac{\bar{\mathbf{u}}' \mathbf{A}_N(f) \mathbf{u}}{\bar{\mathbf{u}}' \mathbf{M}_N(f_N) \mathbf{u}} \leq h_{\max} \frac{\bar{\mathbf{u}}' \mathbf{M}_N(p_s) \mathbf{u}}{\bar{\mathbf{u}}' \mathbf{M}_N(f_N) \mathbf{u}} + \frac{\bar{\mathbf{u}}' h_{\max} \mathbf{R}_N(2s) \mathbf{u}}{\bar{\mathbf{u}}' \mathbf{M}_N(f_N) \mathbf{u}},$$

and

$$\frac{\bar{\mathbf{u}}' (\mathbf{A}_N(f) - h_{\max} \mathbf{R}_N(2s)) \mathbf{u}}{\bar{\mathbf{u}}' \mathbf{M}_N(f_N) \mathbf{u}} \leq h_{\max} \frac{\bar{\mathbf{u}}' \mathbf{M}_N(p_s) \mathbf{u}}{\bar{\mathbf{u}}' \mathbf{M}_N(f_N) \mathbf{u}}.$$

Since K_N and p_s are non-negative, we obtain by (2.4) and by definition of h that

$$h_{\min} p_{s,N}(x) \leq f_N(x) \leq h_{\max} p_{s,N}(x) \quad x \in [0, 2\pi].$$

This implies by definition of $\mathbf{M}_N(f_N)$ that

$$\frac{\bar{\mathbf{u}}' (\mathbf{A}_N(f) - h_{\max} \mathbf{R}_N(2s)) \mathbf{u}}{\bar{\mathbf{u}}' \mathbf{M}_N(f_N) \mathbf{u}} \leq \frac{h_{\max}}{h_{\min}} \frac{\bar{\mathbf{u}}' \mathbf{M}_N(p_s) \mathbf{u}}{\bar{\mathbf{u}}' \mathbf{M}_N(p_{s,N}) \mathbf{u}}$$

and further by (3.3), (3.8) and since $0 < \alpha \leq \beta < \infty$ that

$$\frac{\bar{\mathbf{u}}' (\mathbf{A}_N(f) - h_{\max} \mathbf{R}_N(2s)) \mathbf{u}}{\bar{\mathbf{u}}' \mathbf{M}_N(f_N) \mathbf{u}} \leq \frac{h_{\max}}{\alpha h_{\min}}$$

for all $\mathbf{u} \neq \mathbf{o}_N$. Assume that $\mathbf{R}_N(2s)$ has s_1 positive eigenvalues. Then, by properties of the Rayleigh quotient and by Weyl's theorem [24, p. 184] at most s_1 eigenvalues of $\mathbf{M}_N(f_N)^{-1} \mathbf{A}_N(f)$ are larger than $\frac{h_{\max}}{\alpha h_{\min}}$. Similarly, we obtain by consideration of the left-hand inequality of (3.10) that at most $2s - s_1$ eigenvalues of $\mathbf{M}_N(f_N)^{-1} \mathbf{A}_N(f)$ are smaller than $\frac{h_{\min}}{\beta h_{\max}}$.

2. To show i), we rewrite (3.9) as

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

As in the first part of the proof, we see that this implies

$$\frac{\bar{\mathbf{u}}' \mathbf{A}_N(f) \mathbf{u}}{\bar{\mathbf{u}}' \mathbf{M}_N(f_N) \mathbf{u}} \geq \frac{h_{\min}}{\beta h_{\max}} \frac{\bar{\mathbf{u}}' \mathbf{A}_N(p_s) \mathbf{u}}{\bar{\mathbf{u}}' \mathbf{M}_N(p_s) \mathbf{u}}.$$

Consequently, it remains to show that there exists a constant $0 < c < \infty$ such that

$$\frac{\bar{\mathbf{u}}' \mathbf{A}_N(p_s) \mathbf{u}}{\bar{\mathbf{u}}' \mathbf{M}_N(p_s) \mathbf{u}} \geq \frac{1}{c}.$$

By (3.1), this is equivalent to

$$1 + \frac{\bar{\mathbf{u}}' \mathbf{B}_N(p_s) \mathbf{u}}{\bar{\mathbf{u}}' \mathbf{A}_N(p_s) \mathbf{u}} \leq c.$$

By the special structure of $\mathbf{B}_N(p_s)$ and $\mathbf{A}_N(p_s)$, assertion i) follows as in the proof of Theorem 4.3 in [3]. This completes the proof. \blacksquare

By the following theorem, the “moment property” (3.5) of the kernel is also *necessary* to obtain good preconditioners.

Theorem 3.7 Let $\{\mathbf{A}_N(f)\}_{N \in \mathbb{N}}$ be a sequence of Toeplitz matrices generated by a non-negative function $f \in C_{2\pi}$ which has only a zero of order $2s$ ($s \in \mathbb{N}$) at $x = 0$. Let the grids G_N be defined by (2.7) and (3.4). Assume that $\{K_N\}_{N \in \mathbb{N}}$ is a sequence of even positive reproducing kernels which do not fulfill (3.5). Finally, let $\mathbf{M}_N(f_N)$ be defined by (2.10). Then, for arbitrary $\varepsilon > 0$ and arbitrary $c \in \mathbb{N}$, there exist $N(\varepsilon, c)$ such that for all $N \geq N(\varepsilon, c)$ at least c eigenvalues of $\mathbf{M}_N(f_N)^{-1} \mathbf{A}_N(f)$ are contained in $(0, \varepsilon)$.

The proof follows again the lines of the fundamental paper of F. Di Benedetto [3, Theorem 5.4]. We include the short proof with respect to our background.

Proof: By the proof of Theorem 3.6, we have for all $\mathbf{u} \neq \mathbf{o}$ that

$$\frac{\bar{\mathbf{u}}' \mathbf{A}_N(f) \mathbf{u}}{\bar{\mathbf{u}}' \mathbf{M}_N(f_N) \mathbf{u}} \leq \frac{h_{\max}}{h_{\min}} \frac{\bar{\mathbf{u}}' \mathbf{A}_N(p_s) \mathbf{u}}{\bar{\mathbf{u}}' \mathbf{M}_N(p_{s,N}) \mathbf{u}}.$$

Hence it remains to show that $\mathbf{M}_N(p_{s,N})^{-1} \mathbf{A}_N(p_s)$ has an arbitrary number of eigenvalues in $(0, \varepsilon)$ for N sufficiently large. By (3.2) and [32, Theorem 3.1], we have that

$$\begin{aligned} \mathbf{T}_{N+2s-2} &:= \mathbf{S}_{N+2s-2}^I \operatorname{diag} \left(\left(2 \sin \frac{j\pi}{2(N+2s-1)} \right)_{j=1}^{2s} \right)^{N+2s-2} \mathbf{S}_{N+2s-2}^I \\ &= \mathbf{S}_{N+2s-2}^I \operatorname{diag} \left(\sum_{k=0}^s \alpha_k \cos \frac{jk\pi}{N+2s-1} \right)_{j=1}^{N+2s-2} \mathbf{S}_{N+2s-2}^I \\ &= \frac{1}{2} \operatorname{stoep}(2\alpha_0, \dots, \alpha_s, 0, \dots, 0) - \frac{1}{2} \operatorname{shank}(\alpha_2, \dots, \alpha_s, 0, \dots, 0), \end{aligned}$$

where $\mathbf{S}_{N-1}^I := (2/N)^{1/2} (\sin \frac{(j+1)(k+1)\pi}{N})_{j,k=0}^{N-2}$ is an orthogonal matrix and where $\operatorname{stoep} \mathbf{a}'$ and $\operatorname{shank} \mathbf{a}'$ denote the symmetric Toeplitz matrix and the persymmetric Hankel matrix with first row \mathbf{a}' , respectively. Deleting the first $s-1$ and the last $s-1$ rows and columns of \mathbf{T}_{N+2s-2} we obtain $\mathbf{A}_N(p_s)$. Thus, we have by Courants minimax theorem for the eigenvalues $\lambda_1(\mathbf{A}_N(p_s)) \leq \dots \leq \lambda_N(\mathbf{A}_N(p_s))$ of $\mathbf{A}_N(p_s)$ that

$$\lambda_j(\mathbf{A}_N(p_s)) \leq \lambda_{j+2s-2}(\mathbf{T}_{N+2s-2}) = \left(2 \sin \frac{j+2s-2}{2(N+2s-1)} \right)^{2s} \leq \left(\frac{j+2s-2}{N+2s-1} \right)^{2s}.$$

The later result is due to a technique of D. Bini et al. [7, Proposition 4.2]. Consider $\mathbf{A}_N(p_s) - t\mathbf{M}_N(p_{s,N})$. For $t = 0$, this matrix has positive eigenvalues, while we have for arbitrary $\varepsilon > 0$ that

$$\begin{aligned} \lambda_j(\mathbf{A}_N(p_s) - \varepsilon \mathbf{M}_N(p_{s,N})) &\leq \lambda_j(\mathbf{A}_N(p_s)) - \varepsilon \lambda_{\min}(\mathbf{M}_N(p_{s,N})) \\ &\leq \left(\frac{j+2s-2}{N+2s-1} \right)^{2s} - \varepsilon p_{s,N}(w_N) \\ &= N^{-2s} \left(\left(\frac{j+2s-2}{1 + \frac{2s-1}{N}} \right)^{2s} - \varepsilon \frac{p_{s,N}(w_N)}{N^{2s}} \right). \end{aligned}$$

Since K_N does not fulfill (3.5), we have by Lemma 3.5 that

$$\lim_{N \rightarrow \infty} \frac{p_{s,N}(w_N)}{N^{2s}} = \infty.$$

Thus, for $j \leq c$ independent of N and for sufficiently large $N \geq N(\varepsilon, c)$ the values $\lambda_j(\mathbf{A}_N(p_s) - \varepsilon \mathbf{M}_N(p_{s,N}))$ become negative. The eigenvalues of $\mathbf{A}_N(p_s) - t \mathbf{M}_N(p_{s,N})$ are continuous functions of t . Since the smallest c eigenvalues pass from a positive value for $t = 0$ to a negative value for $t = \varepsilon$, there exist $\varepsilon_1, \dots, \varepsilon_c \in (0, \varepsilon)$ such that $\mathbf{A}_N(p_s) - \varepsilon_j \mathbf{M}_N(p_{s,N})$ has eigenvalue zero. This is equivalent to the fact that $\mathbf{M}_N(p_{s,N})^{-1} \mathbf{A}_N(p_s)$ has an eigenvalue $\varepsilon_j \in (0, \varepsilon)$ and we are done. \blacksquare

The generalization of the above results for generating functions with different zeros of even order

$$f(x) = (x - y_1)^{2s_1} \dots (x - y_m)^{2s_m} \tilde{f}(x) \quad (\tilde{f} > 0)$$

is straightforward (see [18]). By applying the polynomial

$$p(x) := \prod_{i=1}^m p_{s_i}(x - y_i)$$

instead of p_s and following the above lines, we can show that for grids G_N of the form (2.7) with $x_{N,l} \neq y_i$ ($l = 0, \dots, N-1$; $i = 1, \dots, m$) and for kernels K_N fulfilling (3.5) with $s := \max\{s_j : j = 1, \dots, m\}$, there exist constants $0 < \alpha \leq \beta < \infty$ such that for all $x \in G_N$

$$\alpha \leq \frac{(p * K_N)(x)}{p(x)} \leq \beta.$$

4 Jackson polynomials and B -spline kernels

In this section, we consider concrete positive reproducing kernels K_N with property (3.5). The *generalized Jackson polynomials* of degree $\leq N-1$ are defined by

$$J_{m,N}(x) = \lambda_{m,N} \left(\frac{\sin(nx/2)}{\sin x/2} \right)^{2m} \quad (m \in \mathbb{N}),$$

where $n := \lfloor \frac{N-1}{m} \rfloor + 1$ and where $\lambda_{m,N}$ is determined by (2.3) [22, p. 203]. It is well-known [22, p. 204], that the generalized Jackson polynomials $J_{m,N}$ are even positive reproducing kernels which satisfy property (3.5) for

$$m \geq s + 1.$$

In particular, $J_{1,N}$ is the *Fejér kernel* which is related to the optimal circulant preconditioner [19, 15]. However, the Fejér kernel does not fulfill (3.5) for $s \geq 1$ such that we cannot expect a fast convergence of our PCG-method if f has a zero of order ≥ 2 . Our numerical tests confirm this result.

By Theorem 3.6, the generalized Jackson polynomials $K_N = J_{m,N}$ with $m \geq s+1$ can be used for the construction of preconditioners. Note that preconditioners related to Jackson kernels were also suggested in [39]. However, the construction of the Fourier coefficients of $J_{m,N}$ seems to be rather complicated. See also [10]. Therefore we prefer the following B -spline kernels.

The “ B -spline kernels” were introduced by R. Chan et al. in [14]. The authors showed by numerical tests that preconditioners from B -spline kernels of certain order seem to be good candidates for the PCG-method. Applying the results of the previous section, we are able to show the theoretical reasons for these results, at least for the positive B -spline kernels.

Let $\chi_{[0,1]}$ denote the characteristic function of $[0, 1)$. The *cardinal B -splines* N_m ($m \geq 1$) of order m are defined by

$$N_1 := \chi_{[0,1)}, N_{m+1} := \int_0^1 N_1(t) N_m(\cdot - t) dt$$

and their centered version by

$$M_m := N_m\left(\cdot + \frac{m}{2}\right).$$

Note that M_m is an even function with $\text{supp } M_m = [-\frac{m}{2}, \frac{m}{2}]$ and that

$$\int_{-\infty}^{\infty} M_m(t) e^{-ixt} dt = \left(\text{sinc } \frac{x}{2}\right)^m, \quad (4.1)$$

where

$$\text{sinc } x := \begin{cases} \frac{\sin x}{x} & x \neq 0, \\ 1 & x = 0. \end{cases}$$

Let the B -spline kernels $B_{m,N}$ be defined by [14]

$$B_{m,N}(x) := 1 + \frac{2}{M_{2m}(0)} \sum_{k=1}^{N-1} M_{2m}\left(\frac{mk}{N}\right) \cos kx.$$

Note that $B_{1,N}$ again coincides with the Fejér kernel.

For the construction of the preconditioner, it is important, that the Fourier coefficient $c_{N,k} = M_{2m}(\frac{mk}{N})/M_{2m}(0)$ can be computed in a simple way for example by applying a simplified version of de Boor’s algorithm [9, p. 54].

By (4.1), it is easy to check that $B_{m,N}$ is a dilated, 2π -periodized version of $(\text{sinc } \frac{x}{2})^{2m}$, i.e.

$$B_{m,N}(x) = \frac{N}{m} \frac{1}{M_{2m}(0)} \sum_{r \in \mathbb{Z}} \left(\text{sinc } \left(\frac{N}{m} \left(\frac{x + 2\pi r}{2} \right) \right) \right)^{2m}. \quad (4.2)$$

Thus

$$B_{m,N} \geq 0 \quad (m \in \mathbb{N}).$$

Moreover, we obtain similar to the generalized Jackson polynomials:

Lemma 4.1 The B -spline kernels $B_{m,N}$ satisfy (3.5) if and only if $m \geq s + 1$.

Proof: By (4.2), we obtain that

$$\begin{aligned}
\int_{-\pi}^{\pi} t^{2k} B_{m,N}(t) dt &= \frac{N}{m} \frac{1}{M_{2m}(0)} \int_{-\pi}^{\pi} t^{2k} \sum_{r \in \mathbb{Z}} \left(\operatorname{sinc} \left(\frac{N}{m} \left(\frac{t + 2\pi r}{2} \right) \right) \right)^{2m} dt \\
&\leq \frac{N}{m} \frac{1}{M_{2m}(0)} \int_{-\infty}^{\infty} t^{2k} \left(\frac{\sin \left(\frac{N t}{m} \right)}{\frac{N t}{m}} \right)^{2m} dt \\
&= \frac{2}{M_{2m}(0)} \int_{-\infty}^{\infty} \left(\frac{2mu}{N} \right)^{2k} \left(\frac{\sin u}{u} \right)^{2m} du \\
&\leq c N^{-2k} \int_{-\infty}^{\infty} u^{2k-2m} du \leq C N^{-2k}
\end{aligned}$$

for $m \geq k + 1$. Thus, for $m \geq s + 1$ the kernels $B_{m,N}$ satisfy property (3.5). On the other hand, we have that

$$\begin{aligned}
\int_{-\pi}^{\pi} t^{2k} B_{m,N}(t) dt &\geq \frac{N}{m} \frac{1}{M_{2m}(0)} \int_{-\pi}^{\pi} t^{2k} \left(\frac{\sin \frac{N}{m} \left(\frac{t}{2} \right)}{\frac{N}{m} \left(\frac{t}{2} \right)} \right)^{2m} dt \\
&= \frac{2}{M_{2m}(0)} \int_{-N\pi/(2m)}^{N\pi/(2m)} \left(\frac{2mu}{N} \right)^{2k} \left(\frac{\sin u}{u} \right)^{2m} du \\
&= \frac{2 (2m)^{2k}}{M_{2m}(0)} N^{-2k} \int_{-N\pi/(2m)}^{N\pi/(2m)} \frac{(\sin u)^{2m}}{u^{2m-2k}} du.
\end{aligned}$$

If $m \leq k$, then the last integral is not bounded for $N \rightarrow \infty$. Thus, for $m \leq s$, the kernel $B_{m,N}$ does not fulfill property (3.5). ■

By Theorem 3.6, the B -spline kernels $K_N = B_{m,N}$ with $m \geq s + 1$ produce good preconditioners.

5 Generalizations of the preconditioning technique

In this section, we sketch how our preconditioners can be generalized to (real) symmetric Toeplitz matrices and to doubly symmetric block Toeplitz matrices with Toeplitz blocks. We will do this in a very short way since both cases do not require new ideas. However, we have to introduce some notation to understand the numerical tests in Section 7.

Symmetric Toeplitz matrices

First, we suppose in addition to Section 2 that the Toeplitz matrices $\mathbf{A}_N \in \mathbb{R}^{N,N}$ are symmetric, i.e. the generating function $f \in C_{2\pi}$ is even. Note that in this case, the multiplication of a vector with \mathbf{A}_N can be realized using *fast trigonometric transforms* instead of fast Fourier

transforms (see [32]). 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 (2.8), where the Fourier matrix \mathbf{F}_N is replaced by trigonometric matrices corresponding to fast trigonometric transforms. In practice, four discrete sine transforms (DST I – IV) and four discrete cosine transforms (DCT I – IV) were applied (see [46]). Any of these eight trigonometric transforms can be realized with $\mathcal{O}(N \log N)$ arithmetical operations (see for example [2, 44]). Likewise, we can define preconditioners with respect to any of these transforms. In this paper, we restrict our attention to the DST–II and DCT–II, which are determined by the following transform matrices:

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

where $\varepsilon_k^N := 2^{-1/2}$ ($k = 0, N$) and $\varepsilon_k^N := 1$ ($k = 1, \dots, N-1$). Similar to (2.10), (2.8), we introduce the preconditioners (see [31])

$$\begin{aligned} \text{DCT-II} : \quad \mathbf{M}_N(f_N, \mathbf{C}_N^{II}) & := (\mathbf{C}_N^{II})' \text{diag} \left(f_N \left(\frac{l\pi}{N} \right) \right)_{l=0}^{N-1} \mathbf{C}_N^{II}, \\ \text{DST-II} : \quad \mathbf{M}_N(f_N, \mathbf{S}_N^{II}) & := (\mathbf{S}_N^{II})' \text{diag} \left(f_N \left(\frac{l\pi}{N} \right) \right)_{l=1}^N \mathbf{S}_N^{II}. \end{aligned} \tag{5.1}$$

We recall, that for the construction these preconditioners no explicit knowledge of the generating function is required. Since f is even, the grids G_N are simply chosen as $G_N := \{x_{N,l} := \frac{l\pi}{N} : l = 0, \dots, N-1\}$ and $G_N := \{x_{N,l} := \frac{(l+1)\pi}{N} : l = 0, \dots, N-1\}$ for the DCT–II and the DST–II preconditioners, respectively. If $f(x_{N,l}) \neq 0$ ($l = 0, \dots, N$), then we can prove Theorem 3.6 with respect to the preconditioners (5.1) in a completely similar way. We have only to replace the decomposition (3.1) by

$$\begin{aligned} \mathbf{A}_N(f) & = \mathbf{M}_N(f, \mathbf{C}_N^{II}) - \text{shank}(a_1, \dots, a_{N-1}, 0) \\ \mathbf{A}_N(f) & = \mathbf{M}_N(f, \mathbf{S}_N^{II}) + \text{shank}(a_1, \dots, a_{N-1}, 0) \end{aligned}$$

for the DCT–II and for the DST–II, respectively. See also [31].

Remark: Let

$$\mathcal{A}_{O_N} := \{\bar{\mathbf{O}}_N'(\text{diag } \mathbf{d})\mathbf{O}_N : \mathbf{d} \in \mathbb{R}^N\}$$

denote the matrix algebra with respect to the unitary matrix \mathbf{O}_N . Then the *optimal preconditioner* $\mathbf{M}_N \in \mathcal{A}_{O_N}$ of \mathbf{A}_N in \mathcal{A}_{O_N} is defined by

$$\|\mathbf{M}_N - \mathbf{A}_N\|_F = \min\{\|\mathbf{P} - \mathbf{A}_N\|_F : \mathbf{P} \in \mathcal{A}_{O_N}\},$$

where $\|\cdot\|_F$ denotes the Frobenius norm. As mentioned in the previous section, the optimal preconditioner in \mathcal{A}_{F_N} coincides with our preconditioner (2.10) defined with respect to the Fejér kernel $B_{1,N}$ and with $w_N = 0$ in (2.7). It is easy to check (see [33]) that the optimal preconditioner in \mathcal{A}_{O_N} , where $\mathbf{O}_N \in \{\mathbf{C}_N^{IV}, \mathbf{S}_N^{IV}\}$ is equal to our preconditioner $\mathbf{M}_N(f_N, \mathbf{O}_N)$ in (5.1) defined with respect to \mathbf{O}_N and with respect to the Fejér kernel. Unfortunately,

the Fejér kernel preconditioners do not lead to a fast convergence of the PCG–method if the generating function f of \mathbf{A}_N has a zero of order $2s \geq 2$.

In contrast to these results, the optimal preconditioners in \mathcal{A}_{O_N} with \mathbf{O}_N defined by the DCT I – III or by the DST I – III do not coincide with the corresponding Fejér kernel preconditioner $\mathbf{M}_N(f_N, \mathbf{O}_N)$ in (5.1). In literature [6, 3], so–called optimal Tau preconditioners were of special interest. Using our notation, optimal Tau preconditioners are the optimal preconditioners with respect to the DST–I as unitary transform. The optimal Tau preconditioner realizes a fast convergence of the PCG–method if the generating function f of \mathbf{A}_N has only zeros of order $2s \leq 2$ [6].

Block Toeplitz matrices with Toeplitz blocks

Next we are interested in the solution of doubly symmetric block Toeplitz systems with Toeplitz blocks. The construction of preconditioners with the help of reproducing kernels was applied to well–conditioned block Toeplitz systems in [27]. Following these lines, we generalize our univariate construction to ill–conditioned block Toeplitz systems with Toeplitz blocks. In the next Section we will present good numerical results also for the block case. However, in general, it is not possible to prove the convergence of PCG in a number of iteration steps independent of N . Here we refer to [34].

Note that as in the univariate case there exist banded block Toeplitz preconditioners with banded Toeplitz blocks which ensure a fast convergence of the corresponding PCG–method [35]. See also [4, 30].

We consider systems of linear equations

$$\mathbf{A}_{M,N} \mathbf{x} = \mathbf{b},$$

where $\mathbf{A}_{M,N}$ denotes a positive *definite doubly symmetric block Toeplitz matrix with Toeplitz blocks* (BTTB matrix), i.e.

$$\mathbf{A}_{M,N} := (\mathbf{A}_{r-s})_{r,s=0}^{M-1} \quad \text{with} \quad \mathbf{A}_r := (a_{r,j-k})_{j,k=0}^{N-1}$$

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

$$a_{j,k} := \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi} \varphi(s, t) e^{-i(sj+tk)} \, ds \, dt.$$

Note that the multiplication of a vector with a BTTB matrix requires only $\mathcal{O}(MN \log(MN))$ arithmetical operations (see [33]). We define our so–called “*level-2*” preconditioners by

$$\begin{aligned} \mathbf{M}_{M,N}(\varphi_{M,N}, \mathbf{C}_M^{II} \otimes \mathbf{C}_N^{II}) &:= (\mathbf{C}_M^{II} \otimes \mathbf{C}_N^{II})' \operatorname{diag}(\operatorname{col} \left(\varphi_{M,N} \left(\frac{r\pi}{M}, \frac{j\pi}{N} \right) \right)_{j,k=0}^{N-1, M-1}) \times \\ &\quad (\mathbf{C}_M^{II} \otimes \mathbf{C}_N^{II}), \\ \mathbf{M}_{M,N}(\varphi_{M,N}, \mathbf{S}_M^{II} \otimes \mathbf{S}_N^{II}) &:= (\mathbf{S}_M^{II} \otimes \mathbf{S}_N^{II})' \operatorname{diag}(\operatorname{col} \left(\varphi_{M,N} \left(\frac{r\pi}{M}, \frac{j\pi}{N} \right) \right)_{j,k=1}^{N, M}) \times \\ &\quad (\mathbf{S}_M^{II} \otimes \mathbf{S}_N^{II}), \end{aligned} \tag{5.2}$$

with $\varphi_{M,N} = \varphi * K_{M,N}$ and $K_{M,N}(x, y) := K_M(x)K_N(y)$. Here $\operatorname{col}: \mathbb{R}^{N,M} \rightarrow \mathbb{R}^{MN}$ is defined by

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

6 Numerical Examples

In this section, we confirm our theoretical results 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 \mathbf{b} of (2.1) the vector consisting of N entries “1”. The PCG–method started with the zero vector and stopped if $\|\mathbf{r}^{(j)}\|_2/\|\mathbf{r}^{(0)}\|_2 < 10^{-7}$, where $\mathbf{r}^{(j)}$ denotes the residual vector after j iterations.

We restrict our attention to preconditioners (2.10) and (5.1) constructed from B –spline kernels $K_N = B_{m,N}$. The following tables show the number of iterations of the corresponding PCG–method to achieve a fixed precision. The first row of each table contains the exponent n of the transform length $N = 2^n$ in the univariate case and the block length N in the block Toeplitz case. The kernels are listed in the first column and the applied unitary transform in the second column of each table. Here $\mathbf{F}_N^w := \mathbf{W}_N \mathbf{F}_N$ with $\mathbf{W}_N := \text{diag}(e^{-ik\pi/N})_{k=0}^{N-1}$, i.e. $w_N := \pi/N$ in (2.7). For comparison, the second row of each table contains the number of PCG–steps with preconditioner $\mathbf{M}_N(f)$ defined by (2.8). These preconditioners, which can be constructed only if the generating function f is known, were examined in [31].

We begin with symmetric ill–conditioned Toeplitz matrices $\mathbf{A}_N(f)$ arising from the generating functions

i) (see [13, 14, 33]): $f(x) := x^2 \quad (x \in [-\pi, \pi])$.

ii) (see [3, 10, 11, 14, 31, 36]): $f(x) := x^4 \quad (x \in [-\pi, \pi])$.

The Tables 1 and 2 present the number of iteration steps with different preconditioners.

As expected, for $f(x) = x^2$ it is not sufficient to choose a preconditioner based on the Fejér kernel $K_N = B_{1,N}$ and for $f(x) = x^4$ it is not sufficient to choose a preconditioner based on the cubic B –spline kernel $K_N = B_{2,N}$ in order to keep the number of iterations independent of N .

On the other hand, we have a similar convergence behavior for the different unitary transforms. This is no surprise for \mathbf{F}_N^w and for \mathbf{S}_N^{II} . However, for \mathbf{F}_N and for \mathbf{C}_N^{II} , the corresponding grids G_N contain the zero of f , namely $x_{N,0} = 0$. This was excluded in Theorem 3.6. In our numerical tests it seems to play no rule that a grid point meets the zero of f .

Our next example in Table 3 confirms our theoretical results for the function

iii) $f(x) = (x^2 - 1)^2$

with zeros of order 2 at $x = \pm 1$.

Finally, let us turn to BTTB matrices $\mathbf{A}_{N,N}$. In our examples, the matrices $\mathbf{A}_{N,N}$ are generated by the functions

iv) (see [4]): $\varphi(s, t) = s^2 + t^2 + s^2 t^2 \quad (s, t \in [-\pi, \pi])$.

v) (see [30, 31]): $\varphi(s, t) = s^2 t^4 \quad (s, t \in [-\pi, \pi])$.

vi) (see [30, 31]): $\varphi(s, t) = (s^2 + t^2)^2 \quad (s, t \in [-\pi, \pi])$.

These matrices are ill–conditioned and the CG–method without preconditioning, with Strang–type–preconditioning or with optimal trigonometric preconditioning converges very slow (see

K_N	\mathbf{O}_N	4	5	6	7	8	9	10	11	12
f	\mathbf{F}_N^w	4	4	4	5	6	6	6	6	6
$B_{1,N}$	\mathbf{F}_N	7	8	11	12	14	18	22	29	39
$B_{1,N}$	\mathbf{F}_N^w	7	8	9	11	13	17	20	26	37
$B_{1,N}$	\mathbf{C}_N^{II}	7	8	10	11	13	16	20	25	33
$B_{1,N}$	\mathbf{S}_N^{II}	7	8	9	11	14	17	21	27	38
$B_{2,N}$	\mathbf{F}_N	6	6	6	7	7	7	6	6	6
$B_{2,N}$	\mathbf{F}_N^w	6	6	5	5	5	6	6	6	6
$B_{2,N}$	\mathbf{C}_N^{II}	6	6	6	6	6	6	5	5	5
$B_{2,N}$	\mathbf{S}_N^{II}	6	6	5	5	5	7	7	7	7
$B_{3,N}$	\mathbf{F}_N	6	6	6	7	7	7	7	6	6
$B_{3,N}$	\mathbf{F}_N^w	6	6	6	6	5	6	6	6	6
$B_{3,N}$	\mathbf{C}_N^{II}	6	6	6	6	6	6	6	5	5
$B_{3,N}$	\mathbf{S}_N^{II}	6	6	5	7	6	7	7	7	7

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

[30, 33, 4]). Our preconditioning (5.2) leads to the number of iterations in the Tables 4 – 6. Here $B_{k,N,N}(x, y) := B_{k,N}(x) B_{k,N}(y)$.

In [34], we proved that the number of iteration steps of PCG is independent of N in Example iv) and we explained the convergence behavior of PCG for the other examples. To our knowledge, there does not exist a faster PCG–method if the generating function φ is unknown up to now.

Note that by [42, 43] any multilevel preconditioner is not optimal in the sense that a cluster cannot be proper [45].

Summary. We suggested new positive definite w –circulant preconditioners for sequences of Toeplitz systems with polynomial increasing condition numbers. The construction of our preconditioners is based on the convolution of the generating function with positive reproducing kernels and, by working in the Fourier domain, does not require the explicit knowledge of the generating function. As main result we proved that the quality of the preconditioner depends on a “moment property” of the corresponding kernel which is related to the order of the zeros of the generating function. This explains, e.g. why optimal circulant preconditioners arising from convolutions with the Fejér kernels fail to be good preconditioners if the generating function has zeros of order ≥ 2 .

K_N	O_N	4	5	6	7	8	9	10	11	12
f	F_N^w	6	6	6	8	11	11	11	12	14
$B_{1,N}$	F_N	8	15	23	36	61	153	391	> 800	> 800
$B_{1,N}$	F_N^w	8	15	23	36	61	153	390	> 800	> 800
$B_{1,N}$	C_N^{II}	8	13	20	32	53	129	319	> 800	> 800
$B_{1,N}$	S_N^{II}	8	16	24	38	65	158	402	> 800	> 800
$B_{2,N}$	F_N	9	9	11	11	13	15	18	22	27
$B_{2,N}$	F_N^w	9	9	10	10	13	14	17	20	26
$B_{2,N}$	C_N^{II}	8	8	9	9	9	11	13	14	16
$B_{2,N}$	S_N^{II}	10	10	10	11	13	14	18	19	22
$B_{3,N}$	F_N	9	11	11	12	12	12	13	15	14
$B_{3,N}$	F_N^w	9	9	10	10	12	12	13	13	13
$B_{3,N}$	C_N^{II}	8	9	9	9	9	9	10	10	9
$B_{3,N}$	S_N^{II}	10	10	12	12	14	14	14	15	16

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

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K_N	O_N	4	5	6	7	8	9	10	11	12
f	F_N^w	7	5	5	7	8	8	7	7	7
$B_{1,N}$	F_N	7	13	15	20	27	34	46	63	86
$B_{1,N}$	F_N^w	7	14	16	20	26	32	44	59	83
$B_{1,N}$	C_N^{II}	8	13	15	18	25	30	41	55	75
$B_{1,N}$	S_N^{II}	8	14	16	19	26	33	43	57	79
$B_{2,N}$	F_N	8	9	9	9	9	10	9	9	9
$B_{2,N}$	F_N^w	8	9	9	9	9	8	10	9	9
$B_{2,N}$	C_N^{II}	8	8	8	8	9	10	10	9	9
$B_{2,N}$	S_N^{II}	8	10	10	10	9	8	9	9	9
$B_{3,N}$	F_N	8	10	10	10	10	9	9	11	11
$B_{3,N}$	F_N^w	8	10	9	9	9	10	10	9	9
$B_{3,N}$	C_N^{II}	8	9	9	9	9	8	9	10	10
$B_{3,N}$	S_N^{II}	8	11	10	10	10	10	9	9	10

Table 3: $f(x) = (x^2 - 1)^2$ ($x \in [-\pi, \pi]$)

$K_{N,N}$	O_N	8	16	32	64	128	256	512
φ	S_N^{II}	8	9	9	10	10	10	10
$B_{1,N,N}$	S_N^{II}	10	12	14	16	20	26	36
$B_{2,N,N}$	S_N^{II}	10	10	11	11	11	11	11
$B_{3,N,N}$	S_N^{II}	10	10	11	11	11	11	11

Table 4: $\varphi(s, t) = s^2 + t^2 + s^2t^2$ ($s, t \in [-\pi, \pi]$).

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$K_{N,N}$	\mathbf{O}_N	8	16	32	64	128	256	512
φ	\mathbf{S}_N^{II}	13	16	22	29	36	43	52
$B_{1,N,N}$	\mathbf{S}_N^{II}	18	67	184	631	2363	> 3000	> 3000
$B_{2,N,N}$	\mathbf{S}_N^{II}	16	29	39	56	77	106	158
$B_{3,N,N}$	\mathbf{S}_N^{II}	17	29	34	48	63	79	91

Table 5: $\varphi(s, t) = s^2 t^4$ ($s, t \in [-\pi, \pi)$).

$K_{N,N}$	\mathbf{O}_N	8	16	32	64	128	256	512
φ	\mathbf{S}_N^{II}	9	12	14	19	25	35	49
$B_{1,N,N}$	\mathbf{S}_N^{II}	10	19	31	63	144	381	1413
$B_{2,N,N}$	\mathbf{S}_N^{II}	10	13	15	18	26	39	62
$B_{3,N,N}$	\mathbf{S}_N^{II}	10	14	15	18	25	37	48

Table 6: $\varphi(s, t) = (s^2 + t^2)^2$ ($s, t \in [-\pi, \pi)$).

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